Semiconductor Physics Division
Fachverband Halbleiterphysik (HL)

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Overview of Invited Talks and Sessions

(Lecture rooms POT 06, 81, 51, 112, 151, 251, and HSZ 403; Poster P1A, P1C, P2-OG2, and P2-OG3)

Invited Talks

HL 5.1	Mon	9:30–10:00	POT 81	**Van der Waals heterostructures: tunnelling and interaction with light** — •Artem Mishchenko
HL 5.6	Mon	11:30–12:00	POT 81	**Excitons in ultra-thin perovskites & van der Waals crystals** — •Alexey Chernikov
HL 6.1	Mon	9:30–10:00	POT 51	**Optical Coherent Multidimensional Spectroscopy of Semiconductor Nanostructures** — •Steven Cundiff
HL 7.11	Mon	12:30–13:00	POT 151	**Carbon nanotubes as excitonic insulators** — •Massimo Rontani
HL 15.1	Mon	14:45–15:15	POT 81	**2D / 3D Heterostructures for Optoelectronis** — •Max Lemme
HL 15.6	Mon	16:45–17:15	POT 81	**Excitons in colloidal 2D-CdSe nanocrystals** — •Ulrike Woggon
HL 16.1	Mon	14:45–15:15	POT 51	**The role of phonons for the optical control of semiconductor quantum dots** — •Doris Reiter
HL 33.1	Tue	9:30–10:00	POT 81	**Deterministic Single Quantum Dot Devices: Building Blocks for Photonic Quantum Networks** — •Stephan Reitzenstein
HL 34.7	Tue	11:30–12:00	POT 51	**Influence of dark states on excitonic spectra of transition metal dichalcogenides** — •Malte Selig, Dominik Christiansen, Gunnar Berghäuser, Ermin Malic, Andreas Knorr
HL 35.1	Tue	9:30–10:00	POT 151	**Edge conduction in the 2D topological insulator candidate InAs/GaSb** — •Susanne Mueller, Matija Karalic, Christopher Mittag, Lars Tiemann, Thomas Tschirky, Quansheng Wu, Alexey A. Soluyanov, Atin Nath Pal, Christophe Charpentier, Matthias Troyer, Werner Wegscheider, Klaus Ensslin, Thomas Ihn
HL 35.4	Tue	10:30–11:00	POT 151	**Progress in Edge Channel Transport of Two-Dimensional Topological Insulators** — •Hartmut Buhmann
HL 35.5	Tue	11:30–12:00	POT 151	**Transport and capacitance in HgTe-based topological insulators** — •Dieter Weiss
HL 35.7	Tue	12:15–12:45	POT 151	**Giant Spin-Orbit Splitting in Inverted InAs/GaSb Double Quantum Wells** — •Fabrizio Nichele, Morten Kjaergaard, Henri J. Suominen, Rafal Skolasinski, Michael Wimmer, Binh-Minh Nguyen, Andrey A. Kiselev, Wei Yi, Marko Sokolich, Michael J. Manfra, Fanming Qu, Arjan J. A. Beukman, Leo P. Kouwenhoven, Charles M. Marcus
HL 50.1	Wed	9:30–10:00	POT 251	**Photoactivated chemical processes on group III-nitride nanostructures and nanohybrids** — Paula Neuderth, Sara Hölzl, Pascal Hille, Jörg Schörmann, Christian Reitz, Mariona Coll, Jordi Arbiol, Roland Marschall, •Martin Eickhoff
HL 51.1	Wed	9:30–10:00	POT 112	**Coupling atomic and solid state quantum systems** — •Val Zwiller
HL 51.5	Wed	10:45–11:15	POT 112	**Strain-tunable quantum dots interfaced with atomic vapors** — •Rinaldo Trotta
HL 51.6	Wed	11:45–12:15	POT 112	**Atomic-vapor-enabled variable optical delay for triggered single-photons from a semiconductor quantum dot** — •Hüseyin Vural, Jonas Weber, Markus Müller, Simon Kern, Julian Maisch, Matthias Widmann, Robert Löw, Jörg Wrachtrup, Ilja Gerhardt, Simone Portalupi, Michael Jetter, Peter Michler

HL 51.8	Wed	12:30–13:00	POT 112	**Correlating independent spins via single-photon projections** — •Mete Atature
HL 58.1	Wed	14:45–15:15	POT 151	**Towards an ideal semiconductor source of polarization entangled photons** — •Fei Ding
HL 67.5	Thu	10:45–11:15	POT 81	**2D Quasicrystals from Semiconducting Perovskite Oxides** — •Wolf Widdra, Stefan Förster
HL 68.1	Thu	9:30–10:00	POT 51	**Solar-driven photoelectrochemical water splitting and carbon dioxide reduction** — •Joel Ager
HL 68.4	Thu	10:30–11:00	POT 51	**Quantum confined colloidal semiconductor nanocrystals for solar fuels** — •Frank Jäckel
HL 68.7	Thu	12:00–12:30	POT 51	**Photo-electrochemistry modelling beyond idealised surfaces and the computational hydrogen electrode** — •Harald Oberhofer
HL 70.1	Thu	9:30–10:00	POT 251	**Sub-nm probing of Topological insulators and Rashba systems** — •Markus Morgenstern
HL 75.1	Thu	14:45–15:15	POT 151	**Spectroscopy on self-assembled quantum dots: Transport meets optics** — •Martin Geller
HL 83.1	Fri	9:30–10:00	POT 51	**New Frontiers in Quantum Matter Heterostructures** — •Jochen Mannhart

Invited talks of the joint symposium SYLI

See SYLI for the full program of the symposium.

SYLI 1.1	Mon	9:30–10:00	HSZ 02	**Interfacial challenges in solid- state Li ion: some perspectives from theory** — •Alan Luntz, Saskia Stegmaier, Johannes Voss, Karsten Reuter
SYLI 1.2	Mon	10:00–10:30	HSZ 02	**Will solid electrolytes enable lithium metal anodes in solid state batteries?** — •Jürgen Janek, Dominik Weber, Wolfgang Zeier
SYLI 1.3	Mon	10:30–11:00	HSZ 02	**Hybrid Electrolytes for Solid-State Batteries** — •Hans-Dieter Wiemhöfer
SYLI 1.4	Mon	11:15–11:45	HSZ 02	**Neutron diffraction on solid-state battery materials** — •Helmut Ehrenberg, Anatoliy Senyshyn, Mykhailo Monchak, Sylvio Indris, Joachim Binder
SYLI 1.5	Mon	11:45–12:15	HSZ 02	**Sulfate-based Solid-State Batteries** — •Yuki Katoh

Invited talks of the joint symposium SYNS

See SYNS for the full program of the symposium.

SYNS 1.1	Wed	15:00–15:30	HSZ 02	**The Limits to Lithography: How Electron-Beams Interact with Materials at the Smallest Length Scales** — •Karl K. Berggren
SYNS 1.2	Wed	15:30–16:00	HSZ 02	**High precision fabrication for light management at nanoscale** — •Saulius Juodkazis, Armandas Balcytis
SYNS 1.3	Wed	16:00–16:30	HSZ 02	**Directed self-assembly of performance materials** — •Paul Nealey
SYNS 1.4	Wed	16:45–17:15	HSZ 02	**Nanometer accurate topography patterning using thermal Scanning Probe Lithography** — •Armin W. Knoll
SYNS 1.5	Wed	17:15–17:45	HSZ 02	**High resolution 3D nanoimprint lithography** — •Hartmut Hillmer

Invited talks of the joint symposium SYQO

See SYQO for the full program of the symposium.

SYQO 1.1	Thu	9:30–10:00	HSZ 02	**Quantum dot based quantum technologies** — •Pascale Senellart
SYQO 1.2	Thu	10:00–10:30	HSZ 02	**Controlled strong coupling of a single quantum dot to a plasmonic nanoresonator at room temperature** — Heiko Gross, Joachim M. Hamm, Tommaso Tufarelli, Ortwin Hess, •Bert Hecht
SYQO 1.3	Thu	10:30–11:00	HSZ 02	**High efficiency and directional emission from a nanoscale light source in a planar optical antenna** — •Mario Agio
SYQO 1.4	Thu	11:30–12:00	HSZ 02	**Tailoring quantum states by measurement** — •Jörg Wrachtrup
SYQO 1.5	Thu	12:00–12:30	HSZ 02	**Quantum optics and quantum control at the nanoscale with surface plasmon polaritons** — •Stéphane Guérin

Invited talks of the joint symposium SYLM

See SYLM for the full program of the symposium.

SYLM 1.1	Thu	15:00–15:30	HSZ 02	**Light matter interaction in TMDs and their heterostructures** — •Ursula Wurstbauer
SYLM 1.2	Thu	15:30–16:00	HSZ 02	**Quantum optics with deterministically positioned quantum emitters in a two-dimensional semiconductor** — •Brian Gerardot
SYLM 1.3	Thu	16:00–16:30	HSZ 02	**Light-matter coupling with atomic monolayers in microcavities** — •Christian Schneider
SYLM 1.4	Thu	17:00–17:30	HSZ 02	**Properties of Synthetic 2D Materials and Heterostructures** — •Joshua Robinson
SYLM 1.5	Thu	17:30–18:00	HSZ 02	**Exciton spectroscopy in transition metal dichalcogenide monolayers and van der Waals heterostructures** — •Bernhard Urbaszek
SYLM 1.6	Thu	18:00–18:30	HSZ 02	**Strain-induced single-photon emitters in layered semiconductors** — •Rudolf Bratschitsch

Invited talks of the joint symposium SYES

See SYES for the full program of the symposium.

SYES 1.1	Fri	10:30–11:00	HSZ 02	**Going Beyond Conventional Functionals with Scaling Corrections and Pairing Fluctuations** — •Weitao Yang
SYES 1.2	Fri	11:00–11:30	HSZ 02	**Multi-reference density functional theory** — •Andreas Savin
SYES 1.3	Fri	11:30–12:00	HSZ 02	**Density functionals from machine learning** — •Kieron Burke
SYES 1.4	Fri	12:00–12:30	HSZ 02	**Taming Memory-Dependence in Time-Dependent Density Functional Theory** — •Neepa Maitra
SYES 1.5	Fri	12:30–13:00	HSZ 02	**Quantum Embedding Theories** — •Fred Manby

Sessions

HL 1.1–1.3	Sun	16:00–18:15	HSZ 403	**Tutorial: Photocatalysis**
HL 2.1–2.5	Mon	9:30–12:15	HSZ 02	**SYLI: Symposium Interfacial Challenges in Solid-State Li Ion Batteries - Invited talks**
HL 3.1–3.13	Mon	9:30–13:00	HSZ 204	**Transport: Topological Insulators (jointly with DS, MA, HL, O)**
HL 4.1–4.6	Mon	9:30–12:15	CHE 89	**Focused Session: Inhomogeneous Materials for Solar Cells I**
HL 5.1–5.9	Mon	9:30–12:45	POT 81	**Focus Session: Two-dimensional materials I (joined session with TT)**
HL 6.1–6.10	Mon	9:30–12:45	POT 51	**Ultrafast Phenoma I**
HL 7.1–7.11	Mon	9:30–13:00	POT 151	**Spintronics I (joined session with TT)**
HL 8.1–8.8	Mon	9:30–11:45	POT 251	**Photovoltaics**
HL 9.1–9.10	Mon	9:30–12:30	POT 112	**Quantum Dots: Preparation and Characterization**
HL 10.1–10.10	Mon	9:30–12:30	POT 06	**Semiconductor Lasers I**
HL 11.1–11.10	Mon	10:30–13:00	TRE Ma	**Plasmonics and Nanooptics I: Light-Matter Interactions**
HL 12.1–12.10	Mon	10:30–13:00	GER 38	**Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - I**
HL 13.1–13.8	Mon	11:00–13:00	ZEU 260	**Organic Electronics and Photovoltaics I: Light-Emitting Devices**
HL 14.1–14.18	Mon	14:00–18:00	P2-OG3	**Poster: Two-Dimenaional Materials and Topological Insulators**
HL 15.1–15.10	Mon	14:45–18:15	POT 81	**Focus Session: Two-dimensional materials II (joined session with TT)**
HL 16.1–16.8	Mon	14:45–17:30	POT 51	**Ultrafast Phenoma II**
HL 17.1–17.7	Mon	14:45–17:00	POT 151	**Spintronics II (joined session with TT)**
HL 18.1–18.9	Mon	14:45–17:30	POT 06	**Semiconductor Lasers II**
HL 19.1–19.12	Mon	15:00–18:15	HSZ 204	**Transport: Graphene and Carbon Nanostructures (jointly with DY, DS, HL, MA, O)**
HL 20.1–20.9	Mon	15:00–18:15	ZEU 222	**Fundamentals of Perovskite Photovoltaics II (joint session CPP/DS/HL)**
HL 21.1–21.9	Mon	15:00–18:15	ZEU 222	**Fundamentals of Perovskite Photovoltaics II (joint session CPP/DS/HL)**

HL 22.1–22.11	Mon	15:00–18:15	ZEU 260	**Organic Electronics and Photovoltaics II: Doping**
HL 23.1–23.7	Mon	15:00–16:45	TRE Ma	**Plasmonics and Nanooptics II: Light-Matter Interaction**
HL 24.1–24.12	Mon	15:00–18:15	GER 38	**Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - II**
HL 25.1–25.24	Mon	15:00–19:00	P2-OG2	**Poster: Nitrides**
HL 26.1–26.3	Mon	16:30–17:15	CHE 89	**Focussed Session: Frontiers in Exploring and Applying Plasmonic Systems II (Joint Session of CPP, DS, HL, MM, and O, organized by DS)**
HL 27.1–27.6	Mon	17:00–18:30	TRE Ma	**Plasmonics and Nanooptics III: Light-Matter Interaction**
HL 28.1–28.30	Mon	18:30–21:00	P1A	**Poster: Fundamentals of Perovskite Photovoltaics (joint session CPP, DS, HL)**
HL 29.1–29.14	Tue	9:30–13:15	HSZ 103	**Transport: Quantum Coherence and Quantum Information Systems - Theory (jointly with MA, HL)**
HL 30.1–30.10	Tue	9:30–12:30	ZEU 222	**Fundamentals of Perovskite Photovoltaics III (joint session CPP/DS/HL)**
HL 31.1–31.12	Tue	9:30–12:45	ZEU 260	**Organic Electronics and Photovoltaics III: Mobile and Trapped Charges**
HL 32.1–32.6	Tue	9:30–12:45	CHE 89	**Focussed Session: Frontiers in Exploring and Applying Plasmonic Systems I (Joint Session of CPP, DS, HL, MM, and O, organized by DS)**
HL 33.1–33.11	Tue	9:30–13:00	POT 81	**Quantum Dots: Optical Properties I**
HL 34.1–34.12	Tue	9:30–13:15	POT 51	**Two-dimensional materials III (joined session with TT)**
HL 35.1–35.7	Tue	9:30–12:45	POT 151	**Focus Session: Topological Insulators on Coupled Quantum Wells (joined session with TT)**
HL 36.1–36.13	Tue	9:30–13:15	POT 251	**Organic Semiconductors (joined session with CPP, DS)**
HL 37.1–37.10	Tue	9:30–12:30	POT 112	**III-V Semiconductors**
HL 38.1–38.6	Tue	9:30–11:15	POT 06	**Zinc Oxide**
HL 39.1–39.10	Tue	10:30–13:00	TRE Ma	**Plasmonics and Nanooptics IV: Light-Matter Interaction**
HL 40.1–40.9	Tue	10:30–13:00	GER 38	**Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - III**
HL 41.1–41.5	Tue	11:45–13:00	POT 06	**Nitrides: Preparation**
HL 42.1–42.7	Tue	14:00–16:00	ZEU 222	**Fundamentals of Perovskite Photovoltaics IV (joint session CPP/DS/HL)**
HL 43.1–43.8	Tue	14:00–16:00	TRE Ma	**Plasmonics and Nanooptics V: Light-Matter Interaction**
HL 44.1–44.5	Tue	14:45–16:00	POT 81	**Quantum Dots: Optical Properties II**
HL 45.1–45.13	Wed	9:30–13:00	HSZ 03	**Transport: Quantum Coherence and Quantum Information Systems - Experiment (jointly with MA, HL)**
HL 46.1–46.12	Wed	9:30–12:45	HSZ 201	**Transport: Molecular Electronics and Photonics (jointly with CPP, HL, MA, O)**
HL 47.1–47.11	Wed	9:30–12:45	POT 81	**Organic Photovoltaics and Electronics I (joined session with CPP)**
HL 48.1–48.13	Wed	9:30–13:15	POT 51	**Two-dimensional materials IV (joined session with TT)**
HL 49.1–49.11	Wed	9:30–12:45	POT 151	**Quantum Dots: Optical Properties III**
HL 50.1–50.11	Wed	9:30–13:00	POT 251	**Nitrides: Preparation and Characterization**
HL 51.1–51.8	Wed	9:30–13:00	POT 112	**Focus Session: Hybrid Quantum-Dot / Atom Systems**
HL 52.1–52.7	Wed	9:30–11:30	POT 06	**Devices**
HL 53.1–53.8	Wed	10:15–12:45	ZEU 250	**Fundamentals of Perovskite Photovoltaics V (joint session CPP/DS/HL)**
HL 54.1–54.8	Wed	10:30–12:30	TRE Ma	**Plasmonics and Nanooptics VI: Light-Matter Interactions and Characterisation**
HL 55.1–55.9	Wed	10:30–13:00	GER 38	**Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - IV**
HL 56.1–56.9	Wed	10:30–13:00	GER 38	**Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - IV**
HL 57.1–57.10	Wed	14:45–17:45	POT 81	**Organic Photovoltaics and Electronics II (joined session with CPP)**
HL 58.1–58.11	Wed	14:45–18:15	POT 151	**Quantum Dots: Optical Properties IV**
HL 59.1–59.10	Wed	14:45–17:45	POT 251	**Nitrides: Preparation and Characterization II**
HL 60.1–60.12	Wed	15:00–18:30	ZEU 260	**Organic Electronics and Photovoltaics IV: OPV**
HL 61.1–61.12	Wed	15:00–18:00	TRE Ma	**Plasmonics and Nanooptics VII: Applications and Other Aspects**

HL 62.1–62.13	Wed	15:00–18:15	GER 38	**Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - V**
HL 63.1–63.80	Wed	15:00–19:00	P1A	**Poster: Quantum Dots and Optics**
HL 64.1–64.46	Wed	15:00–19:00	P1C	**Poster: Photovoltaics and Optics**
HL 65.1–65.5	Thu	9:30–12:30	HSZ 02	**Quantum Optics on the Nanoscale: From Fundamental Physics to Quantum Technologies (joined session, HL, DS, O, TT, organized by HL)**
HL 66.1–66.8	Thu	9:30–13:00	HSZ 03	**Focus Session on 2D Materials: Ballistic Quantum Transport in Graphene (jointly with DY, DS, HL, MA, O)**
HL 67.1–67.5	Thu	9:30–11:15	POT 81	**Perovskites, Hybrid Photovoltaics and Plasmonics**
HL 68.1–68.7	Thu	9:30–12:30	POT 51	**Focus Session: Semiconductor Materials and Nanostructure for Photocatalysis**
HL 69.1–69.10	Thu	9:30–12:30	POT 151	**Quantum Dots: Transport Properties I**
HL 70.1–70.10	Thu	9:30–12:45	POT 251	**Topological Insulators I (joined session with TT)**
HL 71.1–71.7	Thu	9:30–11:30	POT 112	**Transport Properties**
HL 72.1–72.7	Thu	9:30–11:45	POT 06	**Nitrides: Devices**
HL 73.1–73.13	Thu	10:30–13:45	GER 38	**Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - VI**
HL 74.1–74.5	Thu	12:00–13:15	POT 06	**Group IV: Si/Ge/SiC**
HL 75.1–75.5	Thu	14:45–16:15	POT 151	**Quantum Dots: Transport Properties II**
HL 76.1–76.6	Thu	14:45–16:45	POT 251	**Topological Insulators II (joined session with TT)**
HL 77.1–77.6	Thu	14:45–16:30	POT 112	**Transport in High Magnetic Fields**
HL 78.1–78.6	Thu	15:00–18:30	HSZ 02	**Optics and Light-Matter Interaction with Excitons in 2D Materials (SYLM) (joined session DS, DY, HL, TT, organized by HL)**
HL 79.1–79.31	Thu	15:00–19:00	P2-OG3	**Poster: New Materials**
HL 80.1–80.9	Thu	16:00–18:30	GER 38	**Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - VII**
HL 81.1–81.8	Fri	9:30–11:30	HSZ 03	**Transport: Spintronics, Spincalorics and Magnetotransport (jointly with DS, HL, MA)**
HL 82.1–82.6	Fri	9:30–11:15	POT 81	**Quantum Information Systems**
HL 83.1–83.10	Fri	9:30–12:45	POT 51	**Oxide Semiconductors (joined session with CPP, DS)**
HL 84.1–84.11	Fri	9:30–12:45	POT 151	**Heterostructures and Interfaces**
HL 85.1–85.10	Fri	9:30–12:30	POT 251	**Topological Insulators III (joined session with TT)**
HL 86.1–86.11	Fri	9:30–12:45	POT 112	**New Materials**
HL 87.1–87.10	Fri	9:30–12:30	POT 06	**Carbon: Diamond and others**
HL 88.1–88.10	Fri	10:15–13:15	ZEU 255	**Organic Electronics and Photovoltaics V: OPV**
HL 89.1–89.5	Fri	10:30–13:00	HSZ 02	**Frontiers of Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond**
HL 90.1–90.6	Fri	11:30–13:00	POT 81	**Inhomogeneous Materials for Solar Cells**

Annual General Meeting of the Semiconductor Physics Division

Thursday 18:00–19:00 POT 81

HL 1: Tutorial: Photocatalysis

Time: Sunday 16:00–18:15 Location: HSZ 403

Tutorial HL 1.1 Sun 16:00 HSZ 403

An Introduction to Rechargeable Battery Technology and Current Research Trends — •Bryan McCloskey — Department of Chemical and Biomolecular Engineering, UC, Berkeley, CA, USA — Energy Storage and Distributed Resources Division, LBNL, Berkeley, CA, USA

From electric and plug-in hybrid vehicles gaining a foothold in the automotive market to the 787 airline and Galaxy Note 7 battery fires, battery technology has, for better or worse, found itself in the popular spotlight in recent years. This spotlight is likely to shine brighter in the future, as improvements in both capability and size of portable electronic devices will make batteries and battery research increasingly important in the coming decade. Nevertheless, the 787 and Galaxy Note 7 incidents highlight an interesting dichotomy in battery research: although decades of development have allowed rechargeable batteries to be used in advanced applications, our understanding of how to design a safe, high energy density, low cost rechargeable battery still needs to be improved. This talk will initially give a general introduction to battery technology, including Li-ion batteries, focusing on their chemistry and applications. The second part of the talk will outline research directions associated with improving rechargeable batteries, with a specific emphasis on research activities for advanced materials development, including solid-state batteries and the so-called *beyond Li-ion* chemistries (Li-S, Li-air (O2), and Mg-ion batteries).

Tutorial HL 1.2 Sun 16:40 HSZ 403

Theory and Simulations for All-Solid State Batteries — •Christoph Scheurer — Theoretische Chemie, TU München, Lichtenbergstr. 4, 85748 Garching, Germany

The concept of an All-Solid State Battery (SSB) has recently attracted substantial interest for its potential advantages over conventional liquid electrolyte-based batteries, which are slowly approaching their fundamental limitations. The SSB is often considered inherently safe due to the intrinsic separator function of solid electrolytes, as well as longterm stable, being based exclusively on solid inorganic or polymer electrolytes and electrodes and thus avoiding the use of potentially volatile and flammable organic solvents. The lack of a liquid electrolyte, on the other hand, also poses several challenges like e.g. interfacial resistances or mechanical stress and contact loss at solid-solid interfaces, which need to be fully understood and overcome for a functional, competitive SSB.

In this tutorial we will discuss key topics within the theory of superionic and mixed ionic-electronic conductors to understand the requirements for solid state electrolytes, electrode materials and their interplay. Traditional electrochemical concepts will be connected to recent atomistic simulations employing density functional theory (DFT) electronic structure, force-field based molecular dynamics (MD) and Monte-Carlo (MC), as well as coarse-grained kinetic Monte-Carlo (kMC) computations.

Coffee Break

Tutorial HL 1.3 Sun 17:35 HSZ 403

Solid State Ionics - Mechanisms and Experimental Methods in Battery Research — •Ruediger-A. Eichel — Forschungszentrum Juelich, Institut fuer Energie- und Klimaforschung — RWTH Aachen, Institut fuer Physikalische Chemie

Solid-State Batteries promise safe, long-lived, high volumetric energy density and easily miniaturized (as thin films) devices for energy storage. However, because high currents generally only cross solid-solid interfaces at high transition resistances, current solid-state batteries mainly are limited to low-power densities.

In this contribution, the underlying principles of Solid-State Ionics, i.e. the foundations of charge transport and transfer in the 'bulk' and accross boundaries, are outlined together with an introduction of the most prominent experimental techniques for characterization of these phenomena and mechanisms. Furthermore, recent examples of application in the field of Solid-State Batteries are outlined.

HL 2: SYLI: Symposium Interfacial Challenges in Solid-State Li Ion Batteries - Invited talks

Time: Monday 9:30–12:15 Location: HSZ 02

Invited Talk HL 2.1 Mon 9:30 HSZ 02

Interfacial challenges in solid- state Li ion: some perspectives from theory — •Alan Luntz[1], Saskia Stegmaier[1], Johannes Voss[1], and Karsten Reuter[2] — [1]Stanford University, Stanford, CA, USA — [2]Technical University of Munich, Munich, Germany

Unfortunately, interfacial challenges severely limit power and cycle life in all solid- state Li ion batteries. We use theory to investigate some of the origins of these limitations with both continuum theory and DFT. The obvious ones are electrochemical stability of the electrolyte at the anode/cathode interfaces and mechanical issues relating to maintaining interfacial contact during cycling while inhibiting Li dendrite growth. We are especially trying to understand if any fundamental limitations exist from the structures of the double layers that form at the solid electrolyte- electrode or other interfaces in the solid-state stack. These can be quite different than in conventional liquid Li ion batteries. We use Li3OCl as a prototypical Li ion superionic conductor and discuss its properties and discuss its interface with model electrode interfaces.

Invited Talk HL 2.2 Mon 10:00 HSZ 02

Will solid electrolytes enable lithium metal anodes in solid state batteries? — •Jürgen Janek, Dominik Weber, and Wolfgang Zeier — Institut für Physikalische Chemie, Justus Liebig-Universität, Gießen, Germany

In order to achieve solid state lithium batteries with higher energy densities [1], lithium metal anodes are one of the primary options. However, reversible and morphologically stable plating of thick lithium metal films is difficult, as void formation and dendrite growth may occur - leading to impedance growth and/or short-circuits. Ceramic electrolytes are considered as a potential solution to this problem. In this lecture the interface between solid electrolytes and lithium metal anodes will be discussed in depth, and the occurrence of both thermodynamic and kinetic instabilities will be highlighted. In particular, the existence of SEI ("solid electrolyte interphases"), forming between lithium metal and the solid electrolyte, will be demonstrated for a number of solid electrolytes. It will also be shown that the growth of these SEI layers follows a typical square-root law-type behavior in SEI formation in liquid electrolytes.

[1] J. Janek and W. Zeier, Nat. Energy 1 (2016) 16141

Invited Talk HL 2.3 Mon 10:30 HSZ 02

Hybrid Electrolytes for Solid-State Batteries — •Hans-Dieter Wiemhöfer — Inst. Inorganic & Analyt. Chem., WWU Münster — Helmholtz-Institute Münster

Rechargeable lithium batteries with largely increased energy and power densities are a primary goal at present world wide. At the same time, enhanced safety concerns cause the need to replace current liquid electrolytes by new high performance electrolytes combining higher mechanical, thermal and electrochemical stability. Finally, this leads to the development of hybrid electrolytes. The primary idea is to construct electrolytes fulfilling a multitude of requirements based on a combination of components and phases, often coupled with approaches to achieve stable meso or micro porous networks down to chemically designed nanostructures. Starting from ion conducting inorganic solids and glasses, the combination with polymers and salt-in-polymer systems opens a wide range for possibilities for chemical design, tailoring and fine tuning of electrolyte properties of such hybrid systems. The concept will be illustrated with a number of examples, for instance, self organized block-copolymer networks acting as porous containers for fast ion conducting channels. Future all solid state batteries are expected to profit from hybrid concepts as well. For instance, volume changes during charging/discharging of active electrodes need an elastic polymer network acting as a glue and stabilizing a good contact and

charge transfer kinetics of solid electrolyte/solid electrode interfaces.

15 min. break

Invited Talk HL 2.4 Mon 11:15 HSZ 02

Neutron diffraction on solid-state battery materials — •Helmut Ehrenberg[1], Anatoliy Senyshyn[2], Mykhailo Monchak[1], Sylvio Indris[1], and Joachim Binder[1] — [1]Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM) — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universitaet Muenchen, Garching, Germany

Solid-state batteries are a promising approach to safer electrochemical energy storage and higher energy densities. Bottle necks are interface reactions and transport limitations in the solids. Advanced and optimized materials must provide dedicated properties, for example a good Li-ion conductivity for sufficiently high current densities and only small volume changes to preserve mechanical integrity. Neutron diffraction offers unique features to elucidate the underlying structure-property relationships, which determine the resulting performance parameters on cell level. Selected examples are shown, which demonstrate the capabilities of neutron diffraction to reveal Li-ion diffusion pathways as in the $Li_{1.3}Al_{0.3}Ti_{1.7}(PO_4)_3$ (LATP) superionic conductor, Li occupation numbers at intermediate states of charge as for $LiCoPO_4$ or a comparison of volume changes between commercial and alternative zero-strain electrode materials. The capabilities of solid-state batteries are discussed.

Invited Talk HL 2.5 Mon 11:45 HSZ 02

Sulfate-based Solid-State Batteries — •Yuki Katoh — Toyota Motor Europe NV/SA, Hoge Wei 33, Zaventem, Belgium

Large-scale batteries are in high demand for applications such as plug-in electric hybrid or electric vehicles, and smart electric power grids. The all-solid-state battery is the most promising candidate for future battery systems, due to the high energy density obtaining by direct-series-stacking of the battery cells. However, the poor electrochemical characteristics of the all-solid-state battery, due to higher cell-resistivity than conventional liquid electrolyte batteries, still remain as an unsolved issue. We will demonstrate an all-solid-state battery with extremely high power performance that employs the superionic conductors having the Li10GeP2S12-type crystal structure. The battery can operate over a wide temperature range with extremely high current drains of 3 mAcm-2 (-30 C), 100 mAcm-2 (25 C), and 1000 mAcm-2 (100 C). Careful electrochemical examination of the all-solid-state battery with the same battery configuration as a liquid electrolyte system revealed that the rate characteristics are simply dependent on the difference in state of electrolyte. The vert high power characteristics of solid state battery comes from intrinsic ion transportation mechanism of solid electrolyte.

HL 3: Transport: Topological Insulators (jointly with DS, MA, HL, O)

Time: Monday 9:30–13:00 Location: HSZ 204

HL 3.1 Mon 9:30 HSZ 204

Magnetic excitations in the symmetry protected, topological Haldane phase of $SrNi_2V_2O_8$ — Vladimir Gnezdilov[1,2], Vladimir Kurnosov[2], •Peter Lemmens[1], A. K. Bera[3], A. T. M. N. Islam[3], and Bella Lake[3] — [1]TU-BS, Braunschweig — [2]ILTP Kharkov — [3]HZB Berlin

We report results of a single-crystal Raman scattering study of the coupled spin-1 Haldane chain compound $SrNi_2V_2O_8$. In addition to the one-and two-magnon excitations, broad gapless and temperature dependent continua are detected with light polarization parallel to the basal plane. This feature is discussed in terms of spinon-like excitations related to a symmetry protected topological state, of which the Haldane phase in 1D is a preeminent example.

Work supported by RTG-DFG 1952/1, Metrology for Complex Nanosystems and the Laboratory for Emerging Nanometrology, TU Braunschweig.

HL 3.2 Mon 9:45 HSZ 204

Low-temperature magnetotransport in Mn-doped Bi_2Se_3 topological insulators — V. Tkáč[1], V. Komanicky[2], R. Tarasenko[1], M. Vališka[1], V. Holý[1], G. Springholz[3], V. Sechovský[1], and •J. Honolka[4] — [1]Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, CZ — [2]Institute of Physics, P. J. Šafárik University, SK — [3]Institute of Semiconductor and Solid State Physics, Johannes Kepler University, AT — [4]Institute of Physics, Academy of Sciences of the Czech Republic, CZ

Magnetic impurities can break the time-reversal symmetry of 3D topological insulators (TI), thereby opening an energy gap Δ at the Dirac point of a topological surface state with large consequences for transport properties in the thin film limit. In magnetotransport a transition from weak antilocalisation to weak localisation is expected, strongly dependent on contributions from possible coexisting 2D quantum well and bulk states. We present a low-T magnetotransport study ($T = 0.3$ K - 300 K, $B_{max} = 14$ T) of MBE-grown Bi_2Se_3 films of 20 nm - 500 nm thickness with varying Mn concentrations up to 8% and Curie temperatures $T_C = 5-7$ K [1,2]. The results are interpreted following mainly theory by Lu et al. [3] as a competition of quantum corrections to the conductivity σ (phase coherence length $l_\phi \propto T^{-1/2} \sim 50-150$nm for pure Bi_2Se_3) and 2D e-e interaction corrections both in the ferro- and paramagnetic phase.

[1] M. Valiska et al., Appl. Phys. Lett. 108, 262402 (2016).
[2] R. Tarasenko et al., Physica B 481, 262 (2016).
[3] H.-Z. Lu et al., Phys. Rev. Lett. 112, 146601 (2014).

HL 3.3 Mon 10:00 HSZ 204

Proximity-induced superconductivity and quantum interference in topological crystalline insulator SnTe devices — •Robin Klett[1], Joachim Schönle[2], Denis Dyck[1], Karsten Rott[1], Shekhar Chandra[3], Claudia Felser[3], Wolfgang Wernsdorfer[2], and Günter Reiss[1] — [1]CSMD, Bielefeld University, Germany — [2]CNRS, Institut Neél, France — [3]MPI for Chemical Physics of Solids, Germany

Topological states of matter host a variety of new physics that is promising for future technology. Among these phenomena, the emergence of metallic symmetry-protected topological surface states (TSS) are of major interest. The coupling of topological matter to a nearby superconductor is forsaken to host unconventional proximity-induced superconductivity. We demonstrate the fabrication of superconducting Quantum interference devices (SQUIDs) out of SnTe/Nb hybrid structures. Our findings show strong proximity-induced superconductivity in the surface of SnTe. Transport contributions of Majorana Bound States are predicted to enter with a shift in periodicity to DC SQUID experiments. The Analysis of the SQUID response suggest the absence of periodicity shifts, but show additional features expected for TSS carried supercurrents, such as unconventional Fraunhofer shapes.

HL 3.4 Mon 10:15 HSZ 204

Emergence of topological and topological crystalline phases in $TlBiS_2$ and $TlSbS_2$ — •Udo Schwingenschlögl, Qingyun Zhang, and Yingchun Cheng — King Abdullah University of Science and Technology (KAUST), Physical Science and Engineering Division (PSE), Thuwal 23955-6900, Saudi Arabia

Using first-principles calculations, we investigate the band structure evolution and topological phase transitions in $TlBiS_2$ and $TlSbS_2$ under hydrostatic pressure as well as uniaxial and biaxial strain. The phase transitions are identified by parity analysis and by calculating the surface states. Zero, one, and four Dirac cones are found for the (111) surfaces of both $TlBiS_2$ and $TlSbS_2$ when the pressure grows, which confirms trivial-nontrivial-trivial phase transitions. The Dirac cones at the $\bar{M}$ points are anisotropic with large out-of-plane component. $TlBiS_2$ shows normal, topological, and topological crystalline insulator phases under hydrostatic pressure, thus being the first compound to exhibit a phase transition from a topological to a topological crystalline insulator. [1] Scientific Reports **5**, 8379 (2015)

HL 3.5 Mon 10:30 HSZ 204

Perfect filter for triplet superconductivity on the surface of a 3DTI — •Daniel Breunig[1], Pablo Burset[1], François Crépin[2], and Björn Trauzettel[1] — [1]Institute for Theoretical Physics and

Astrophysics, Wuerzburg University, 97074 Wuerzburg, Germany — [2]Laboratoire de Physique Théorique de la Matière Condensée, UPMC, Sorbonne Universités, 75252 Paris, France

We study a NSN junction on the surface of a 3D topological insulator (TI), where N is a normal region and S is a s-wave proximity-induced superconducting region. Spin-orbit coupling in the TI breaks spin rotational symmetry and induces unconventional triplet superconductivity.

From the anomalous Green function, we identify the singlet and triplet pairing amplitudes and perform a symmetry classification on these quantities. Pauli exclusion principle demands the antisymmetry of the Green function under simultaneous exchange of its space, time and spin variables. The pairing amplitudes can thus be classified as ESE, OSO, ETO or OTE. Here, the first (last) letter specifies the time/frequency (parity) symmetry (Even or Odd) and the second one describes the spin (Singlet or Triplet). A special feature of our system is the emergence of the exotic odd-frequency pairing.

Interestingly, we find that for a bipolar junction, where the chemical potentials in the N leads only differ in their signs, the non-local singlet pairing amplitude is completely suppressed and only triplet pairing occurs. As a result, the non-local conductance across the junction can be dominated by purely spin triplet crossed Andreev reflections, while electron cotunneling is absent.

HL 3.6 Mon 10:45 HSZ 204

Ferromagnetic transition and fluctuation-induced Dzyaloshinskii-Morya interaction at the surface of three-dimensional topological insulators — •Flavio Nogueira[1], Ferhat Katmis[2], and Ilya Eremin[2] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum — [2]Deparment of Physics and Francis Bitter Magnet Laboratory, Massachusetts Institute of Technology

A ferromagnetic insulator (FMI) proximate to the surface of a three-dimensional topological insulator (TI) generate a gap in the spectrum of surface Dirac fermions, provided an out-of-plane exchange exists. We study the ferromagnetic transition in TI-FMI structures and show that fluctuations from Dirac fermions induce a Dzyaloshinskii-Morya (DM) interaction in the effective free energy of the FMI. This DM interaction arises only if the chemical potential is nonzero. Thus, if the proximity effect gaps the Dirac fermions, this means that the Fermi level must be outside the gap in order for a DM term to be induced. We also show that the Curie temperature of the ferromagnetic state at the interface between the TI and FMI is necessarily higher than the bulk Curie temperature of the FMI. This result is corroborated by recent experiments in Bi_2Se_3-EuS bilayer structures. These results imply an interface critical behavior very different from the bulk FMI.

HL 3.7 Mon 11:00 HSZ 204

A time-reversal symmetric topological magnetoelectric effect in 3D topological insulators — •Heinrich-Gregor Zirnstein and Bernd Rosenow — Institut für Theoretische Physik, Universität Leipzig, Germany

One of the hallmarks of time-reversal symmetric (TRS) topological insulators in 3D is the topological magnetoelectric effect (TME). So far, a time-reversal breaking variant of this effect has been discussed, in the sense that the induced electric charge changes sign when the direction of an externally applied magnetic field is reversed. Theoretically, this effect is described by the so-called axion term. Here, we discuss a time-reversal symmetric TME, where the electric charge depends only on the magnitude of the magnetic field but is independent of its sign. We obtain this non-perturbative result by a combination of analytic and numerical arguments, and suggest a mesoscopic setup to demonstrate it experimentally.

In particular, we show that threading a thin magnetic flux tube of one flux quantum through the material and applying a uniform electric field will induce a half-integer charge $\Delta Q = e/2 \operatorname{sgn} \mathbf{E}_z$ on the surface of the topological insulator. The sign of the induced charge is independent of the direction of the magnetic field.

15 min. break.

HL 3.8 Mon 11:30 HSZ 204

Single-electron injection in the edge states of a 2D topological insulator — •Giacomo Dolcetto and Thomas Schmidt — Physics and Materials Science Research Unit, University of Luxembourg

The realization of single-electron sources in integer quantum Hall systems has paved the way for exploring electronic quantum optics experiments in solid-state devices. Recently, two-dimensional topological insulators have also been considered as an interesting playground for implementing electron quantum optics. Here, two electron waveguides emerge at the edge, one for spin-up and one for spin-down electrons. Scattering between the two channels is strongly suppressed and phase-coherent ballistic transport is predicted. In this talk I will characterize the injection of single Kramers pairs from a mesoscopic capacitor: a periodic voltage drive results in the emission of periodic trains of electron and hole Kramers pairs. Due to spin-momentum locking and to the geometry of the device, the injected state is in general a superposition of many different orthogonal states, thus representing an interesting playground not only to study the transport properties, but also to investigate and to measure the entanglement production.

HL 3.9 Mon 11:45 HSZ 204

Odd-frequency superconductivity at the Helical Edge of a 2D Topological Insulator — •Felix Keidel[1], Pablo Burset[1], François Crépin[2], and Björn Trauzettel[1] — [1]Institute for Theoretical Physics and Astrophysics, Würzburg University, 97074 Würzburg, Germany — [2]Laboratoire de Physique Théorique de la Matière Condensée, UPMC, Sorbonne Universités, 75252 Paris, France

By virtue of the basic laws of quantum mechanics, the Pauli principle demands the Cooper pairs in superconductors to be odd under exchange of the two constituent electrons. Consequently, even-parity singlets are formed in conventional s-wave superconductivity. Exotic unconventional pairing symmetries emerge once the classification is extended to frequency, additionally to orbital and spin degrees of freedom.

In our work, we study a helical edge of a two-dimensional topological insulator in proximity to an s-wave superconductor and ferromagnetic insulators. While helicity and the magnetic field induce triplet correlations in addition to the inherited singlet pairing, both even- and odd-parity contributions arise since translational invariance and inversion symmetry are broken. In such a hybrid junction, odd-frequency amplitudes thus occur naturally as all combinations of spin and parity symmetry appear. On the basis of a Green's function analysis, we find signatures of these unconventional pairing amplitudes in the local density of states and in the non-local conductance. Strikingly, our method allows to track the emergence of unconventional superconductivity and make a connection to transport and pairing properties of the system.

HL 3.10 Mon 12:00 HSZ 204

Parity anomaly driven topological transitions in magnetic field — •Jan Böttcher, Christian Tutschku, and Ewelina M. Hankiewicz — Institut für Theoretische Physik und Astronomie, Uni Würzburg, 97074 Würzburg, Germany

Recent developments in solid state physics give a prospect to observe the parity anomaly in (2+1)D massive Dirac systems. We show, that the charge neutrality condition for a quantum anomalous Hall (QAH) state in orbital magnetic fields gets modified by an additional term originating from an intrinsic Chern-Simons term in the one loop Lagrangian. This can be utilized to experimentally differentiate the QAH from the quantum Hall (QH) state at charge neutrality [1]. As a result, an experimental signature of the QAH phase in magnetic fields is a long $\sigma_{xy} = e^2/h$ ($\sigma_{xy} = -e^2/h$) plateau in $Cr_x(Bi_{1-y}Sb_y)_{2-x}Te_3$ (HgMnTe quantum wells). Furthermore, we predict a new transition between the quantum spin Hall (QSH) and the QAH state in magnetic fields without magnetic impurities but driven by effective g-factors and particle-hole asymmetry.

[1] J. Böttcher, C. Tutschku, E. M. Hankiewicz, arXiv:1607.07768v1

HL 3.11 Mon 12:15 HSZ 204

Tunable edge states and their robustness towards disorder — •Maik Malki and Götz S. Uhrig — Lehrstuhl für Theoretische Physik 1, TU Dortmund, Germany

The interest in the properties of edge states in Chern insulators and in $\mathbb{Z}_2$ topological insulator has increased rapidly in recent years. We present calculations on how to influence the transport properties of chiral and helical edge states by modifications of the edges in the Haldane and in the Kane-Mele model. The Fermi velocity of the chiral edge states becomes direction-dependent as does the spin-dependent Fermi velocity of the helical edge states. Moreover, it is possible to tune the Fermi velocity by orders of magnitude. Additionally, we explicitly investigate the robustness of edge states against local disorder. The edge states can be reconstructed in the Brillouin zone in presence of disorder. The influence of the width and of the length of the system is studied as well as the dependence on the strength of the disorder.

HL 3.12 Mon 12:30 HSZ 204

Instability of interaction-driven topological insulators against disorder — Jing Wang[1,2], Carmine Ortix[1,3], Jeroen van den Brink[1], and •Dmitri Efremov[1] — [1]IFW Dresden, Germany — [2]University of Science and Technology of China, Hefei, China — [3]Utrecht University, Netherlands

We analyze the effect of disorder on the weak-coupling instabilities of quadratic band crossing point (QBCP) in two-dimensional Fermi systems, which, in the clean limit, display interaction-driven topological insulating phases. In the frame of the weak-coupling renormalization group procedure, which treats fermionic interactions and disorder on the same footing, we test all possible instabilities and identify the corresponding ordered phases in the presence of disorder for both single-valley and two-valley QBCP systems. We find that disorder generally has a strong influence on the stability of the interaction-driven topological insulating phases – it strongly suppresses the critical temperature at which the topologically non-trivial order sets in – and can even trigger a phase transition to different, topologically trivial, ordered phases.

HL 3.13 Mon 12:45 HSZ 204

Effect of disordered geometry on transport properties of three dimensional topological insulator nanowires — •Emmanouil Xypakis[1], Jun Won Rhim[1], Roni Ilan[2], and Jens H. Bardarson[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden — [2]Department of Physics, University of California, Berkeley, California

Three dimensional topological insulator nanowires are materials which, while insulating in the bulk, have a metallic boundary described by a two dimensional Dirac Hamiltonian with antiperiodic boundary conditions. Transport properties of this system have been extensively studied in the limit where the surface manifold is conformally at (e.g., a cylinder) in the presence of a random disordered scalar potential. In this talk I will discuss how this picture is altered when a more realistic surface manifold is chosen, such as a cylinder with a randomly fluctuating radius.

HL 4: Focused Session: Inhomogeneous Materials for Solar Cells I

Although multinary compound semiconductors exhibit a variety of inhomogeneities - such as strong local concentration fluctuations, built-in vertical concentration gradients, rough interfaces, and a high density of grain boundaries - they are among the leading solar cell technologies. In this focused session, the impact of inhomogeneities on the carrier transport in solar cells shall be addressed with emphasis on material growth, characterization, and modeling. Therefore, state-of-the-art research and challenges will be highlighted for a broad range of related materials such as chalcopyrites, kesterites, perovskites, and group III-nitrides.

Organizers: Roland Scheer (MLU Halle Wittenberg), Frank Bertram (OvGU Magdeburg), and Jürgen Christen (OvGU Magdeburg)

Time: Monday 9:30–12:15 Location: CHE 89

Topical Talk HL 4.1 Mon 9:30 CHE 89

Inhomogeneities in chalcopyrites and kesterites — •Claudia S. Schnohr — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Thin film solar cells based on $Cu(In,Ga)(Se,S)_2$ have reached a record efficiency of 22.6 %, thus closing the gap to silicon-based technology. $Cu_2ZnSn(Se,S)_4$ has also attracted great attention as non-toxic, earth-abundant alternative and a record efficiency of 12.6 % has already been demonstrated. Both material systems typically feature inhomogeneities such as grain boundaries, interfaces, and compositional variations, that may deteriorate or improve the device performance. We therefore applied high-resolution X-ray fluorescence analysis using a synchrotron nanobeam to study the elemental composition of chalcopyrite- and kesterite-type thin films on a micrometer and submicrometer scale. To that end, thin cross section lamellas were prepared with a focused ion beam system. For $Cu(In,Ga)(Se,S)_2$, the depth-dependent Ga gradient shows a strong dependence on the growth conditions in a sequential two-stage process. Furthermore, we find subtle lateral variations in the material composition and a significant In enrichment for some of the grain boundaries. For highly non-stoichiometric $Cu_2ZnSn(Se,S)_4$, different binary secondary phases coexist within a distance of only a few micrometers and the local compositions of the kesterite-type domains differ tremendously from the integral layer composition. Detailed knowledge of these compositional variations, which directly affect the electronic properties of the material, will thus help to exploit the full potential of chalcopyrite- and kesterite-based thin film solar cells.

Topical Talk HL 4.2 Mon 10:00 CHE 89

Impact of growth condition on defect generation in Cu(In,Ga)Se2 — •Takeaki Sakurai[1], Muhammad Islam[1], Akira Uedono[1], Shogo Ishizuka[2], Hajime Shibata[2], Shigeru Niki[2], and Katsuhiro Akimoto[1] — [1]University of Tsukuba, Tsukuba, Japan — [2]National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan

Characterization of defects in Cu(In,Ga)Se2 (CIGS)-based solar cells is an important research subject for understanding its carrier recombination processes. In this decade, the optical and electrical response of the defect states have been intensely studied using various analytical methods. Nevertheless, the origin and distribution of the defects in CIGS have not been fully understood yet due to its complex device structures and multinary compositions. During the growth of CIGS, in particular, segregation of the secondary phase, selenization, and alkali metal diffusion occur, and the difficulty in the control of the growth process mainly results in fluctuation of their optoelectronic properties. Therefore, a systematic study on the relation between the thin film growth and the generation of defects is necessary. In this study, we have investigated the impact of growth condition (Se flux and Ga concentration) on defect generation in CIGS by using various characterization techniques. We want to point out that the defect level centered around 0.8 eV from the valence level may act as a recombination center at room temparature. We will discuss whether this defect level acts as a recombination ceneter by using two-wavelength excited photoluminescence method.

HL 4.3 Mon 10:30 CHE 89

On the impact of material inhomogeneities on the time-resolved luminescence decay — •Matthias Maiberg, Torsten Hölscher, and Roland Scheer — Institute of Physics, Martin-Luther-University Halle-Wittenberg, 06120 Halle, Germany

Time-resolved luminescence is the method of choice for determination of material parameters, e.g. the minority carrier lifetime in a semiconductor. However, due to the size of the excited area the obtained data are mostly mean values averaged over a typical region of $10^4\,cm^{-2}$. In our work, we study the impact of lifetime fluctuations, band gap inhomogeneities, and potential fluctuations on the time-resolved luminescence decay by means of three-dimensional simulation. It turns out that inhomogeneous charge carrier lifetimes will increase the luminescence decay time, if the ratio of the structure size and the average diffusion length is larger than 1. For ratios smaller than 1, however, inhomogeneous charge carrier lifetimes will lead to reduced luminescence decay times. In contrast to the strong impact of lifetime inhomogeneities, band gap fluctuations are shown to have a negligible effect on the luminescence decay. In the end, it is demonstrated that the effect of potential fluctuations, which numerous of the thin-film semiconductors are prone to, is rather similar to that of space charges in a semiconductor junction. In particular the decay time will always be smaller than the recombination lifetime due to occuring drift effects. For this

reason, potential fluctuations may not explain the often observed long decay times in compensated semiconductors such as $Cu(In,Ga)Se_2$ or $Cu_2ZnSnSe_4$.

15 min. break.

Topical Talk HL 4.4 Mon 11:00 CHE 89

Inhomogeneities in chalcopyrites for solar cells — •Daniel Abou-Ras — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Thin-film solar cells with polycrystalline Cu(In,Ga)(S,Se)2 absorber layers have exhibited record conversion efficiencies of up to 22.6%. Although parallel to the substrate, the concentrations of the matrix elements in these Cu(In,Ga)(S,Se)2 thin films do not vary substantially, obvious inhomogeneities are the [In]/[Ga] and also (in case S is present) [S]/[Se] gradients perpendicular to the substrate. Moreover, also indications for various net doping concentrations in neighboring grains have been reported, which may be explained by locally varying point-defect concentrations. On the (sub)nanometer scale, compositional variations at different line and planar defects in Cu(In,Ga)(S,Se)2 thin films have been detected. The present contribution will give an overview of all these imhomogeneities existing on different length scales, but all affecting the potential landscape of chalcopyrite-type Cu(In,Ga)(S,Se)2 absorber layers.

Topical Talk HL 4.5 Mon 11:30 CHE 89

Understanding the defects in Cu(In,Ga)Se2 solar cell: a correlative microscopy approach — •Oana Cojocaru-Mirédin[1], Torsten Schwarz[2], Roland Mainz[3], and Daniel Abou-Ras[3] — [1]University of RWTH Aachen, I. Institut of Physics, Sommerfeldstraße 14, 52056 Aachen, Germany — [2]Max-Planck Institut für Eisenforschng, Max-Planck Straße 1, 40237 Düsseldorf, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, D-14109 Berlin, Germany

In Cu(In,Ga)Se2 solar cells, interfaces between individual layers in a thin-film stack, such as p-n heterojunctions, or structural defects such as grain boundaries or stacking faults, often influence substantially the performance of the device [1]. To further develop these solar devices, one needs to understand the relationship between structural and chemical properties for specific interfaces and defects. Diffraction techniques in transmission electron microscopy or scanning electron microscopy are excellent tools for structural investigations, i.e., the crystallographic structure of stacking faults and grain boundary. The present work shows an advanced, correlative study combining atom-probe tomography and various electron microscopy techniques on defects in Cu(In,Ga)Se2 absorber. Indeed, different approaches for determining structural and chemical property relationships will be presented. The experimental results to be presented will also be compared directly with the existing theoretical models on defects and phase formation in photovoltaic materials.

[1] M. Müller et al., Journal of Applied Physics 115 (2014) 023514.

HL 4.6 Mon 12:00 CHE 89

Controllable crystallization of chalcogenide thin films for photovoltaic and electrical applications — •Ilia Korolkov, Michel Cathelinaud, Xian-Hua Zhang, and Jean-Luc Adam — Verres et céramique, ISCR, Université de Rennes 1, Rennes, France

Chalcogenide materials (i.e. materials containing sulfur (S), selenium (Se) and/or tellurium (Te)) are of great importance in the context of solar energy harvesting because of their suitable electronic properties such as extended absorption spectrum, direct band gap and high absorption coefficient.

In this work we present the investigation on chalcogenide thin films of 40Sb2Se3-40GeSe2-20CuI composition, which upon the crystallization showed the formation of the conductive percolation network formed by Sb2Se3 rods covered with Cu2GeSe3 microcrystals. We optimized targets composition varying the amount of iodine and copper iodide. Various deposit and heating treatment regimes were applied as well. We revealed an important role of the iodine which dopes Sb2Se3, increasing drastically its conductivity and serving as an electron donor. We established that pre-deposit of a very thin film of CuI (about 3nm) prior to a major thin film deposit influences positively on crystallization and conductive channels formation during the heating treatment. A simple photovoltaic cell of [ITO|ZnO (or Sb2Se3 : I)|40Sb2Se3-40GeSe2-20CuI|Au] configuration shows the short circuit current up to 10mA/cm2 and open circuit voltage up to 0,2V.

HL 5: Focus Session: Two-dimensional materials I (joined session with TT)

Time: Monday 9:30–12:45 Location: POT 81

Invited Talk HL 5.1 Mon 9:30 POT 81

Van der Waals heterostructures: tunnelling and interaction with light — •Artem Mishchenko — School of Physics and Astronomy, The University of Manchester, Manchester, UK

When graphene or other conducting 2D crystals are separated by an atomically thin insulating 2D crystal (e.g. hexagonal boron nitride), quantum mechanical tunnelling leads to the appreciable interlayer current between the two 2D conductors due to the overlap of their wave functions. These tunnel devices reveal exciting physics and great potential for applications: resonant tunnelling, negative differential conductance, light emission and detection, to name a few. Here, I will update on a current status and perspectives of tunnelling devices and quantum wells based on 2D materials assembled into van der Waals heterostructures. Particularly, I will present the results on tunnelling in mono- and bilayer graphene, tunnelling in 2D crystal-based quantum wells, and tunnelling in superconducting 2D materials. I will overview such effects as momentum and chirality conservation, phonon- and impurity-assisted tunnelling. Furthermore, interaction with light (i.e. photovoltaics, solar cells, light emission, lasing and plasmonics) within these heterostructures will be discussed. Finally, possible practical applications will be outlined.

HL 5.2 Mon 10:00 POT 81

Quantum emission from low dimensional materials — •Nathan Chejanovsky[1,2], Youngwook Kim[2], Andrea Zappe[1], Rainer Stöhr[1], Felipe Favaro de Oliveira[1], Durga Dasari[1,2], Amit Finkler[1], Jurgen H. Smet[2], and Jörg Wrachtrup[1,2] — [1]3rd Physics Institute and Research Center SCoPE, University of Stuttgart, 70569 Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

Quantum emitters (QEs) in semi-conductors are at the forefront of optical research. 3D solid state systems [1] and quantum dots [2] are known sources of QEs. Nevertheless, quantum dots have constraints on temperature operation, broad linewidths and emission intermittency rendering these systems problematic. 3D systems suffer from light scattering and are difficult to process into tailored nano-structures.

Low dimensional wide band-gap materials (e.g. Van der Waals crystals) open possibilities for circumventing these obstacles, accessing intra-band gap states using sub-band gap excitation. Fulfilling this criteria, hexagonal boron nitride (h-BN), hosts room temperature QEs. [3] I summarize developments in this field and present results from our recent publication: [3] connecting structural features and QE location, generation of QEs using chemical etching/ion irradiation and analyzing their spectral features and photodynamics.

[1] Jelezko, F. et al. phys. stat. sol. (a) 2006, 203(13), 3207-3225
[2] Lodahl, P. et al. Reviews of Modern Physics 2015, 87 (2), 347-400
[3] Chejanovsky, N. et al. Nano letters 2016, 16, 7037-7045

HL 5.3 Mon 10:15 POT 81

Layered semiconductors coupled to an optical microcavity — •Michael Förg[1], Hisato Yamaguchi[2], David Hunger[3,4], and Alexander Högele[1] — [1]Fakultät für Physik and Center for NanoScience (CeNS), Ludwig-Maximilians-Universität München, Germany — [2]Materials Physics and Applications Division, Los Alamos National Laboratory, USA — [3]Ludwig-Maximilians-Universität München, Schellingstr. 4, München, Germany — [4]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, Garching, Germany

Two-dimensional atomic crystals of transition metal dichalcogenides exhibit remarkable optoelectronic properties in the limit of direct band-gap monolayers [1]. Bilayer heterostructures, on the other hand, feature long-lived indirect excitons potentially viable for studies of con-

densation phenomena [2]. In the scope of this work we investigate excitons in CVD grown layered semiconductors coupled to an optical microcavity. In our experiments we use a tunable open-access cavity with one curved fiber-based mirror and one planar mirror which supports laterally extended semiconductor flakes. This configuration allows us to combine controlled inter-mirror spacing with lateral scanning capabilities. While the former parameter is used to explore the light-matter coupling as a function of the cavity length, the latter enables two-dimensional cavity imaging of extended monolayer flakes to probe variations in the local crystal quality and the dielectric environment.

[1] Xu et al., Nat. Phys. 10, 343 (2014)
[2] Rivera et al., Nat. commun. 6 (2015)

HL 5.4 Mon 10:30 POT 81

Understanding single-photon emission from defects in hexagonal boron nitride — •Sten Haastrup and Kristian S. Thygesen — Center for Atomic-Scale Materials Design, Department of Physics, Technical University of Denmark

Point defects in sheets of hexagonal boron nitride have recently been studied as potential single-photon emitters: Experimental studies have shown that the emission from point defect color centers has extremely narrow bandwidth and mainly takes place in the zero phonon line. From an engineering perspective, a high-quality source of single photons would be extremely useful for many applications including quantum computing and quantum communications. Currently, it is not clear which defect systems in boron nitride have the right properties for use as single-photon emitters; different experimental studies have observed emission at very different energies, indicating that multiple different defect states can produce single photons. This is the starting point for our investigation into which properties of defects are important for single-photon emission, and which properties of boron nitride make it suitable as host. We have used density functional theory to explore the potential energy surfaces of the ground- and lowest excited states around different point defects in hBN. Our calculations shed light on the observed narrow band nature of the emission lines and indicate potential routes for tuning emission energy, line width and lifetime.

HL 5.5 Mon 10:45 POT 81

On the Dynamics of Excitons in Perovskite Nanoplatelets — •Alexander F. Richter[1,2], Verena A. Hintermayr[1,2], Florian Ehrat[1,2], Bernhard Bohn[1,2], Thomas Simon[1,2], Lakshminarayana Polavarapu[1,2], Alexander S. Urban[1,2], and Jochen Feldmann[1,2] — [1]Chair of Photonics and Optoelectronics, Department of Physics and Center for Nanoscience (CeNS), Ludwig-Maximilians-Universität München (LMU), Amalienstraße 54, 80799 Munich, Germany — [2]Nanosystems Initiative Munich (NIM), Schellingstraße 4, 80799 Munich, Germany

Organic-inorganic halide perovskites have received great attention in the past few years due to their remarkably high solar energy conversion efficiency. Their functionality is even more widespread showing vast improvements in light-emitting applications, especially in the form of nanocrystals. We have successfully synthesized two-dimensional perovskite nanoplatelets with a controllable thickness down to a single unit cell. This leads to exciton binding energies in the hundred meV range. Here, we present experimental results on the dynamics of excitons in such nanoplatelets. Time-resolved photoluminescence reveals an increased exciton recombination rate with decreasing crystal thickness. In addition, we derive exciton-phonon scattering rates from a linewidth analysis of linear optical spectra. These results are compared to exciton dephasing rates obtained by transient four-wave-mixing experiments.

Coffee break

Invited Talk HL 5.6 Mon 11:30 POT 81

Excitons in ultra-thin perovskites & van der Waals crystals — •Alexey Chernikov — Department of Physics, University of Regensburg, Germany

Excitons, as first introduced by J. Frenkel in 1931, are fundamental quasiparticles in semiconductors, composed from an excited electron and the remaining hole with an effective positive charge bound together by the Coulomb interaction. The excitons strongly influence the materials‘ response to external fields and perturbations, and are of particular importance for a variety of applications, including solar cells, light emitters, lasers, modulators, and detectors. In addition, they play a major role in more advanced concepts, such as entangled photons from biexciton sources, excitonic qubits, carrier multiplication, and Bose-Einstein condensation.

In this talk, I will focus on the properties of excitonic particles in nanostructured two-dimensional materials: single layers of semiconducting organic-inorganic perovskites and van der Waals crystals as thin as a single unit cell. I will discuss the nature of an unusually strong and unconventional Coulomb interaction shared by these systems and demonstrate how it results in exciton binding energies as large as 0.5 eV with highly efficient light-matter interaction, largely determining the optical response of these ultra-thin layers. Finally, I will outline how the excitons can be externally tuned either by electrical and optical injection of charge carriers or through the dielectric engineering of the environment in heterostructures.

HL 5.7 Mon 12:00 POT 81

Carrier dynamics in MoS2 — •Michael Lorke, A. Steinhoff, M. Florian, C. Gies, M. Roesner, T. Wehling, and F. Jahnke — Institute for Theoretical Physics, University of Bremen, Germany

In the context of the current interest in transition-metal dichalcogenides, we study the optical generation and relaxation of excited carriers and their influence on optical properties. In these two-dimensional atomically thin semiconductors, the Coulomb interaction is known to be much stronger than in quantum wells of conventional semiconductors like GaAs, as witnessed by the up to 50 times larger exciton binding energy. The question arises, whether this translates into equivalently faster carrier-carrier Coulomb scattering of excited carriers. We answer this question by combining ab-initio band-structures and single-particle wave functions with kinetic equations for the Coulomb-induced carrier scattering in the full Brillouin zone, We find an ultrafast redistrubution of carriers into different valleys of the band structure on a 100fs timescale. The other main source of carrier relaxation is the interaction of the excited carriers with phonons. To analyze carrier-phonon scattering and dephasing, we solve kinetic equations, based on ab-initio carrier-phonon interaction matrix elements, both for carriers and phonons, including heating effects due to the excitation of non-equilibrium phonons. We find that within 100fs the electrons have relaxed into the valleys of the bandstructure, demostrating fast carrier dynamics, which is accompanied by the generation of non-equilibrium phonons. This process is followed by carrier cooling on a timescale of about 1ps, which is consistent with recent experimental findings.

HL 5.8 Mon 12:15 POT 81

Optical Properties of WSe_2 monolayers on metal films — •Laxmi Narayan Tripathi, Oliver Iff, Simon Betzold, Sven Hoefling, and Christian Schneider — Technische Physik and Wilhelm-Conrad-Roentgen Research Center for Complex Material Systems, Universitaet Wuerzburg, Wuerzburg, Am Hubland, D-97074 Germany

Single photon generation is essential for quantum communications. For efficient quantum communication devices, a core requirement are single photon sources which are stable, bright, and which can be replicated. Recently, quantum light emission from inorganic two dimensional layers of transition metal dichalcogenides (TMDC), such as WSe_2, has been demonstrated.

In this contribution, we present our spectroscopy results from a metal-TMDC hybrid device. We performed low temperature (5K) photoluminescence measurement on a WSe_2 monolayer transferred mechanically on metal surface and obtained stable and sharp emission features as compared to bare TMDC monolayer on dielectric substrate. The nanoscale metal surface sample were prepared in the group of Prof Dai-Sik Kim, Seoul National University, South Korea. We envisage that the results will find application in quantum photonics.

HL 5.9 Mon 12:30 POT 81

Tamm-Plasmon Exciton-Polaritons with a WS2 monolayers at room temperature — •Sebastian Stoll[1], Nils Lundt[1], Christian Schneider[1], and Sven Höfling[1,2] — [1]Technische Physik and Wilhelm-Conrad-Röntgen Research Center for Complex Material Systems, Universität Würzburg, D-97074 Würzburg, Am Hubland, Germany — [2]SUPA, School of Physics and Astronomy, University of St. Andrews KY 16 9SS, UK

We demonstrate the formation of room temperature Tamm-plasmon Exciton-polaritons with a WS2 monolayer. Due to their high oscillator strength and stable excitonic complexes at 300 K, transition metal dichalcogenide monolayers have awaken strong interest in the field of

light-matter interaction at high temperatures. Recently, WS2 was brought into the strong coupling regime by embedding it into both an open-cavity [1] and a Fabry-Perot-cavity consisting of two silver mirrors [2]. In this experiment, the use of a Tamm structure provides us with a narrower cavity linewidth and thus with a higher cavity Q-factor. The exciton-polariton dispersion was measured by momentum-resolved PL spectroscopy. The acquired dispersion shows the expected avoided crossing behaviour of the two polariton branches and yields a Rabi splitting of around 27 meV. References: [1] L.C. Flatten et al., Scientific Reports 6, 33134 (2016) [2] S. Wang et al., Nano Letters 16, 7 (2016)

HL 6: Ultrafast Phenoma I

Time: Monday 9:30–12:45 Location: POT 51

Invited Talk HL 6.1 Mon 9:30 POT 51

Optical Coherent Multidimensional Spectroscopy of Semiconductor Nanostructures — •Steven Cundiff — University of Michigan, Ann Arbor, Michigan, USA

Optical coherent multidimensional spectroscopy excels at removing the effects of inhomogeneity and revealing the details of coupling for resonant excitations. In semiconductors, the excitations are typically excitons. In nanostructures, inhomogeneity arises due to size and alloy fluctuations, while coupling can arise due to many-body interactions.

In quantum wells, coherent two-dimensional spectroscopy reveals the essential role of many-body interactions, both in terms of the nonlinear response of the exciton resonance and coupling between peaks. Disorder arises because of fluctuations in the well width, and 2D spectroscopy can monitor the migration of excitons among localization sites.

For very thin quantum wells, strongly localized, quantum-dot like states, are present. Using high spatial resolution, it is possible to isolate these states and observe many-body coupling that occurs due to carriers present in the quantum-well states.

Self-organized quantum dots display strong inhomogeneous broadening, which usually prevents the observation of coherent effects, such as Rabi oscillations, in an ensemble measurement. However, 2D spectroscopy allows an individual frequency group to be isolated, which in turn means that clear Rabi flopping can be observed. Furthermore, coherent control of the biexcitonic state is possible due to the broad bandwidth of the excitation pulses.

HL 6.2 Mon 10:00 POT 51

Localized High-Harmonic Generation in Semiconductor Nanostructures — •Murat Sivis[1,2], Marco Taucer[2], Kyle Johnston[2], Giulio Vampa[2], André Staudte[2], Andrei. Yu. Naumov[2], David. M. Villeneuve[2], Paul B. Corkum[2], and Claus Ropers[1] — [1]4th Physical Institute - Solids and Nanostructures, Georg-August University, Göttingen, Germany — [2]Joint Attosecond Science Laboratory, National Research Council of Canada and University of Ottawa, Ottawa, Canada.

High-harmonic generation (HHG) in solid-state systems, as recently demonstrated in semiconductors[1–3], enables the transfer of gas-phase attosecond spectroscopy techniques to condensed matter. In general, HHG is sensitive to the electronic structure of the generation medium and the local driving laser field. Both of these properties can be routinely tailored in solids by modifying the chemical composition and the microstructure. Here, we study HHG in nanostructured zinc oxide and silicon crystals. We use wavelength-selective microscopic imaging to characterize the harmonics (at 2 μm driving wavelength) and find enhanced emission in nanofabricated grating structures as well as in gallium-implanted patterns. Our results illustrate novel means to control HHG and to use the harmonic emission as a unique local probe to investigate structural, chemical or electronic dynamics in solid-state systems.

[1]S. Ghimire *et al.* Nat. Phys. **7**, 138-141 (2011).
[2]O. Schubert *et al.* Nat. Photon. **8**, 119-123 (2014).
[3]G. Vampa *et al.* Nature **522**, 462-464 (2015).

HL 6.3 Mon 10:15 POT 51

Atomistic modeling of exciton and charge dynamics in a ZnO nanocrystal — •Dirk Ziemann and Volkhard May — Institut für Physik, Newtonstr. 15, Humboldt Universität zu Berlin, D-12489 Berlin, Germany

There is an increasing interest in ZnO semiconductor materials due to, i. a., its wide band gap and large exciton binding energy. Especially ZnO nanostructures are promising candidates for modern optical and opto electronic devices. For a quantitative understanding of the processes and time scales in theses systems an atomistic description of realistic systems, which are tens of nanometers in size and consist of thousands of atoms, is needed.

Therefor, in this talk the dynamics of excitons and charges in a spherical ZnO nanocrystal (10.000 atoms) will be discussed. The dynamics are described by a stochastic Schrödinger equation taking the initial photoexcitation and the subsequent relaxtion via electron/exciton phonon interaction into acount. The electronic and phononic states are modeled by the density functional based tight binding (dftb) method, which deals with huge systems and is still able to consider, e. g., surface effects, ligands und defects on an atomistic level. Excitonic states are calculated with a configuration interaction (CI) approach.

HL 6.4 Mon 10:30 POT 51

Terahertz narrowband-pump broadband-probe spectroscopy of intersubband transitions in a wide single quantum well — •Johannes Schmidt, Stephan Winnerl, Emmanouil Dimakis, Harald Schneider, and Manfred Helm — Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Electron relaxation dynamics of intersubband transitions (ISBT) in quantum wells can cover a broad range from ps to ns time scales, dependent on the transition energy compared to the LO-phonon energy [1]. Most of previous studies used various types of narrowband interband or intraband spectroscopy, where only one transition can be studied at a time. We have developed a setup that allows for narrowband THz pumping using the free electron laser FELBE together with broadband THz probing employing time-domain spectroscopy, and thus enabling us to record the full spectral relaxation dynamics under resonant pumping.

We study a 40 nm wide modulation doped single GaAs quantum well; this guarantees a homogeneous intensity over the active structure (which is not the case in multi quantum wells). To improve the sensitivity of the measurements, we modulate the electron density using proper gate voltages.

THz absorption of the 1-2 ISBT is seen at 2.15 THz and the 2-3 transition is observed at 3.4 THz. While pumping the 1-2 transition resonantly, a relaxation time of 1100 ps is probed. We will also report on the full probe spectra, on excitation of the 2-3 transition, and we are searching for pump-induced quantum coherent effects.

HL 6.5 Mon 10:45 POT 51

Phonon Wave Packet Emission Signatures in Four-Wave Mixing Micro-Spectroscopy of Single Quantum Dots — •Daniel Wigger[1], Tomasz Jakubczyk[2,3], Valentin Delmonte[2,3], Quentin Mermillod[2,3], Doris E. Reiter[1], Jacek Kasprzak[2,3], and Tilmann Kuhn[1] — [1]Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [2]Univ. Grenoble Alpes, F-38000 Grenoble, France — [3]CNRS, Institut Néel, "Nanophysique et Semiconducteurs" Group, F-38000 Grenoble, France

Four-Wave Mixing (FWM) micro-spectroscopy is a powerful tool to investigate the level structure of single emitters. This knowledge is essential for the use of single emitters in quantum technological applications. We investigate single self-assembled Quantum Dots (QDs), which stand out as scalable solid state single emitters but suffer from their inevitable coupling to lattice vibrations. The optical excitation of the QD exciton on the ps timescale leads to the generation of travelling phonon wave packets [1]. This generation of phonons results in a loss of coherence in the excitonic subsystem. For ultrafast excitations this is directly reflected in a rapid drop of the FWM signal. We present a combined theoretical and experimental study on the temperature dependence of the corresponding FWM signals [2].

[1] Wigger et al., J. Phys.: Condens. Matter 26, 355802 (2014)

[2] Jakubczyk et al., ACS Photonics (2016)

Coffee Break

HL 6.6 Mon 11:30 POT 51

Ultrafast Extreme-UV ARPES Study of the Transition-Metal Dichalcogenide $MoSe_2$ — •Jan Heye Buss[1], Julian Maklar[1], Frederic Joucken[1], Yiming Xu[1], He Wang[1], Changhyun Ko[2], Sefaattin Tongay[2], Junqiao Wu[2], and Robert A. Kaindl[1] — [1]Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, USA — [2]Dept. of Materials Science and Engineering, University of California, Berkeley, USA

Semiconducting transition-metal dichalcogenides exhibit intriguing physical properties, including a large spin-orbit splitting, strong Coulomb interactions, and optical access to the valley degree of freedom. Important insight into the fundamental microscopic interactions can be obtained via studies of the momentum-resolved non-equilibrium carrier dynamics. Here, we present time-resolved ARPES investigations of $MoSe_2$ crystals using high-repetition-rate extreme-UV femtosecond pulses, enabling us to track the electron dynamics within the full Brillouin zone with high sensitivity. After resonantly driving excitons at the K-point, the transient ARPES signals reveal a rapid time evolution governed by inter-valley scattering to the conduction band minimum on a 70-fs time scale. We will discuss the momentum-space dynamics as well as distinct temporal and spectral features that yield first evidence for the observation of excitons via angle-resolved photoemission spectroscopy.

HL 6.7 Mon 11:45 POT 51

Ultrafast electron transfer-induced CO_2 activation at a ZnO surface — •Lukas Gierster, Sesha Vempati, and Julia Stähler — Department of Physical Chemistry, Fritz-Haber-Institute of the Max-Planck-Society, Faradayweg 4-6, 14195 Berlin, Germany

Since many years, ZnO has been used as a catalyst which facilitates the conversion of carbon dioxide into valuable chemicals such as methanol [1]. CO_2, which is the most stable carbon oxide species, needs to be activated in order to start hydrogenation. Recent experimental and theoretical work showed that CO_2 adsorbs in a bent configuration with tridentate chemical binding on the ZnO (10-10) surface [1]. However, the energies of the frontier molecular orbitals of the adsorbed CO_2 molecules in the chemical reaction are still not known. We investigate this question using two-photon photoelectron spectroscopy (2PPE), which gives access to occupied and unoccupied electronic states and the dynamics therein. Static photoelectron spectroscopy shows that the work function of the surface increases considerably upon CO_2 adsorption possibly due to a (partial) reduction of the molecules and their dipole moment. A time-resolved pump-probe experiment suggests that electrons are injected from the ZnO substrate into the CO_2 molecules after above band gap photoexcitation of the substrate. The injected electrons populate the CO_2 LUMO, which subsequently shifts down in energy. This leads to a built up of an electronic state just below the Fermi energy within few picoseconds, which is likely to be related to the activated CO_2 molecules.

[1] K. Kotsis, et al., Z. Phys. Chem. 222, 891-915 (2008).

HL 6.8 Mon 12:00 POT 51

Complete Analysis of a transmission electron diffraction pattern of a molybdenum disulphide-graphite heterostructure — •Marlene Adrian, Arne Senftleben, Silvio Morgenstern, and Thomas Baumert — University of Kassel, Institute of Physics (CINSaT), D-34132 Kassel, Germany

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 in the group of 2D layered materials, the combination opens a new pathway towards ultrasmall electronic devices. In this contribution we present a complete mathematical description of multilayer heterostructures and a full characterisation of their diffraction patterns. A 27 nm thick molybdenum disulphide-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 6.9 Mon 12:15 POT 51

Ultrafast transmission electron microscopy using laser-triggered field emitters — •Thomas Danz, Armin Feist, Nora Bach, Nara Rubiano da Silva, Marcel Möller, Sascha Schäfer, and Claus Ropers — IV. Physical Institute – Solids and Nanostructures, University of Göttingen, Germany

Ultrafast transmission electron microscopy (UTEM) is a promising approach to investigate ultrafast processes with nanometer spatial resolution [1]. Using the versatile imaging, diffraction, and spectroscopy capabilities of such an instrument, structural, electronic, and magnetic dynamics can be probed in a laser pump/electron probe scheme [2].

The pulsed electron source of the Göttingen UTEM project employs linear photoemission from a nanoscopic Schottky emitter, delivering highly coherent electron pulses with down to 200 fs pulse duration, 0.6 eV energy width, and sub-1 nm focused beam diameter [3]. We present first applications, as well as prospects and challenges of the UTEM in ultrafast electron imaging, diffraction, energy loss spectroscopy (EELS), and holography, and discuss approaches to reversibly drive electronic and structural phase transitions in inhomogeneous systems.

[1] A. H. Zewail, Science **328**, 187 (2010)
[2] A. Feist *et al.*, in preparation
[3] A. Feist *et al.*, arXiv:1611.05022

HL 6.10 Mon 12:30 POT 51

A combined approach of k.p-perturbation theory and semiconductor Bloch equations for the analysis of ultrafast photocurrents — •Reinold Podzimski[1], Huynh Thanh Duc[2], and Torsten Meier[1] — [1]Department Physik and Center of Optoelectronics and Photonics Paderborn (CeOPP), Universität Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany; — [2]Ho Chi Minh City Institute of Physics, Vietnam Academy of Science and Technology, Mac Dinh Chi Street 1, District 1, Ho Chi Minh City, Vietnam;

In unbiased non-centrosymmetric semiconductors electronic currents can be generated directly by optical laser pulses. Combining k.p-perturbation theory with the semiconductor Bloch equations provides an approach to theoretically describe these photocurrents in bulk and quantum well systems [1,2]. We investigate shift and rectification currents in bulk GaAs and GaAs quantum well systems. The transparent approach of the semiconductor Bloch equations allows to identify the microscopic origin of several phenomena. Using a geodesic grid for the discretization of the **k**-space we are able to include the Coulomb interaction and to investigate excitonic contributions.

[1] R. Podzimski, H. T. Duc, and T. Meier, Proc. SPIE **97460W**, 9746 (2016).
[2] H. T. Duc, R. Podzimski, S. Priyadarshi, M. Bieler, and T. Meier, Phys. Rev. B **94**, 085305 (2016).

HL 7: Spintronics I (joined session with TT)

Time: Monday 9:30–13:00 Location: POT 151

HL 7.1 Mon 9:30 POT 151

Dynamical spin-orbit-based spin transistor — •Fahriye Nur Gürsoy[1,2], Phillipp Reck[1], Cosimo Gorini[1], Klaus Richter[1], and Inanç Adagideli[2] — [1]Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany — [2]Faculty of Engineering and Natural Sciences, Sabanci University, Orhanli-Tuzla, Istanbul, Turkey

Spin-based devices are highly important for the future of information technology. In this project we focus on a mesoscopic 2-Dimensional Electron Gas (2DEG) with time-dependent Rashba spin-orbit interaction, which can be engineered via an AC top gate.

Spin-orbit coupling in 2DEGs can be rewritten in terms of appropriate SU(2) gauge fields, so as to clearly identify the relevant Onsager symmetries [1, 2].The latter can then be exploited for the realisation of spin transistor devices, in particular when the spin-orbit interaction is non-homogeneous through the sample [1]. On the other hand, a dynamical Rashba interaction was suggested as a generator of spin-motive forces. Here we merge the two concepts, and explore the possibilities of realising a spin transistor in a quantum coherent sample driven by a time-dependent Rashba field. We follow a mixed analytical-numerical approach, and compute the (spin) conductance and the pumping (spin) current of the periodically driven system with the Floquet Hamiltonian method [3].

[1] I. Adagideli, et al., Phys. Rev. Lett. 108, 236601 (2012).
[2] C. Gorini, et al., Phys. Rev. Lett. 109, 246604 (2012).
[3] J. H. Shirley, Phys. Rev. 138, B979 (1965).

HL 7.2 Mon 9:45 POT 151

Coherent electron Zitterbewegung triggered by ps optical pulses — •Manfred Ersfeld[1], Ivan Stepanov[1], Alexander V. Poshakinskiy[2], Mihail Lepsa[3], Eugeneous L. Ivchenko[2], Sergey A. Tarasenko[2], and Bernd Beschoten[1] — [1]2nd Institute of Physics and JARA-FIT, RWTH Aachen University, D-52074 Aachen, Germany — [2]Ioffe Institute, 194021 St Petersburg, Russia — [3]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich GmbH, Germany

Zitterbewegung is a direct consequence of relativistic quantum mechanics which predicts that free Dirac electrons exhibit a rapid trembling motion even in the absence of external forces. Recent theoretical studies have shown that electrons in III-V semiconductors also exhibit Zitterbewegung caused by the spin orbit interaction. Here we probe the Zitterbewegung of electrons in n-type InGaAs as an AC electric current. We trigger the coherent electron Zitterbewegung by optical initialization of an ensemble of electron spins in the same spin states and control the frequency of electron oscillations in real space by tuning the Larmor spin precession frequency in an external magnetic field.

HL 7.3 Mon 10:00 POT 151

On the link between charge- and spin-dynamics in PBTTT — •Uday Chopra[1], Erik R. McNellis[1], Denis Andrienko[2], Pascal Kordt[2], and Jairo Sinova[1] — [1]Johannes Gutenberg University, Mainz, Germany — [2]Max Planck Institute for Polymer Research, Mainz, Germany

In the nascent field of organic spintronics, charge- and spin-dynamics are strongly linked. We study this relationship in a high-mobility[1], spin-conducting polymer[2], PBTTT, using a newly developed multi-scale modelling framework. High mobility ($\sim$ 1 $cm^2V^{-1}s^{-1}$) in PBTTT along the $\pi - \pi$ stacking direction is attributed to its highly ordered structure and hence the strong transfer integrals in the same direction. However, the mechanism for spin transport and its correlation with electron transport is still unclear. We demonstrate the anisotropy in electron dynamics of PBTTT by calculating electron transfer rates for morphologies of different sizes and extent of disorder in the backbone using Marcus theory and Kinetic Monte Carlo (KMC) as implemented in VOTCA-CTP[3] and showing the field and temperature dependence of mobility along different crystalline axes. In addition to it, we present an approach for spin transport in organic semiconductors build on top of VOTCA-CTP via first-principles modelling of spin relaxation mechanisms which allows us an uprecedented insight into the explicit dependence of spin- on charge-dynamics and the parameters that correlate them. [1] McCulloch et al., Nat. Mater., 2006, 5, 328. [2] Watanabe et al., Nat. Phys., 2014, 10, 308. [3] V. Rühle et al. J Chem. Theory Comput., 2011, 7, 3335.

HL 7.4 Mon 10:15 POT 151

Theory of current-induced spin polarisations in a 2DEG — Amin Maleki[1], •Cosimo Gorini[2], Ka Shen[3], Ilya V. Tokatly[4,5], Giovanni Vignale[6], and Roberto Raimondi[1] — [1]CNISM e Dipartimento di Fisica, Università Roma Tre, Rome, Italy — [2]Institut für Theoretische Physik, Universität Regensburg, Regensburg, Germany — [3]Kavli Institute of NanoScience, Delft University of Technology, Delft, Netherlands — [4]Nano-Bio Spectroscopy group, Dpto. Fisica de Materiales, Universidad del País Vasco, San Sebastián, Spain — [5]IKERBASQUE, Bilbao, Spain — [6]Department of Physics and Astronomy, University of Missouri, Columbia, Missouri, USA

The Bloch equations for the spin dynamics of a 2DEG are derived in the presence of intrinsic (Rashba and Dresselhaus) and extrinsic (impurities) spin-orbit coupling. In comparison to previous analyses, we find new terms arising from the interplay between the two types of spin-orbit interaction. These influence current-induced spin polarisations (CISP), which are shown to have a more complex symmetry with respect to that of the internal Rashba-Dresselhaus field. Our results are derived both diagrammatically and via a semi/quasi-classical approach, based on a SU(2) gauge formulation of spin-orbit coupling.

HL 7.5 Mon 10:30 POT 151

Toward accurate calculation of diffusive spin transport starting from realistic Hamiltonians. Applications to electrons, excitons, and topological insulators. — •Vincent Sacksteder[1] and Yasufumi Araki[2] — [1]W155 Wilson Building, Royal Holloway University of London, Egham Hill, Egham, TW20 0EX, United Kingdom — [2]Creative Interdisciplinary Research Division, Tohoku University

Spin-orbit couplings, in the presence of an electric current, can generate strong spin currents with possible applications to magnetic domain switching in new memory devices. This talk will focus on a coarse-graining strategy which starts from realistic Hamiltonians describing spin and scattering at the atomic scale, and derives spin diffusion equations suitable for modeling a spintronics device. After reviewing the standard formalism, we outline how spin diffusion coefficients can be calculated either analytically or numerically, in either magnetized or unmagnetized systems. We present results for spin lifetimes, spin polarization production, and characteristic spatial patterns in electron gases, excitons, and topological insulators.

HL 7.6 Mon 10:45 POT 151

Charge- and Spin Dynamics in Organic Spintronics from First-Principles Theory: VOTCA-STP — •Erik R. McNellis[1], Shayan Hemmatiyan[1,2], Amaury Melo Souza[1], Sebastian Müller[1], Sergei A. Egorov[1,3], Denis Andrienko[4], and Jairo Sinova[1] — [1]Johannes Gutenberg University, Mainz, Germany — [2]Texas A & M University, College Station, USA — [3]University of Virginia, Charlottesville, USA — [4]Max-Planck-Institute for Polymer Research, Mainz, Germany

Novel high-mobility materials based on organic molecules bring a host of advantages in spintronic applications. In organics, spin- and charge dynamics are intimately linked. Ideally, such materials should be theoretically modeled using realistic structural models with atomic resolution, and field- and spin-orbit coupling (SOC) effects calculated from state-of-the-art first-principles theory.

We present a multi-scale framework for modeling of spin-dynamics in organics, implemented on top of the electron dynamics given by the VOTCA-CTP package[1]. This development allows us to accurately treat the balance of SOC phenomena in realistic morphologies, while observing the link between charge- and spin-dynamics directly.

Our results include a complete map of the spin-relaxation in Alq_3 - the organic spintronics fruit-fly - as a function of charge concentration and temperature. Additionally, insights into the highly spin conducting polymer PBTTT will be presented, along with developments towards treating the spin Hall and Nernst effects.

1. V. Rühle et al., J Chem. Theory Comput. **7**, 3335 (2011)

Coffee Break

HL 7.7 Mon 11:30 POT 151

Control of spin helix symmetry in semiconductor quantum wells by crystal orientation — •Paul Wenk, Michael Kammermeier, and John Schliemann — Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

We investigate the possibility of spin-preserving symmetries due to the interplay of Rashba and Dresselhaus spin-orbit coupling in n-doped zinc-blende semiconductor quantum wells of general crystal orientation. It is shown that a conserved spin operator can be realized if and only if at least two growth-direction Miller indices agree in modulus. We determine the appropriate requirements on the axial symmetric Rashba and Dresselhaus contributions and discuss the impact of cubic Dresselhaus terms which break this symmetry. We observe that including the latter commonly inhibits a perfect realization of the persistent spin helix symmetry except for two specific directions, i.e., [110] and [111]. Furthermore, by analyzing the spectrum of the spin diffusion equation, we show that besides the cases of perfect spin-preserving symmetries, the spin of the long-lived homogeneous spin state relaxes about a factor 2 faster than for the helical spin state. To support experimental probing, we additionally provide analytical expressions for the weak (anti)localization correction and the characteristic shift of the magnetoconductivity minima [2] which show an imprint of the peculiar symmetry.

[1] M. Kammermeier *et al.*, Phys. Rev. Lett. **117**, 236801 (2016)
[2] K. Yoshizumi *et al.*, Appl. Phys. Lett. **108**, 132402 (2016).

HL 7.8 Mon 11:45 POT 151

Hidden orbital polarization in centrosymmetric materials — •Ji Hoon Ryoo and Cheol-Hwan Park — Department of Physics & Astronomy, Seoul National University 1 Gwanak-ro, Gwanak-gu, Seoul 08826, Korea

Until recently, the possibility of spatial spin distribution in centrosymmetric and non-magnetic materials was largely dismissed, because their electronic bands are degenerate even if spin-orbit coupling is strong. However, Zhang et al. [1] has pointed out that even in those materials, the degenerate Bloch states can have spin polarization localized at different sites in real space, significantly broadening the scope of spintronics to materials with inversion symmetry. On the other hand, the orbital magnetic moment could play as an important role as the spin moment in the magnetization of solids, in both equilibrium and non-equilibrium situations [2-5]. In this talk, we report that the hidden, or sublattice-dependent orbital polarization of Bloch states can be large in common centrosymmetric materials, and suggest some implications of this finding to photoemission spectroscopies and antiferromagnetic information technology.

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HL 7.9 Mon 12:00 POT 151

Improving and tailoring the magnetic properties of thin Fe layers by making use of exchange coupling — •Markus Ehlert, Helmut Körner, Thomas Hupfauer, Markus Schitko, Christian Back, 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 Fe layers by making use of the exchange coupling between soft magnetic Fe and hard magnetic Dysprosium (Dy). Microstructured thin films of Fe, Dy, and Fe-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 AMR effect. By analyzing and comparing the corresponding AMR data we show that the presence of a Dy layer on top of the Fe layer significantly influences and enhances the magnetic properties of the Fe layer. We also investigated the temperature dependence of this effect and its dependence on the thickness of the Fe layer. All experimental results can consistently be explained with the model of the AMR effect and are also confirmed by corresponding SQUID measurements of full film samples.

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

HL 7.10 Mon 12:15 POT 151

First principles calculations to address key spin relaxation mechanisms in organic semiconductors — •Amaury de Melo Souza[1], Sergei Ergorov[2], Pedro Brandimarte[3], Sebastian Mueller[1], Uday Chopra[1], Shayan Hemmatiyan[4], Denis Andrienko[5], Ilja Mueller[1], Jairo Sinova[1], and Erik McNellis[1] — [1]Johannez Gutenberg University, Mainz, Germany — [2]University of Virginia, Charlottesville, USA — [3]University del Pais Vasco, San Sebastian, Spain — [4]Texas A&M University, College Station, USA — [5]Max Planck Institute for Polymers, Mainz, Germany

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 able to study spin transport in the presence of anisotropy, thermal effects, magnetic and electric field effects in realistic morphologies of amorphous organic systems. In this talk, we present in detail first-principles calculations combined with perturbation theory in order to extract the relevant quantities required to address key spin relaxation mechanisms, namely, spin flip due to spin-orbit coupling, intra-site spin relaxation due to spin-orbit coupling and electron-phonon coupling and exchange mediated transport. Finally, we apply our approach to a realistic morphology of Alq3 (Tris(8-hydroxyquinolinato)aluminum) and identify which spin relaxation mechanism is dominant in this system.

Invited Talk HL 7.11 Mon 12:30 POT 151

Carbon nanotubes as excitonic insulators — •Massimo Rontani — CNR-NANO, Modena, Italy

Fifty years ago Walter Kohn speculated that a zero-gap semiconductor might be unstable against the spontaneous generation of excitons—electron-hole pairs bound together by Coulomb attraction. The reconstructed ground state would then open a gap breaking the symmetry of the underlying lattice, a genuine consequence of electronic correlations.

I will show that this 'excitonic insulator' is realized in zero-gap carbon nanotubes, by presenting results of first-principles calculations performed by means of many-body perturbation theory as well as quantum Monte Carlo. The excitonic order modulates the charge between the two carbon sublattices of the armchair tube, opening an experimentally observable gap which scales as the inverse of the tube radius and weakly depends on the axial magnetic field.

These findings invalidate the common wisdom that the ground state of armchair carbon nanotubes is a Luttinger liquid. I will discuss the physical origin of this conclusion, related to the strong e-h binding in quasi-1D and the almost unscreened long-range interactions in undoped nanotubes. Finally, I will propose independent experimental tests to discriminate between the excitonic insulator and the Luttinger liquid at strong coupling (Mott insulator).

This work is performed together with Daniele Varsano, Sandro Sorella, Davide Sangalli, Matteo Barborini, Stefano Corni, and Elisa Molinari.

HL 8: Photovoltaics

Time: Monday 9:30–11:45 Location: POT 251

HL 8.1 Mon 9:30 POT 251

Light enhanced degradation of Cu(In,Ga)Se_2 investigated by time-resolved photo-luminescence and X-ray photoelectron spectroscopy — •Torsten Hölscher, Stefan Förster, Thomas Schneider, Setareh Zahedi-Azad, Eva Maria Zollner, Matthias Maiberg, and Roland Scheer — Martin-Luther-University Halle-Wittenberg, Germany

Cu(In,Ga)Se_2 (CIGSe) as absorber material for thin-film solar cells is known to degrade when exposed to air. So far, only little is known about the underlying surface processes. A method of choice for such an investigation is time-resolved photoluminescence (TRPL), which gives insight into the recombination kinetics of minority charge carriers. In our work, we have applied TRPL to CIGSe layers grown on molybdenum covered soda lime glass. The results show a strong decrease of the minority carrier lifetime after 10 till 60 min illumination with white light (1 sun) under ambient conditions. Measurement of X-ray photoelectron spectroscopy reveals an increase of the Na 1s and O 1s peak on the CIGSe surface. The position of the O 1s peak is centered at 531.7 eV, which we refer to the Na–O-CIGSe bonding complex. Based on TRPL and XPS we propose a light enhanced formation of this Na–O-CIGSe complex on the surface as the origin of the degradation. This model may also explain the often observed – "laser degradation" – during TRPL measurements. In the end, we discuss the influence of this degradation effect on the solar cell performance.

HL 8.2 Mon 9:45 POT 251

Optoelectronic properties of a-Si:H and a-Si:H/c-Si interfaces from first principles — •Philippe Czaja[1], Urs Aeberhard[1], Massimo Celino[2], and Simone Giusepponi[2] — [1]IEK-5 Photovoltaics, Forschungszentrum Jülich, Germany — [2]ENEA Casaccia, Italy

In order to optimize the optoelectronic properties of novel solar cell architectures, such as the amorphous-crystalline interface (a-Si:H/c-Si) in silicon heterojunction devices, we calculate and analyze the local microscopic structure at the interface and in bulk a-Si:H, in particular with respect to the impact of material inhomogeneities. The microscopic information is used to extract macroscopic material properties, and to identify localized defect states, which govern the recombination properties encoded in quantities such as capture cross sections used in the Shockley-Read-Hall theory.

To this end, atomic configurations for a-Si:H and a-Si:H/c-Si interfaces are generated using molecular dynamics. Density functional theory calculations are then applied to these configurations in order to obtain the electronic wave functions. These are analyzed and characterized with respect to their localization and their contribution to the (local) density of states. GW calculations are performed for the a-Si:H configuration in order to obtain a quasi-particle corrected absorption spectrum. The results suggest that the quasi-particle corrections can be approximated through a scissors shift of the Kohn-Sham energies.

HL 8.3 Mon 10:00 POT 251

Investigation of the Loss Mechanisms in $CuInS_2$/ZnO Nanocrystal Solar Cells — •Dorothea Scheunemann, Sebastian Wilken, Holger Borchert, and Jürgen Parisi — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, 26111 Oldenburg

Heterojunction solar cells based on colloidal nanocrystals have shown remarkable improvements in performance in the last decade. This progress was accompanied by a deeper understanding of the underlying physical processes in nanocrystal solids and devices. However, the vast majority of these studies is focused on two materials, PbS and PbSe. In contrast, there is still a lack of such detailed knowledge in case of other materials, as for example copper-based compounds, which show lower power conversion efficiencies when incorporated into solar cells. Here, we present a detailed study on the photocurrent loss mechanisms in nanocrystalline $CuInS_2$/ZnO heterojunction solar cells by combining steady-state characterization methods with transient photocurrent and photovoltage measurements. We demonstrate the presence of two different loss mechanisms: An extraction barrier at the $CuInS_2$/ZnO interface, which can be reduced upon illumination with UV light, as well as significant trap-assisted recombination in the $CuInS_2$ layer. The presented results confirm the potential of heterojunctions made from $CuInS_2$ and ZnO nanocrystals in solution producible solar cells, but also clearly highlight the importance of a substantial reduction of sub-band gap states to improve the performance.

HL 8.4 Mon 10:15 POT 251

First-principles modeling the alkali-metal post-deposition treatment of CIGS solar cells — •Maria Fedina, Hannu-Pekka Komsa, Ville Havu, and Martti Puska — Department of Applied Physics, Aalto University, P.O. Box 11000, Espoo, Finland

The efficiency of the Cu(In,Ga)Se_2 (CIGS) solar cell has increased significantly during the last few years thanks to the post-deposition treatment (PDT) by alkali metals. The PDT process results in formation of alkali metal impurities inside the CIGS grain interiors (GIs) and near grain boundaries (GB) We have calculated formation energies and migration barriers for Li, Na, K, Rb, and Cs impurities in bulk $CuInSe_2$ (CIS) within the framework of the density-functional theory. We will discuss the interplay between the alkali metal impurities and the native point defects in CIS. Moreover, the most important parameters of the secondary phases, such as lattice constants, band gaps, and heats of formation have been calculated. Mechanisms for secondary phase formation in CIGS will be discussed. Due to low free energies at surfaces and GBs, alkali metal atoms accumulate preferably at GBs and near the CIGS surface resulting in possible formation of secondary phases. We have calculated formation energies of alkali metal impurities also near different types of GBs and close to the surface, and we will discuss the prominent trends between different alkali metal atoms.

Coffee Break

HL 8.5 Mon 10:45 POT 251

Theoretical analysis of an Intermediate Band in Sn-doped Hematite with Wide-spectrum Solar Response — Wilayat Khan[1] and •Jan Minar[2] — [1]New Technologies-Research Center, University of West Bohemia, Univerzitní 8, 306 14 Plzen*, Czech Republic — [2]Department of chemistry and Center for NanoScience, LMU Munich, Butenandtstra*e 11, 81377 M*unchen, Germany

Hematite α-Fe2O3 is exposed to be an efficient photocatalytic material for water splitting process under visible light. We have further improved the photocatalytic activity of Hematite by varying Tin (Sn) concentration substituted for Fe in pristine hematite. Experimental measurements on the Sn doped Fe2O3 and a brief theoretical study on the density of states (DOS) have been reported in the previous studies, but further detail insight into the optoelectronic and spectroscopic properties is still missing. Here we obtained the accurate insulating character and feature the electronic structure and other key properties of pristine and Sn doped Fe2O3 by the combination of on-site Hubbard interaction and generalized gradient approximation within WIEN2k code. The electronic structures explore the engineering of the orbitals around the Fermi level due to increase in the concentration of Sn in Fe2O3, and the expected reduction in the band gap is also attributed to the corresponding contents of Sn. The electronic structure of doped hematite introduces an intermediate band (IB) and absorption edge is shifted to the infrared regime. In addition, the Fe-K edge and Fe-L2,3 edge were also calculated using the SPR-KKR code.

HL 8.6 Mon 11:00 POT 251

Preparation and Analysis of In_2S_3:V Intermediate Band Thin-Film Absorbers for Solar Cells — •Leonard Wägele[1], Tanja Jawinski[1,2], Christoph Bahret[1], Holger von Wenckstern[2], Marius Grundmann[2], and Roland Scheer[1] — [1]Institute of Physics, Martin-Luther-University Halle-Wittenberg, 06120 Halle, Germany — [2]Institute of Experimental Physics II, University of Leipzig, 04103 Leipzig, Germany

To achieve higher energy conversion efficiencies above the Shockley-Queisser limit, one can use larger band gap materials provided with an intermediate band. This allows the absorption of low energy photons via the intermediate band, while high energy photons can generate charge carriers with reduced thermalization losses. One theoretically suitable material for such a device is In_2S_3 combined with transition metals. We grow thin-film In_2S_3:V with physical co-evaporation from the elements. We use SEM, EDX, XRD and Raman spectroscopy to study the structural changes of vanadium variations. We show that

vanadium is successfully incorporated into the In_2S_3 structure. Furthermore, UV-VIS-NIR spectroscopy, photoluminescence and photoconductivity are used to study the electro-optical properties of the material. We find that the absorption increases slightly with incorporated vanadium, while the below band gap photoluminescence decreases. Additionally, we show results from In_2S_3:V p-i-n solar cells utilizing both SnO:F and ZnO:Al as n-TCOs and ZnCo2O4 and NiO as p-TCOs. EQE and JV-measurements reveal the formation of functioning solar cells with so far low short circuit currents.

HL 8.7 Mon 11:15 POT 251

Investigating photocurrents on a micrometer scale: Ultrabroadband reflection microscopy and photo-current imaging of structured thin-film solar cells — •Moritz Gittinger[1], Regina-Elisabeth Ravekes[2], Ralf Vogelgesang[1], Martin Vehse[2], Carsten Agert[2], Christoph Lienau[1], and Martin Silies[1] — [1]AG Ultrafast Nano-Optics, Carl von Ossietzky Universität Oldenburg, Germany — [2]Next Energy EWE Research Centre for Energy Technology, Oldenburg, Germany

Silicon thin-film solar cells are promising candidates in the quest for higher quantum efficiencies. Currently, though, they still suffer from an inefficient light coupling due to the thin, sub-μm thick absorber material. Light trapping using honeycomb-structured ZnO electrodes appear to be a low-cost and large-scale approach to significantly increase the external quantum efficiency (EQE) of the cell [1]. Here, we present a fast optical far-field technique to map simultaneously the locally-induced photocurrent in and the reflected light from these honeycomb-structured films with varying honeycomb dimensions with micrometer resolution and in a broad spectral range. We observe locally varying photocurrents and reflection signals that reflect the periodic variation of local optical density of states of the two-dimensional honeycomb pattern of the cell. The local fluctuations are quantitatively analyzed in terms of a one-parameter scaling theory for random light localization [2] and are correlated to the EQE of the cell. [1] R.-E. Nowak et al., IEEE Journal of Photovoltaics 5, 479 (2015) [2]Th. M. Nieuwenhuizen, M.C.W. van Rossum, PRL 74, 2674 (1995)

HL 8.8 Mon 11:30 POT 251

Many-body effects in X-ray absorption spectra of the sulfur $L_{2,3}$ edge in Cu_2ZnSnS_4 — •Archana Manoharan[1], Lorenzo Pardini[1], and Claudia Draxl[1,2] — [1]Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany — [2]European Theoretical Spectroscopic Facility (ETSF)

The kesterite material Cu_2ZnSnS_4 (CZTS) is a promising candidate as an absorber layer for solar-cell applications. In the present work, we study its structural, electronic, and X-ray absorption properties using a first-principles approach. We explore the X-ray absorption spectra at the sulfur $L_{2,3}$ edge in CZTS by solving the Bethe-Salpeter equation (BSE) and compare them to corresponding binary phases, i.e., ZnS and SnS_2. Special emphasis is put on the spin-orbit coupling between the S $2p_{1/2}$ and $2p_{3/2}$ core states. In comparison to the independent-particle approximation, the inclusion of Coulomb interaction redshifts the absorption edge in all three materials. In case of CZTS, a bound exciton is found. It is formed by transition from the S $2p_{3/2}$ core state. The second peak with excitonic character is due to the mixing of excitation channels of the L_2 and L_3 edges. In the binary phases, a bound state is observed in SnS_2 but not in ZnS. We assign the bound exciton in CZTS to hybridisation of Sn with S. The calculated BSE results are in good agreement with experimental spectra.

HL 9: Quantum Dots: Preparation and Characterization

Time: Monday 9:30–12:30 Location: POT 112

HL 9.1 Mon 9:30 POT 112

Fabrication of spectrally homogeneous quantum dot micropillar laser arrays as a nanophotonic hardware for reservoir computing — •Jan Grosse[1], Tobias Heuser[1], Arsenty Kaganskiy[1], Daniel Brunner[2], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin, Germany — [2]FEMTO-ST, Département d'Optique, 15B Avenue des Montboucons, 25030 Besançon, France

Reservoir computing is a machine learning approach for a new way of efficient data processing. In this promising computing scheme, inspired by the neurons in the brain, the interaction of a network of nodes, called the reservoir, is evaluated by a trained readout to enable applications like fast speech recognition. To realize this concept with optically coupled nodes, a nanophotonic hardware implementation is of particular interest. Here, we report on the growth and fabrication process of spectrally homogeneous 2D arrays of up to 900 quantum dot micropillar lasers. Using diffractive coupling and sophisticated external optics [1], lasers in such arrays will form a nonlinear optical reservoir network. To enable this appealing application, spectral inhomogenities of the vertical laser structure, grown by MOCVD, are compensated by precisely adjusting the radius of individual micropillars [2] via high-resolution electron beam lithography to achieve an overall spectral homogeneity better than 200 μeV in the dense micropillar laser array.

References

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[2] S.Reitzenstein, A.Forchel, J.Phys.D.Appl.Phys. 43, 033001 (2010)

HL 9.2 Mon 9:45 POT 112

Fluorescence behavior of semiconductor nanoparticles in vicinity of plasmonic metals — •Simon Schneider, Elvira Kröger, Xiao Tang, Christian Strelow, Tobias Kipp, and Alf Mews — Institute of Physical Chemistry, University of Hamburg, Grindelallee 117, 20146 Hamburg, Germany

Interactions of plasmonic metal nanoparticles with semiconductor nanoparticles greatly influence the fluorescence behavior of the latter. If introduced to a plasmonic resonant system, the rate of spontaneous emission can be enhanced (Purcell effect). Here, the distance between the metal- and semiconductor nanoparticles has a huge influence on the fluorescence behavior of the whole system, direct contact of the two parts leads to complete fluorescence quenching. We control the distance between metal and CdSe/CdS semiconductor dot-in-rod (DR) structures on the nanometer scale using a silica shell around the DRs as a dielectric spacer and investigate the effect of attached plasmonic metals (Ag & Au) on the fluorescence behavior of the DRs. Metal nanoparticles of 2-3 nm in diameter only showed little to no effect whereas the growth of a continuous gold shell around the DRs doubled the fluorescence-decay rate.

HL 9.3 Mon 10:00 POT 112

P-doping of Silicon Nanocrystals: Free Carriers vs. Defects — •Daniel Hiller[1], Julian Lopez-Vidrier[1], Sebastian Gutsch[1], Margit Zacharias[1], Keita Nomoto[2,3], and Dirk König[3] — [1]Laboratory for Nanotechnology, IMTEK, University of Freiburg, Germany — [2]The University of Sydney, Australia — [3]University of New South Wales (UNSW), Sydney, Australia

We study the size limitations of conventional P-doping of ultra-small Si volumes using Si nanocrystals (Si NCs) of 2-5 nm as a model system. Theoretical studies predicted that P-doping of Si nanocrystals fails due to self-purification, increased formation energies of substitutional P-atoms, and increased ionization energies of donor electrons due to quantum- and dielectric confinement. However, several groups reported a quenching of photoluminescence (PL) from Si NCs by P-doping and attributed that to non-radiative Auger recombination with donor electrons. In this work, we address this contradiction. We disprove the self-purification effect by atom probe tomography (APT) measurements [1]. However, a correlation of APT-statistics, PL- and I-V-measurements reveals that the PL quenching cannot be explained by free carriers. X-ray absorption (XAS) measurements at the P-K-edge indicate that the majority of P-atoms in Si NCs is not ionized at 300 K [3]. I-V shows that P-ionization requires 100-500 meV depending on the NC size [2]. Using density functional theory (DFT) simulations [3], we explain the PL-quenching by P-induced defect states.

[1] Phys. Status Solidi RRL (2016), DOI: 10.1002/pssr.201600376 [2] Appl. Phys. Lett. 106, 113103 (2015) [3] Sci. Rep. 5, 09702 (2015)

HL 9.4 Mon 10:15 POT 112

Electrical characterization of sub-20 nm silicon nanowires

fabricated using electron beam lithography and inductively coupled plasma etching — •Muhammad Bilal Khan, Dipjyoti Deb, Yordan M. Georgiev, and Artur Erbe — Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany.

Scaling down of CMOS faces strong challenges due to which new materials, enhanced functionality and new device concepts have gained importance. These concepts include undoped silicon nanowire based reconfigurable devices, which can be programmed as p-FET or n-FET by controlling the electrostatic potential applied via gate electrodes. In this work, electrical characterization of undoped sub-20 silicon nanowires (SiNWs) is reported. SiNWs are fabricated on intrinsic silicon-on-insulator (SOI) substrates in <110> and <100> crystal directions by a top down approach. Hydrogen silsesquioxane (HSQ), a negative tone electron beam resist, is used for nano- patterning and as a hard mask for etching. Nanowire etching process is optimized using an inductively coupled plasma (ICP) source and $C_4F_8/SF_6/O_2$ mixed gas recipe at 18 ^oC. These NWs are oxidized to form a SiO_2 shell and subsequently silicidized. For silicidation, the SiO_2 shell is wet etched at pre-defined positions followed by Nickel (Ni) sputtering and diffusion which yield silicide-silicon (Schottky) junctions. Ni is used for silicidation to selectively control the charge carriers injection at the junctions. Different silicidation progress and charge carrier transport was observed in <110> and <100> crystal directions.

HL 9.5 Mon 10:30 POT 112

Monolithical integration of III-V Quantum Dots into Silicon towards a new silicon based material platform for optoelectronics — •Marc Sebastian Wolf and Johann Peter Reithmaier — Technische Physik, Institute of Nanostructure Technologies and Analytics (INA), CINSaT, University of Kassel

Beyond the successful integration of III-V light emitting material on silicon by wafer-bonding or direct planar growth by using thick relaxation layers, no approach yet is fully process compatible with silicon fabrication technologies. To avoid III-V processing, a new hybrid material based on III-V quantum dots (QDs) embedded in a silicon matrix is under investigation (Benyoucef et al., pss a 211, 817 (2014). A key parameter is the development of core-shell QDs directly grown on silicon surfaces, which could be already successfully demonstrated at low-density structures (Benyoucef et al., APL 102, 132101 (2013)). In this work, the III-V quantum dots are grown in a solid source molecular beam epitaxy system directly on the silicon substrate and subsequently capped with Silicon. The growth and characterisation of InAs/GaAs quantum dots with densities of $> 10^{10} cm^{-2}$ on the silicon surface will be discussed. Additionally, photocurrent measurements of InAs nanocluster monolithically embedded in a silicon p-i-n diode will be shown.

HL 9.6 Mon 10:45 POT 112

MOVPE grown InAs quantum dots on InGaAs/GaAs metamorphic buffers — •Susanne Schreier, Matthias Paul, Fabian Olbrich, Jonatan Höschele, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und funktionelle Grenzflächen, Universität Stuttgart and Research Centers SCoPE and IQ^{ST}, Allmandring 3, 70569 Stuttgart

In the last years the interest in quantum computing and cryptography and therefore the need for single-photon sources increased strongly. InAs semiconductor quantum dots (QDs) are promising candidates for sources of entangled or indistinguishable photons due to their good optical properties. The implementation in glass fiber networks requires emission wavelengths of 1310 nm (O-band) and 1550 nm (C-band), corresponding to the dispersion and absorption minima. To reach these wavelengths the typical emission energies of InAs QDs need to be red shifted. This can be realized by reducing the lattice mismatch between GaAs and InAs by the use of an InGaAs metamorphic buffer layer below the QDs. The buffer layer functions, similar to InP substrates, to reduce the strain in the QDs. This leads to a reduction of the effective band gap and to an increase in size of the QDs, which results in a lower emission energy. In contrast to InP substrates, the extraction efficiency for photoluminescence (PL) measurements can be enhanced by AlAs/GaAs distributed Bragg reflectors below both the metamorphic buffer and the QDs. The characterization involves XRD and AFM to investigate the structural properties and PL to investigate the optical properties of the InAs QDs.

Coffee Break

HL 9.7 Mon 11:30 POT 112

Single shot spin readout in a 3D crystalline transistor — •Matthias Koch[1,2], Eldad Peretz[2,3], Joris G. Keizer[2], and Michelle Y. Simmons[2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft — [2]University of New South Wales — [3]Bar Ilan University

Atomic-scale fabrication has recently been demonstrated in silicon using scanning tunneling microscope (STM) hydrogen resit lithography[1]. Dopants can be placed in silicon with atomic precision to fabricate a single atom transistor[2], where a single atom controls the device opacity. Scalable architectures, i.e. based on cross wires, demand from hydrogen resist lithography to separate the individual elements of the electronic circuit on different planes. Here, we demonstrate a new fabrication recipe by performing single shot spin readout with a vertically aligned top gate. The additional device layer does not cause instabilities which reflects in a high readout fidelity of 97%. Our results show that hydrogen resist lithography can be extended easily to multiple planes, a premises for the development of complex device architectures.

[1] A. Fuhrer, M. Füchsle, T. C. G. Reusch, B. Weber, and M. Y. Simmons, Nano Letters 9, 707 (2009)

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HL 9.8 Mon 11:45 POT 112

Quantum Dots grown by Local Droplet Etching on GaAs (111)A Substrates — •Julian Ritzmann[1], Nand Lal Sharma[2], Dirk Reuter[2], Carolin Lüders[3], Jörg Debus[3], Arne Ludwig[1], and Andreas D. Wieck[1] — [1]Ruhr-Universität Bochum, D-44780 Bochum — [2]Universität Paderborn, D-33098 Paderborn — [3]Technische Universität Dortmund, D-44227 Dortmund

The generation of entangled photon pairs is a key to practical quantum communications. In the case of biexcitons in SK-grown quantum dots (QD), the fine structure splitting (FSS) of the energy levels causes the transition paths of biexciton and exciton to be distinguishable. Therefore, we need quantum dots with strongly reduced FSS. This was theoretically proposed and experimentally shown for GaAs quantum dots on (111)A-oriented AlGaAs by droplet epitaxy (DE)[1]. However, these QDs exhibit a strong distribution in size resulting in rather broad photoluminescence (PL) spectra. Nearly uniform quantum dots were achieved by filling up nanoholes on (001)-oriented Al(Ga)As with GaAs achieving a PL linewidth of less than 10 meV[2]. These nanoholes were generated via local droplet etching (LDE) of gallium droplets on an Al(Ga)As surface. Our approach is to use LDE for the growth of uniform, triangular QDs on (111)A-oriented substrates with low density and reduced FSS. Here, we present a study on different parameters for the LDE and LDE QD process on GaAs (111)A surfaces using atomic force microscopy, PL and micro-PL.

[1] T. Mano et al., Appl. Phys. Express 3, 065203 (2010).

[2] Ch. Heyn et al., Appl. Phys. Lett. 94, 183113 (2009).

HL 9.9 Mon 12:00 POT 112

Efficient deterministic single-photon sources based on quantum-dots in suspended circular Bragg grating cavities — •Tobias Heuser, Arsenty Kaganskiy, Esra B. Yarar Tauscher, Ronny Schmidt, Anna Musial, Sven Rodt, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin, Germany

Applications in the field of quantum communication will benefit strongly from deterministic single-photon sources (SPSs) based on single semiconductor quantum dots (QDs). Such non-classical light sources feature close to ideal single-photon emission as well as photon-indistinguishability. However, maximizing the photon extraction efficiency of these sources remains an important issue.

Here, we report on the implementation of a highly efficient semiconductor QD-based SPS using a circular Bragg grating which is patterned into a suspended membrane. The high refractive index contrast at the grating leads to in-plane light confinement as well as vertically asymmetric out-of-plane scattering. Maximizing the photon extraction efficiency by finite element simulations of the device geometry yields values up to even 80%. To implement this approach with a high device yield, we apply deterministic high-resolution in-situ electron beam lithography [1] at cryogenic temperatures. In this way, specific QDs can be pre-selected according to their position and emission energy to ensure spatial and spectral matching for optimal extraction efficiency.

References
[1] M. Gschrey, Appl. Phys. Lett. ,vol. 102, p. 251113, 2013

HL 9.10 Mon 12:15 POT 112

Investigating the crystal structure of CdSe and CdTe semiconductor nanowires — •Philip Harder, Tobias Redder, Andreas Nielsen, Tobias Kipp, and Alf Mews — Institut für Physikalische Chemie, Universität Hamburg, Grindelallee 117, 20146 Hamburg, Deutschland

The Solution-Liquid-Solid method allows to synthesize CdSe and CdTe nanowires with very small diameters (below 10 nm), that have interesting optical and electronical properties. These properties mainly depend on the ligands on the surface and the crystal structure, i. e. the zincblende to wurtzite ratio. We developed a method to determine the ratio in these nanowires via powder X-ray diffraction measurements. The analysis of the experimental powder diffraction patterns was carried out via genetic evolutional algorithms and the results were correlated with high resolution TEM measurements. We acknowledge financial support by the DFG via KI 1257/2 and ME 1380/16-3.

HL 10: Semiconductor Lasers I

Time: Monday 9:30–12:30 Location: POT 06

HL 10.1 Mon 9:30 POT 06

Carrier dynamics in tunnel-injection quantum-dot structures — •Stephan Michael, Michael Lorke, Christian Carmesin, and Frank Jahnke — Institute of Theoretical Physics, University of Bremen, P.O. Box 330440, 28334 Bremen, Germany

For tunnel-injection (TI) quantum-dot (QD) lasers record high small signal modulation bandwidth up to 15 GHz and also high performance of 1.55 μm InAs QDs on InP-based hetero-structures (1) were reported, which shows the enormous application potential for high-speed optical communication networks. The optimal design of future TI lasers benefits from a detailed understanding of the physics and the interplay of various interaction processes involved in such TI devices. We investigated theoretically the carrier dynamics in TI structures by explicitly calculating carrier-phonon and carrier-carrier scattering processes using a material realistic model of the electronic structure based on a discretized Kane Hamiltonian. In doing so, we shed light on the underlying tunneling processes and highlight the importance of hybridized states for high scattering rates. We further specify criteria based on our microscopic calculation to engineer optimal scattering pathways necessary to obtain TI structures for high-speed laser devices.

(1) S. Bhowmick, M. Z. Baten, T. Frost, B. S. Ooi, and P. Bhattacharya, IEEE JQE **50**, NO. 1 7-14 (2014)

HL 10.2 Mon 9:45 POT 06

Simulation of monolithically integrated GaAs-AlGaAs core-shell nanowire lasers on silicon waveguides — •Jochen Bissinger, Thomas Stettner, Tobias Kostenbader, Daniel Ruhstorfer, Gregor Koblmueller, and Jonathan Finley — Walter Schottky Institut, Technische Universität München, Am Coulombwall 4, 85748 Garching

III-V semiconductor nanowire (NW) lasers monolithically integrated on silicon have attracted attention as potential on-chip light sources for optical interconnects. Their unique one-dimensional geometry is both an active gain medium and a natural Fabry-Pérot cavity. However, direct integration of NW-lasers on silicon (Si) is challenging due to the poor modal reflectivity at the NW-Si interface. Recently, we demonstrated how by patterning nano-apertures in a thick SiO_2-interlayer at the NW-Si interface, low-order mode lasing is observed with high β-factors [1]. Such schemes also enable the integration of NW lasers on silicon-on-insulator waveguides and suggest the feasibility of NW-based photonic devices.

In this contribution we simulated the optical loss of GaAs-based NW lasers and their coupling behaviour to a Si-waveguide in dependence of the different design parameters of the system. The performance of the device is found to be mainly affected by the type of lasing mode and the thicknesses of the SiO_2-interlayer and the Si-waveguide. These studies therefore serve as a guideline in the construction of optimized NW lasers on SOI waveguides for future on-chip optical interconnects.
[1] B. Mayer et al., Nano Lett., 16 (1), pp 152-156 (2016).

HL 10.3 Mon 10:00 POT 06

The impact of detuning on the performance of semiconductor disk lasers — Fan Zhang[1], Christoph Möller[1], Martin Koch[1], Stephan Koch[1], •Arash Rahimi-Iman[1], and Wolfgang Stolz[1,2] — [1]Department of Physics and Materials Sciences Center, Philipps-Universität Marburg, D-35032 Marburg, Germany — [2]NAsP III/V GmbH, Hans-Meerwein-Straße, D-35032 Marburg, Germany

After two decades of research and development, semiconductor disk lasers (SDLs), also referred to as vertical-external-cavity surface-emitting lasers (VECSELs), are recognized as advanced light sources offering a high-power output and excellent beam quality, while the lasing wavelength can be set by semiconductor bandgap engineering. In this work, we focus on an important, yet less-discussed factor, namely the detuning in SDLs. It is defined as the wavelength difference between the material gain and the longitudinal confinement factor (LCF) at room temperature. Due to device-to-device fluctuations, it is difficult to conduct direct experimental studies on the detuning. Therefore, a new approach is promoted to achieve different detunings from the same gain chip: by altering the cavity angle of a V-shaped cavity in which the VECSEL chip serves as a folding mirror. As the negative detuning is raised from -20 nm to -37 nm, a significant increment of the maximum output power by 70% is observed, while the lasing threshold is elevated from 7.4 W to 25.6 W due to the increased detuning. Yet, the modification of the intra-cavity incidence angle on the chip also leads to a shift of the emission wavelength of about 16 nm and enhances the tunability to 34 nm.

HL 10.4 Mon 10:15 POT 06

The MECSEL: A new laser concept towards AlGaInP-based direct laser emission in the orange spectral range — •Raffael Pecoroni, Hermann Kahle, Roman Bek, 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

The new MECSEL (membrane external-cavity surface-emitting laser) concept consists of an active region without integrated DBR (distributed Bragg reflector), sandwiched in between two intra-cavity heat spreaders. The advantage now is that unusual material combinations can be used as active regions as growth restrictions due to lattice mismatch do not play a role anymore. Furthermore, no limitation of absorbing DBR layers have to be taken into account. This allows us now to reach for example the orange spectral range with an AlGaInP-based active region. Here, we include $Al_{0.33}GaInP$ quantum wells into $Al_{0.55}GaInP$-barrier layers, release wet-chemically etched the substrate and sandwich it between intra-cavity heat spreaders. First characterization measurements of the gain membranes and the operation as vertical emitting laser will be presented.

HL 10.5 Mon 10:30 POT 06

Quantum dot micropillar lasers subject to time-delayed optical feedback — •Steffen Holzinger[1], Xavier Porte[1], Benjamin Lingnau[2], Kathy Lüdge[2], Christian Schneider[3], Martin Kamp[3], Sven Höfling[3,4], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Germany — [2]Institut für Theoretische Physik, Technische Universität Berlin, Germany — [3]Technische Physik, Julius-Maximilians-Universität Würzburg, Germany — [4]School of Physics and Astronomy, University of St Andrews, Scotland

The chaotic dynamics of feedback-coupled semiconductor lasers have been so far mainly experimentally studied in the classical regime. Electrically pumped quantum dot micropillar lasers provide an advantageous platform for the realization of feedback experiments in the regime of few photons, where single emitter effects and high spontaneous emission noise become prominent. In these structures two linear, orthogonally polarized lasing modes compete for a common gain medium, resulting in characteristic switching dynamics above the lasing threshold. Using an external cavity, we experimentally and theoretically investigate the influence of the feedback strength, external cavity length and

polarization on the optical spectrum as well as the switching dynamics of the lasing modes.

Coffee Break

HL 10.6 Mon 11:15 POT 06

Generation of high frequency oscillations independently of the external cavity length in a semiconductor laser with optical feedback — •Chi-Hak UY[1], Lionel WEICKER[1], Martin VIRTE[2], Emeric MERCIER[1], Delphine WOLFERSBERGER[1], and Marc SCIAMANNA[1] — [1]LMOPS, CentraleSupélec, 2 rue Edouard Belin 57000 Metz FRANCE — [2]Brussels Photonic Team, Department of Applied Physics and Photonics (B-PHOT TONA), Vrije Universiteit Brussels, Pleinlaan 2, 1050 Brussels, Belgium

We numerically investigate the external cavity modes generated by a semiconductor laser subject to a phase-conjugate optical feedback (PCF). We explore the effects of both the cavity length and the feedback rate on the frequency of the external cavity modes which are periodical solutions in PCF configuration. From this analysis, we observe that a short cavity does not necessarily leads to higher frequency oscillations and highlight that the key parameter for the generation of such solutions is the feedback rate. Indeed, independently of the time delay the feedback strength fixes the frequency of the solutions obtained. Finally, we investigate the Hopf bifurcations and their frequencies and deduct the frequency of the external cavity modes expected.

HL 10.7 Mon 11:30 POT 06

Mode-locking dynamics and pulse train stability of monolithic two-section quantum-well semiconductor lasers emitting at 1070 nm with different lengths and gain-to-absorber section length ratios — •Christoph Weber[1], Andreas Klehr[2], Andrea Knigge[2], and Stefan Breuer[1] — [1]Institute of Applied Physics, Technische Universität Darmstadt, Schlossgartenstr. 7, 64289 Darmstadt, Germany — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Gustav-Kirchhoff-Straße 4, 12489 Berlin, Germany

We experimentally investigate the mode-locking (ML) dynamics of passively mode-locked multi-section multi quantum well narrow ridge waveguide semiconductor lasers emitting at a peak wavelength of 1070 nm. ML stability is quantified by pulse train timing jitter (TJ) as well as the relative amplitude jitter (AJ) in dependence on laser biasing by gain injection current and absorber reverse bias voltage. Initial results on pulse train stability analysis have been presented in C. Weber et al., Proc. SPIE, 9892-77, 2016, and on mode-locking stability of a quantum well laser in C. Weber et al., Proc IEEE Internat. Conf. on Transparent Optical Networks, We.P.29, 2016. In this contribution, lasers with different total cavity lengths and absorber to gain section length ratios are studied and regimes of stable and unstable emission are identified by stability analysis, and studies on average and peak optical power, pulse width and pulse repetition rate, enabling a direct comparison of ML regimes.

HL 10.8 Mon 11:45 POT 06

k-space engineering of laser modes in organic microcavities with photonic lattices — •Mona Kliem, Andreas Mischok, Hartmut Fröb, and Karl Leo — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Technische Universität Dresden, 01062 Dresden

Microcavities (MCs) offer a flexible playground to study photon and polariton dispersion in a tunable potential landscape. In vertical MCs, confined photons exhibit a parabolic dispersion relation and in turn behave similarly to other parabolic particles such as free electrons, albeit with an approx. 10^{-5} times smaller effective mass, leading to very low condensation and/or lasing thresholds. By adding a silver layer inside of an organic MC, we observe the formation of Tamm-plasmon-polariton states, shifting the cavity potential to lower energies. Consequently, patterning this thin silver layer enables us to manipulate the potential landscape and create periodic photonic lattices in 2D and 3D, exhibiting Bloch-like band structures in both k_x and k_y direction. The silver layer is photolithographically structured on top of a distributed Bragg reflector (DBR) to achieve micron-scale stripe-, hole- and dot-like patterns, arranged in square and hexagonal arrays before finishing the sample with a $\lambda/2$ active layer and top DBR. We study the effect of these photonic lattices on the full in-plane MC dispersion via tomographic micro-photoluminescence measurements and observe novel lasing modes at band edges of the resulting energy diagram. By choosing the right design parameters of the silver pattern we are able to directly engineer and control the lasing performance of our MCs.

HL 10.9 Mon 12:00 POT 06

Intensity and Wavefront Analysis of Multimode Semiconductor Lasers — •Inga-Maria Eichentopf and Martin Reufer — Hochschule Ruhr West, Institut Naturwissenschaften, Mülheim an der Ruhr, Germany

To analyse the beam characteristics of laser sources wavefront measurements using a Shack-Hartmann Sensor became an established way for nearly Gaussian beams. The aim of our research is to transfer this method to broad area semiconductor lasers. The multimode lasers we utilize in our studies are based on the material system of GaAs emitting light in the near infrared. For this type of laser the number and structure of optical modes is affected by electrical as well as thermal effects inside the laser resonator. Thereby the changes in modal composition can be detected instantaneously through the deformation of the wavefront. For our investigations we use a so called Gaussian telescope setup to magnify the cross section of the laser beam and to increase the length of spatial transition from optical near to far field. This approach is used to analyze the emission evolution of high power laser diodes which emit a multitude of optical modes.

HL 10.10 Mon 12:15 POT 06

Analysis of ultra-low threshold lasing from a nanobeam laser with a quantum-well gain material — •Frederik Lohof[1], Stephan Jagsch[2], Noelia Vico Triviño[3], Gordon Callsen[2], Stefan Kalinowski[2], Ian Rousseau[3], Jean-François Carlin[3], Raphaël Butté[3], Axel Hoffmann[2], Nicolas Grandjean[3], Frank Jahnke[2], Stephan Reitzenstein[1], and Christopher Gies[1] — [1]Institute for Theoretical Physics, University of Bremen, Germany — [2]Institute of Solid State Physics, Technische Universität Berlin, Germany — [3]Institute of Physics, École Polytechnique Féderal de Lusanne, Switzerland

The ongoing quest for miniaturization of laser structures is a driving factor in applied semiconductor physics. Cavities with large Q factors and low mode volume strongly funnel the emission into the laser mode, thereby approaching the thresholdless regime ($\beta \approx 1$). A recent addition are nanobeam cavities that offer great potential for silicon-integrated nanophotonics and on-chip structures. For such a design we develop and evaluate a quantum-mechanical laser theory that facilitates quantitative predictions of the emission output and the autocorrelation function $g^{(2)}$. Our device uses a quantum-well gain material. While typical QW edge-emitting lasers operate with $\beta < 10^{-3}$, the nanobeam cavity exhibits high β and vanishing threshold in the emission output, in which case $g^{(2)}$ has become an established tool to identify lasing. Building on a formalism employed for high-Q quantum-dot nanolasers, we calculate $g^{(2)}$ for a QW gain material to reveal the laser transition and to evaluate device characterisitics.

HL 11: Plasmonics and Nanooptics I: Light-Matter Interactions

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

HL 11.1 Mon 10:30 TRE Ma

Nanoplasmonics from large-scale ab initio calculations: opposite trends in Ag and Na clusters — •Marc Barbry[1], Peter Koval[2], Natalia E. Koval[1], Javier Aizpurua[1], and Daniel Sánchez[1,2] — [1]Material Physics Center, San Sebastián, Spain — [2]Donostia International Physics Center, San Sebastián, Spain

An accurate description of electronic excitations is indispensable for understanding material properties and designing nanoscale devices. For instance, using large-scale TDDFT calculations, we have recently demonstrated the importance of taking into account the details of the atomic-scale structure [1] and the quantization of electron transport [2] in metal nanostructures in order to accurately describe their plasmonic properties. In this contribution we will compare the surface plasmon resonance of sodium and silver clusters within the same framework of *iterative* TDDFT [3]. Recent progress in our implementation made it possible to perform calculations of large clusters of diameters ranging from a few Å to 4–5 nm, counting up to 5000 silver atoms and using only modest computational resources (a 32-core node with 500GB RAM). With these new capabilities, we have characterized the size-scaling of the SPR frequency for both sodium and silver clusters. As expected these two materials show opposite behaviours that can be related to the different spill out of charge at the surface and to the additional screening created by the 4*d* electrons in silver.

[1] M. Barbry *et al. Nano Letters*, **15** (2015) 3410. [2] F. Marchesin *et al. ACS Photonics*, **3** (2016) 269. [3] P. Koval *et al. J. Phys.: Condens. Matter*, **28** (2016) 214001.

HL 11.2 Mon 10:45 TRE Ma

Mueller matrix investigation of gold gratings — •Meng Wang, Anja Löhle, Bruno Gompf, Martin Dressel, and Audrey Berrier — 1. Physikalisches Institut and Research Center SCoPE, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Surface plasmon polaritons (SPPs), dispersive collective electron excitations propagating along metal-dielectric interfaces leading to strong field confinement, are powerful ways to control the electromagnetic field. They foster promising applications, e.g., in sensing and nanophotonics. In this work, a plasmonic one-dimensional grating fabricated by evaporating gold thin films on an elastomer is investigated by Mueller Matrix (MM) spectroscopic ellipsometry, a powerful tool to characterize the interaction of nanostructured objects with polarized light. All 16 MM elements were measured in reflection. To evaluate the respective role of specific features, such as plasmonic modes, anisotropy, material absorption, or simply diffraction orders, the optical response was measured at various angles of incidence and different azimuthal orientations over a broad frequency range. Hence, the complex interactions resulting from the interplay of these excitations can be unravelled. Modelling of the optical properties based on a biaxial model completes the study. Anisotropy, SPPs, diffraction orders and inter-band transition are distinguished from their different dispersive behaviour and explain all MM features. This knowledge can help to better understand how to tailor the specific excitations and provides guidelines for the design of novel optical functionalities using nanostructured materials.

HL 11.3 Mon 11:00 TRE Ma

Pump-probe nanoscopy with NIR to deep THz radiation — •F. Kuschewski[1], S.C. Kehr[1], J. Döring[1], N. Awari[2], B. Green[2], S. Kovalev[2], M. Gensch[2], and L.M. Eng[1] — [1]Institut für Angewandte Physik, TU Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf

Recently, scattering-type scanning near-field infrared microscopy (s-SNIM) was successfully combined with pump-probe experiments pushing the temporal resolution of s-SNIM down to a few fs [1]. That combination offers spectacular possibilities to explore the dynamics of nanoscale physical devices, but usually shows a low optical contrast due to high background signals. We analyzed the frequency spectrum in pump-probe s-SNIM finding sidebands to the main carrier frequency that provide a much higher signal-to-noise ratio, as proven both by simulations and recent experiments [2]. Experimentally a greatly increased contrast in the 1st order sideband was found [2], that now has been extended up to the 5th order, applying s-SNIM to a structured gold/semiconductor sample. Note that our approach is applicable to the broad spectral range from visible to THz wavelengths.

[1] M. Wagner et al. *Nano Lett.* **14**, 894 (2014).
[2] F. Kuschewski et al. *Sci. Rep.* **5**, 12582 (2015).

HL 11.4 Mon 11:15 TRE Ma

Photon emission from plasmonic tunnel junctions including a microscope tip and metallic quantum wells — •Tomoki Sueyoshi, Peter-Jan Peters, and Richard Berndt — Institut für Experimentelle und Angewandte Physik, CAU Kiel, Germany

Radiative decay processes involving tunneling electrons are studied by probing light emission from metallic quantum-well (QW) junctions in a scanning tunneling microscope. The electronic states of Pb QWs on Ag(111) are controlled with the number of Pb layers and identified by scanning tunneling spectroscopy. The luminescence from the tip-QW-metal junctions involves radiative decay of tip-induced localized plasmons excited by inelastic tunneling electrons. The observed optical spectra reflect the plasmon density of states in the junctions. In addition, intense emission is observed from transitions of tunneling electrons between unoccupied QW states. These results demonstrate plasmon-assisted luminescence induced by tunneling electrons in the QW tunnel junctions.

HL 11.5 Mon 11:30 TRE Ma

Temporal dynamics of nanowire based lasers — •Robert Röder[1], Themistoklis Sidiropoulos[2], Rupert F. Oulton[2], and Carsten Ronning[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Germany — [2]Imperial College London, UK

Reinforced work in the field of nanophotonics for on-chip integrated optical components is urgent to provide novel approaches for optical data processing which can circumvent the forthcoming limitations of conventional electronic circuits. Here, II-VI compound semiconductor nanowires (NW) provide robust high optical gain and show beneficial Fabry-Pérot resonator properties allowing low threshold NW lasing at room temperature [Geburt et al, Nanotechnology 23, 365204 (2012)] and even continuous wave emission [Röder et al, Nano Letters 13, 3602 (2013)]. Yet, optical confinement in semiconductor NWs, and thus there size, is diffraction limited. However, plasmonic lasers using semiconductor NWs as gain medium have generated significant interest, since the optical mode size in these systems is far below the vacuum wavelength. By exploiting the natural non-linearity of the laser process itself, we investigate the laser dynamics of both photonic [Röder et al, Nano Lett. 15, 4637 (2015)] and plasmonic NW lasers [Sidiropoulos et al., Nat. Phys. 10, 870 (2014)], which are of high interest for concepts of ultrafast optical switching, nanosensing and nanospectroscopy.

HL 11.6 Mon 11:45 TRE Ma

Using plasmonic nanoantennas to read out the orbital angular momentum of light — •Richard M. Kerber[1], Jamie M. Fitzgerald[2], Sang Soon Oh[2], Ortwin Hess[2], and Doris E. Reiter[1,2] — [1]Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany — [2]Department of Physics, The Blackett Laboratory, Imperial College London, South Kensington Campus, London SW7 2AZ, United Kingdom

The orbital angular momentum of light has recently been recognized as a new degree of freedom to encode information in communication technology. One way to determine the orbital angular momentum of light is to destroy the helical wavefront of the light beam. We here propose an alternative way to read out the orbital angular momentum of light using plasmonic nanoantennas by converting the phase information into spectral information without losing the phase properties of the beam. Using the excitation of bright and dark modes of a plasmonic nanoantenna, which exhibit different resonant wavelengths, the determination of the value of orbital angular momentum of the light beam becomes possible. Exemplary considering rotation-symmetrical nanorod antennas we show that their scattering cross-section is sensitive to the value of orbital angular momentum combined with the polarization of an incident orbital angular momentum light beam. For the simulation of the scattering cross-section we use the boundary element method and further predict the orbital angular momentum dependence of the excited modes with an analytical line antenna model.

HL 11.7 Mon 12:00 TRE Ma

Temporal characteristics of intense tunable pulses from an in-

frared free-electron laser — •Riko Kiessling, Sandy Gewinner, Wieland Schöllkopf, Martin Wolf, and Alexander Paarmann — Fritz-Haber-Institut der MPG, Berlin

For the generation of coherent radiation in the infrared region, the free-electron laser (FEL) posseses unique properties regarding intensity, wavelength tunability and short pulse durations. Covering the spectral range from 3 to 50 μm, the IR FEL at the Fritz Haber Institute is dedicated to (non-)linear spectroscopy of vibrational resonances in molecules, clusters and solid matter.

Here, we present the first cross-correlation measurements of the ps FEL pulses with a synchronized fs fiber oscillator via sum-frequency generation in nonlinear media. The observed FEL pulse intensity envelope confirms a lasing behavior typical for oscillator-type FELs [1]. Also, the influence of the FEL cavity detuning on the temporal shape, duration and fluctuation of the IR pulse is discussed. Using a differential cross-correlation scheme [2] will allow the exact determination of the absolute timing between accelerator-based and table-top optical pulses, which enables time-resolved studies of FEL-induced transient processes in solid-state systems.

[1] Knippels et al., PRL 83, 1578 (1999)
[2] Schulz et al., Nat. Commun. 6, 5938 (2015)

HL 11.8 Mon 12:15 TRE Ma

Tip modified fluorescence — •Jonas Albert and Markus Lippitz — Experimental Physics III, University of Bayreuth, Germany

In Near Field Microscopy the near field interaction is used to overcome the diffraction limit. We utilise the near-field interaction to modify fluorescence of our samples by the presence of the near-field probe, a metal coated AFM-tip. First experiments on CdSe nanocrystals show significant changes in the fluorescence lifetime dependent on the distance between crystal and a gold-tip.

Furthermore the optical fields at the near-field probe are confined in a space much smaller than the wavelength and therefore showing a high field gradient on the nanometer scale. We are using the optical field gradients to enhance dipole forbidden transitions in coherent excitonic systems, such as wire-like molecular aggregates.

HL 11.9 Mon 12:30 TRE Ma

Strongly Enhanced Mid-Infrared Second Harmonic Generation from Weak Optical Phonon Modes — •Alexander Paarmann, Ilya Razdolski, Sandy Gewinner, Wieland Schöllkopf, and Martin Wolf — Fritz-Haber-Institut, Berlin, Germany

Mid-infrared second harmonic generation (SHG) spectroscopy [1] provides a unique access to optical phonon resonances in the nonlinear-optical response of polar dielectrics, representing an alternativ spectroscopic approach to established techniques like infrared or Raman spectroscopy. Specifically, the SHG signal is sensitive not only to resonances in the nonlinear susceptibility, but also to the local electromagnetic fields determined by the linear optics. Here, we demonstrate how this intertwined sensitivity can be exploited for enhancement of the SHG specfically for weak oscillators.

Our experiments employ intense, tunable and narrowband mid-infrared pulses from a free-electron laser to acquire SHG excitation spectra from 4H-SiC with the c-axis of the uniaxial crystal in the surface plane [2]. Depending on the crystal azimuthal angle, we observe sharp enhancement of the SHG yield at the frequency of a weak zone-folded mode that exists in 4H-SiC due to the layer stacking along the c-axis. Perspectives are discussed on how to use this effect to detect periodic lattice distortions in strongly correlated insulators.

[1] Paarmann et al., Appl. Phys. Lett. 107, 081101 (2015), [2] Paarmann et al., Phys. Rev. B 94, 134312 (2016)

HL 11.10 Mon 12:45 TRE Ma

A near field study on the transition from localized to propagating plasmons on 2D nano-tips — •Thorsten Weber[1,2], Thomas Kiel[3], Stephan Irsen[2], Kurt Busch[3,4], and Stefan Linden[1] — [1]Physikalisches Institut, Universität Bonn, Nußallee 12, D-53115 Bonn, Germany — [2]Electron Microscopy and Analytics, Center of Advanced European Studies and Research, Ludwig-Erhard-Allee 2, D-53175 Bonn, Germany — [3]Institut für Physik, Humboldt-Universität Berlin, Newtonstraße 15, D-12489 Berlin, Germany — [4]Max-Born-Institut, Max-Born-Straße 2A, D-12489 Berlin, Germany

Plasmonic nano-structures have the unique capability to concentrate light in nanometric volumes. One approach to use this capability is based on resonant plasmonic nanostructures like rod nanoantennas or split ring resonators. In these resonant structures, hot spots of the electromagnetic field are created by localized particle plasmons. Another approach is utilizing non-resonant structures, such as nano-tips, on which propagating surface plasmons are excited at the wider end and travel towards the tip's apex.

Here, we report on a near field study of two-dimensional plasmonic gold nano-tips using electron energy loss spectroscopy in combination with scanning transmission electron microscopy, as well as discontinuous Galerkin time-domain calculations. With increasing nanotip size, we observe a transition from localized particle plasmons on resonant nano-tips to non-resonant propagating surface plasmons on large nanotips. Furthermore we demonstrate that nano-tips with a groove cut can support both localized and propagating plasmons.

HL 12: Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - I

Time: Monday 10:30–13:00 Location: GER 38

HL 12.1 Mon 10:30 GER 38

DFT wants U: Embedded-cluster calculations of surface oxygen vacancies at TiO_2 with Hubbard-corrected DFT — •Matthias Kick, Karsten Reuter, and Harald Oberhofer — Technische Universität München

Surface oxygen vacancies, in particular their nature as charge trapping centers, play an inportant role for many oxide materials properties. However, addressing them with first-principles density-functional theory (DFT) computations remains a challenge. At least Hubbard corrected DFT+U is required to achieve an appropriate electron localization. At the same time, the large dielectric constant of polarizable oxides like TiO_2 leads to a strong polarization response. As a result supercells of increasing size are necessary in order to avoid spurious interactions between periodic images in case of charged defects, rendering the conventional periodic boundary condition supercell approach impractical.

Full DFT+U functionality has been implemented in the all-electron electronic structure code FHI-aims. Combined with the solid state (QM/MM) embedding functionality in FHI-aims, this yields a numerically most efficient approach to treat aperiodic aspects at oxide surfaces. We illustrate this by calculating neutral and charged states of the surface oxygen vacancy at rutile TiO_2 (110). We systematically assess the reliability and computational efficiency by comparing to hybrid-level DFT calculations and calculations performed in conventional supercells.

HL 12.2 Mon 10:45 GER 38

Hubbard interactions from density-functional perturbation theory — •Iurii Timrov, Matteo Cococcioni, and Nicola Marzari — Theory and Simulation of Materials (THEOS), and NCCR-MARVEL, École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

DFT+U, together with its V and J extensions, is a simple and powerful tool to model systems containing partially-filled manifolds of localized states [1]. However, the Hubbard parameters are often - and in our view incorrectly - treated semi-empirically. Conceptual and practical methods to determine e.g. the Hubbard U parameter have nevertheless been introduced long ago, based either on the constrained random-phase approximation (cRPA) or on linear-response theory [2]. These approaches make DFT+U a fully first-principles and self-contained method, but are often overlooked due to their cost or complexity. Here, we introduce a computationally inexpensive and straightforward approach to determine the linear-response U, hitherto obtained from the difference between bare and self-consistent inverse electronic susceptibilities evaluated from supercell calculations. By recasting these calculations in the language of density-functional perturbation theory we remove the need of supercells, and allow for a fully automated determination of susceptibilities and Hubbard parameters. Such de-

velopments open the way for deployment in high-throughput studies, while providing the community with a simple tool to calculate consistent values of U for any system at hand. [1] V. Anisimov et al., PRB 44, 943 (1991), [2] M. Cococcioni et al., PRB 71, 035105 (2005).

HL 12.3 Mon 11:00 GER 38

Time-evolution using full configuration interaction quantum Monte Carlo — •Kai Guther[1], Werner Dobrautz[1], Olle Gunnarsson[1], and Ali Alavi[1,2] — [1]Max-Planck Institute for Solid State Research, Stuttgart, Germany — [2]University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, United Kingdom

We report on a new method to perform real-time quantum evolution of a fermionic system using the full configuration interaction quantum Monte Carlo method [1]. To stabilize the algorithm, a slow simultaneous imaginary-time evolution is performed, yielding properties for times slightly rotated into the complex plane.

We employ this technique to compute Green's functions and therefore by means of analytic continuation also spectral weight functions. We demonstrate the applicability of the algorithm using the examples of the 2D-Hubbard model and the carbon dimer, showing that the algorithm can in principle be used as an Anderson solver for DMFT and is capable of obtaining photoemission spectra of ab-initio systems.

[1] G.H. Booth, A.J.W. Thom and A. Alavi, J. Chem. Phys. 131, 054106 (2009)

HL 12.4 Mon 11:15 GER 38

Laplace-transformed MP2 with localized Resolution of Identity for molecular and periodic systems — •Arvid Ihrig, Igor Ying Zhang, and Matthias Scheffler — Fritz-Haber-Institut, Berlin, Germany

The self-interaction error is a well-known problem in (semi)local functionals in density-functional theory (DFT) and to a lesser extend also in hybrid functionals. It leads to a quantitatively and sometimes even qualitatively wrong description. One possible remedy is the 2nd order Moller-Plesset perturbation theory (MP2) and the double-hybrid DFT methods based on it. However, the time and memory requirements prevent their routine-usage for large molecular and condensed-matter systems.

In this work we combine our localized Resolution of Identity (RI-LVL) [1] and its favourable memory requirements with the low-order scaling of the Laplace-transformed MP2 (LT-MP2) [2]. Our highly parallelizable LT-MP2 implementation in a numeric atom-centered orbital (NAO) framework allows us to treat both cluster and periodic models in the same computational environment. We demonstrate the accuracy and other features of our implementation for examples of water clusters and TiO_2 surfaces with small absorbed molecules. We furthermore present a way how the distance-dependent integral screening [3] from the Ochsenfeld group can be generalized to periodic systems.

[1] Ihrig et al., New J. Phys. 17, 093020 (2015)
[2] P. Ayala et al., J. Chem. Phys. 110, 3660 (1999)
[3] S. Maurer et al., J. Chem. Phys. 136, 144107 (2012)

HL 12.5 Mon 11:30 GER 38

Bond Disproportionation in Rare-Earth Nickelates: Describing Lattice Distortions within DFT+DMFT — •Alexander Hampel and Claude Ederer — Materials Theory, ETH Zürich, Switzerland

Perovskite rare-earth nickelates, $R\mathrm{NiO_3}$, display a rich and only partially understood phase diagram, where all compounds with R from Pr to Lu undergo a metal-insulator transition (MIT), that is accompanied by a structural distortion. This distortion breaks the symmetry between formerly equivalent Ni sites and can (in the simplest picture) be understood as a charge disproportionation of the Ni^{3+} cations into Ni^{2+} and Ni^{4+}. Here, we use density functional theory (DFT) and its extensions (DFT+U, DFT+DMFT) combined with symmetry-based distortion mode analysis to explore the interplay between lattice distortions, magnetic order and electronic correlation effects in rare-earth nickelates. Thereby, we want to explore the capabilities of the DFT+DMFT method to describe complex materials with coupled electronic and structural degrees of freedom by comparing with DFT+U results and available experimental data.

HL 12.6 Mon 11:45 GER 38

Density matrix embedding theory for coupled fermion-boson systems — •Teresa E. Reinhard[1], Uliana Mordovina[1], Heiko Appel[1], Joshua S. Kretchmer[2], Garnet K. L. Chan[2], and Angel Rubio[1,3] — [1]Max Planck Institut für Struktur und Dynamik der Materie, Hamburg — [2]Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena — [3]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian

We analyze strongly correlated fermion-boson systems by extending Density Matrix Embedding Theory (DMET) from the purely electronic case [1] to coupled fermion-boson systems. DMET is a novel embedding theory which uses the Schmidt decomposition to divide the treated system into an impurity and a bath part. We project the bath part into the part of the Fock space that contains the entanglement with the impurity region and then solve this much smaller entangled system with exact diagonalization and DMRG.

With this technique, we treat lattice systems of Hubbard-Holstein type, where fermions and bosons are coupled by a bilinear Froehlich coupling. As we choose coherent states for the bosonic basis set, it is convenient to apply our approach to electron-phonon as well as to electron-photon systems.

By using a DMRG solver for the DMET algorithm, an accurate treatment of 2 dimensional systems becomes feasible.

[1] G. Knizia, G. K.-L Chan, Phys. Rev. Lett 109, 186404, (2012)

HL 12.7 Mon 12:00 GER 38

Vertex function of homogeneous electron gas — •Yaroslav Pavlyukh — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, P.O. Box 3049, 67653 Kaiserslautern, Germany — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany

We present a systematic study of the vertex function correction in homogeneous electron gas at metallic densities [1]. Contrary to a popular belief the vertex function not only provides corrections to the well known plasmon or particle-hole pair scatterings, but also gives rise to new physical processes such as generation of two plasmon excitations or the transformation of the initial one-particle state into a two-particles-one-hole state. Using a merger of the many-body perturbation and scattering theories, which is a distinct feature of our method, it is shown that additional scattering channels are responsible for the bandwidth reduction (as observed in photoemission experiments on bulk sodium), appearance of the secondary plasmonic satellite below the Fermi level and lead to a substantial modification of the electron spectral function.

[1] Y. Pavlyukh, A.-M. Uimonen, G. Stefanucci, R. van Leeuwen, Phys. Rev. Lett. **117**, 206402 (2016)

HL 12.8 Mon 12:15 GER 38

Coupled-Cluster approaches for molecules and solids in the numeric atom-center orbital framework — •Tonghao Shen, Igor Ying Zhang, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, DE

As a well-established and successful wave-function theory hierarchy in quantum chemistry, the coupled-cluster (CC) ansatz is attracting increasing attention in computational materials science [1]. However, compared to traditional density-functional approximations, CC approaches face much greater challenges regarding numerical implementation, bassis-set accuracy and efficiency, in particular for solids [2]. In this report, we present a highly parallel implementation of the CC approaches with singles, doubles and perturbative triples, CCSD(T), in the numeric atom-center orbital (NAO) framework. This implementation allows CCSD(T) simulations to be carried out using both cluster and periodic models in a single computational environment. Taking some popular quantum-chemistry test sets (S22, ISO34, and CYCONF), we demonstrate that CCSD(T) with correlation-consistent NAO basis sets [3] can provide accurate reference data for molecular properties. Our solid-state examples include elemental and binary crystals, as Ne (fcc), C, Si (diamond), LiF, MgO (rocksalt), and BN (zincblende).

HL 12.9 Mon 12:30 GER 38

Implementation of the SU(2) Symmetry in FCIQMC using the Graphical Unitary Group Approach — •Werner Dobrautz[1] and Ali Alavi[1,2] — [1]Max-Planck-Institut für Festkörperforschung — [2]Department of Chemistry, University of Cambridge

The Full Configuration Interaction Quantum Monte Carlo (FCIQMC) algorithm [1] is a projector QMC method, previously formulated in the total anti-symmetric space of Slater Determinants, based on the imaginary-time Schrödinger equation to obtain the ground state of a system in the long-time limit.

By formulating the method in eigenfunctions of the $\hat{S}^2$ spin-operator via the Graphical Unitary Group Approach [2] we can make use of the block-diagonal form of spin-preserving, non-relativistic Hamiltonians for different values of the total spin. This allows us to lift possible near degeneracies of low-lying excitations of different spin sectors, calculate spin-gaps more easily and obtain the physical correct ground-state, without spin-contamination, and identify its total spin quantum number.

Our method does not rely on expanding the spin-eigenfunctions in linear combinations of Slater Determinants and thus does not hit an exponential bottle neck and can be applied to system sizes larger than previously reachable with similar approaches.

[1] G. Booth, A. Thom and A. Alavi, J. Chem. Phys. **131**, 054106 (2009)
[2] I. Shavitt, Int. J. Quantum Chem. Symp., **11:** 131 (1977); Int. J. Quantum Chem. Symp., **12:** 5 (1978)

HL 12.10 Mon 12:45 GER 38

A study of the dense uniform electron gas with high orders of coupled cluster — •Verena Andrea Neufeld and Alex James William Thom — University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, United Kingdom

We used the recently developed stochastic coupled cluster method [Phys. Rev. Lett. (2010) 105, 263004 and J. Chem. Phys. (2016) 144, 084108] to benchmark the dense uniform electron gas (UEG). The aim was to make predictions about what truncation level of coupled cluster is needed to reach sufficient accuracy in electronic correlation energies for a range of electron densities. This will aid our future studies of solids with stochastic coupled cluster.

We take advantage of sparsity in wavefunctions by doing coupled cluster stochastically. In this study, we used coupled cluster truncation levels up to CCSDTQ5, that includes single, double, triple, quadruple and quintuple excitations directly. We considered the 14 electron UEG with Wigner-Seitz radius in the range 0.5 to 5.0 a.u.. We applied coupled cluster truncations from CCSD to CCSDTQ5 and extrapolated to the complete basis set size limit. By comparing the differences in energy calculated with CCSD to CCSDTQ5, we learn what truncation level is necessary for sufficient accuracy. What truncation level is needed, is dependent on the level of correlation, which decreases with electron density. We are therefore able to relate the degree of correlation linked to electron density to the level of coupled cluster needed for accuracy. This information will prove valuable when tackling periodic solids that can be approximated by the UEG.

HL 13: Organic Electronics and Photovoltaics I: Light-Emitting Devices

Time: Monday 11:00–13:00 Location: ZEU 260

HL 13.1 Mon 11:00 ZEU 260

Two-color warm white hybrid OLEDs from thermally activated delayed fluorescence — •Ludwig Popp[1], Paul Kleine[1], Reinhard Scholz[1], Ramunas Lygaitis[1,2], Olaf Zeika[1], Axel Fischer[1], Simone Lenk[1], and Sebastian Reineke[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, TU Dresden, Germany — [2]Kaunas University of Technology, Lithuania

Thermally activated delayed fluorescence (TADF) takes place in organic molecules where the energy splitting between the lowest excited singlet and triplet states (ST-splitting, ΔE_{ST}) remains sufficiently low. A newly designed sky-blue TADF emitter with an emission maximum at a wavelength of 500 nm reaches a photoluminescence quantum yield of 70% and an external quantum efficiency (EQE) of up to 14.5% in actual organic light-emitting devices (OLEDs).

In this work we use the sky-blue TADF molecule to build warm white hybrid OLEDs by combination with the red phosphorescent emitter $Ir(MDQ)_2(acac)$. Due to the very broad TADF emission, covering a majority of the high-energy visible spectrum, a dedicated deep blue emitter is becoming obsolete for reaching high color rendering indices (CRI > 80).

Furthermore, we demonstrate deeper insight into the energy transfer mechanisms in this hybrid TADF/phosphorescence approach. Time-correlated single photon counting enables to determine the actual exciton decay pathways and delivers a detailed understanding of the excitonic interplay between the particular excited states.

HL 13.2 Mon 11:15 ZEU 260

Conjugation induced thermally activated delayed fluorescence — •Paul Kleine[1], Qiang Wei[2], Yevhen Karpov[2], Xianping Qiu[2], Hartmut Komber[2], Karin Sahre[2], Anton Kiriy[2], Ramunas Lygaitis[1], Simone Lenk[1], Brigitte Voit[2], and Sebastian Reineke[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Dresden, Germany — [2]Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany

Thermally activated delayed fluorescence (TADF) has seen tremendous research efforts in the last years. It represents an alternative to phosphorescent emitter materials in organic light-emitting diodes, assuring 100% internal quantum efficiency via effective reverse intersystem crossing of barely radiative triplet to emissive singlet states. While many small molecules have been reported to show efficient TADF, reports on polymers sporting TADF are rare. Up to now, publications cover concepts only, where TADF chromophores are linked to polymer networks, retaining their monomeric properties. In this talk, we discuss a novel strategy that unlocks an additional molecular design rule reserved exclusively for polymeric materials. A π-conjugated cyclic polymer composed of non-TADF building blocks was developed. Conjugation induced HOMO destabilization leads to a decreased singlet-triplet splitting and efficient TADF in the polymer, while the repeating unit shows only inefficient phosphorescence. This conjugation induced TADF concept represents a novel molecular design rule particularly for solution-processable polymeric materials.

HL 13.3 Mon 11:30 ZEU 260

Investigation of organic light emitting diodes based on thermally activated delayed fluorescence via magnetic resonance methods — •Nikolai Bunzmann[1], Sebastian Weissenseel[1], Benjamin Krugmann[1], Jeannine Grüne[1], Stefan Väth[1], Andreas Sperlich[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 Bayern), 97074 Würzburg

Organic light emitting diodes (OLEDs) based on thermally activated delayed fluorescence (TADF) exhibit a high upconversion rate from non-emissive triplet to emissive singlet states due to a small energy splitting ΔE_{ST} between the respective states. Consequently, the internal quantum efficiency (IQE) of such devices is strongly enhanced. However, the underlying mechanism of reverse intersystem crossing (RISC) is naturally spin forbidden, wherefore spin sensitive measurement methods are desirable in order to elucidate the TADF process. Therefore, we use electrically and electroluminescence detected magnetic resonance (EDMR, ELDMR) techniques. Hereby, transitions between triplet substates, which are split in an external magnetic field, are driven by microwaves, applied via a non-resonant stripline. We evaluate the dependence of multi-frequency ELDMR and EDMR spectra on changes in experimental conditions in order to obtain detailed information about the investigated spin system. Thereby we contribute to a better understanding of the TADF mechnism, which is crucial in order to further improve the performance of OLED based light sources.

HL 13.4 Mon 11:45 ZEU 260

Orientation of Phosphorescent Dopants in Organic Vapor Phase Deposited Films — •Thomas Lampe[1], Matthew J. Jurow[3], Francisco F. Navarro[2], John Facendola[2], Tobias D. Schmidt[1], Peter I. Djurovich[2], Mark E. Thompson Thompson[2], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Department of Chemistry, University of Southern California, Los Angeles, California 90089, United States — [3]The Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States

Organic vapor phase deposition (OVPD) is an efficient film deposition technique for the preparation of organic thin films. However, the atmospheric conditions during deposition differ from the common thermal evaporation in high vacuum. To investigate the effects of these differences on heteroleptic phosphor orientation in organic guest-host

systems we deposited films via OVPD while controlling the substrate temperature during deposition. The measurement of the alignment of the emissive transition dipole moments in samples deposited at room temperature leads to results comparable to preparation via thermal evaporation. Deposition of the film on a cooled substrate reveals a thermally activated behaviour of the molecular alignment process at low temperatures. The confirm an earlier model for the molecular alignment of heteroleptic phosphopors and give further insight into the physical properties of this phenomenon.

[1] M. Jurow, et. al.: *Nature Mat.* **15** (2015), 85-91

HL 13.5 Mon 12:00 ZEU 260

Magnetic resonance at ultra-small fields in PPV-based OLEDs — •Hermann Kraus, Viola Zeller, Sebastian Bange, and John M. Lupton — Universität Regensburg, Universitätsstraße 31, 93053 Regensburg, Deutschland

Large magnetoresistance and magnetoluminescence effects which arise, for example, due to spin-dependent recombination rates are well-known for OLEDs, although models are still under debate given that they remain hard to verify from a measurement of integrated current and luminance. At very low fields a change in the sign of magnetoresistance appears: the so called ultra-small magnetic field effect for which also several models exist.

Spin resonance of paramagnetic species enables direct manipulation of charge carrier and excitonic precursor spins but most work on spin resonance in OLEDs was done at external magnetic fields on the order of several hundred millitesla. While it is also possible to perform these experiments at fields down to a few millitesla it was believed that resonance effects disappear once the external field is of the same order of magnitude as the internal hyperfine fields. We show that electron spin resonance signals are detectable through both the current and the electroluminescence at ultra-small fields corresponding to a few MHz resonance frequency. This demonstration provides insights into the ultra-small magnetic field effect in magnetoresistance as well as testing the principles of magnetic resonance for very low Zeeman splitting.

HL 13.6 Mon 12:15 ZEU 260

Ultrathin metal electrode for bottom-emitting OLEDs on buckled substrates — •Yungui Li, Toni Bärschneider, Paul-Anton Will, Yuan Liu, Simone Lenk, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonics Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, 01062 Dresden, Germany

We here report our investigations on nanometer thick, composite ultrathin metal electrodes used in organic light-emitting diodes (OLEDs) comprising buckled substrates. The thin metal electrodes are made of 1 nm molybdenum trioxide (MoO3), 2 nm gold, and 3-15 nm of silver. A composite electrode with 9 nm silver based on flat glass substrate shows a maximum transparency of about 80% at 455 nm and a sheet resistance of 10 Ω/sq. With reactive-ion etching process, a buckled surface with depths around 50 to 100 nm is designed to extract the trapped light of bottom-emitting OLEDs since total internal reflection in flat device. When the thin metal electrode is utilized for green bottom-emitting OLEDs, the devices show a maximum external quantum efficiency of 17.5% for buckled OLEDs while in contrast only 13.8% for flat devices. Compared to flat devices, buckled devices show the same level of leakage current and better color stability at different angles. The results confirm the high potential of composite thin metal systems as alternative electrode for OLEDs, with the capability of application for bottom- and top-emitting OLEDs on patterned surfaces.

HL 13.7 Mon 12:30 ZEU 260

Impact of charge carrier injection on single-chain photophysics of conjugated polymers — •Felix J. Hofmann, Jan Vogelsang, and John M. Lupton — Universität Regensburg

Charges in conjugated polymer materials have a strong impact on the photophysics and their interaction with the primary excited state species has to be taken into account in understanding device properties. Here, we employ single-molecule spectroscopy to unravel the influence of charges on several photoluminescence (PL) observables. The charges are injected either stochastically by a photochemical process, or deterministically in a hole-injection sandwich device configuration. We find that upon charge injection, besides a blue-shift of the PL emission and a shortening of the PL lifetime due to quenching and blocking of the lowest-energy chromophores, the non-classical photon arrival time distribution of the multichromophoric chain is modified towards a more classical distribution. Surprisingly, the fidelity of photon antibunching deteriorates upon charging, whereas one would actually expect the number of chromophores to be reduced. A qualitative model is presented to explain the observed PL changes. The results are of interest to developing a microscopic understanding of the intrinsic charge-exciton quenching interaction in devices.

HL 13.8 Mon 12:45 ZEU 260

Optical Detection of the Magnetic Field Effect in OLEDs with Metal-Free Dual Singlet-Triplet Emitters — •Wolfram Ratzke[1], Lisa Schmitt[2], Hideto Matsuoka[2], Christoph Bannwarth[2], Marius Retegan[3], Jonas Zipfel[1], Sebastian Bange[1], Philippe Klemm[1], Frank Neese[3], Stefan Grimme[2], Olav Schiemann[2], John Lupton[1], and Sigurd Höger[2] — [1]University of Regensburg, Germany — [2]University of Bonn, Germany — [3]MPI Mühlheim an der Ruhr, Germany

Even though the magnetic field effect of organic light emitting diodes (OLEDs) has been investigated for more than one decade it is still difficult to identify the underlying mechanisms. Furthermore, theories are discussed which are based on the magnetic field dependent formation of singlet and triplet excited states in order to explain the change in the device resistance without a simultaneous experimental access to all three observables. The spin states can be measured by detecting the fluorescence and phosphorescence but so far this was always restricted to the exclusive observation of pure singlet or triplet emission by investigating different molecular systems, and hence a coherent statement is not possible. Recently, we have developed metal-free OLED emitters which exhibit simultaneous fluorescence and phosphorescence, even at room temperature. These materials can give insight into the change of spin-state statistics when an external magnetic field is applied, and offer a new perspective to distinguish between different field regimes and spin-dependent mechanisms which lead to the magnetic field effect.

HL 14: Poster: Two-Dimenaional Materials and Topological Insulators

Time: Monday 14:00–18:00 Location: P2-OG3

HL 14.1 Mon 14:00 P2-OG3

Disentangling electronic and phonon contributions to the photoexcited stress in bulk WSe_2 — •Marc Herzog[1], Alexander von Reppert[1], Jan-Etienne Pudell[1], Ehren Mannebach[2], Clara Nyby[3], Friederike Ernst[4,5], Aaron Lindenberg[2,5,6], and Matias Bargheer[1,7] — [1]Dept. of Physics and Astronomy, Univ. of Potsdam — [2]Dept. of Materials Science and Engineering, Stanford Univ. — [3]Dept. of Chemistry, Stanford Univ. — [4]Dept. of Applied Physics, Stanford Univ. — [5]PULSE Institute, SLAC — [6]Stanford Institute for Materials and Energy Sciences, SLAC — [7]Helmholtz Center Berlin for Materials and Energy

Transition metal dichalcogenides (TMDCs) have attracted much technological and scientific interest due to their finite band gaps and the complex interplay of electronic, lattice and spin degrees of freedom. With regard to optoelectronic applications it is important to understand the coupled non-equilibrium dynamics of the different degrees of freedom in TMDCs. We address this issue by investigating the structural response of WSe_2 to ultrashort photoexcitation at different photon energies using time-resolved x-ray diffraction. Two independent stress components are identified: (i) a negative electronic stress through modification of the van der Waals interaction between neighboring layers by photocarriers and (ii) a positive phononic stress. The ultrafast negative stress launches coherent compressive hypersound waves and decays on a timescale of 50 ps revealing the photocarrier lifetime. The relative ratio of negative and positive stress components depends on excitation density and photon energy.

HL 14.2 Mon 14:00 P2-OG3

Polarized hot carrier photoluminescence in graphene —

•Thomas Danz, John H. Gaida, Claus Ropers, and Sascha Schäfer — IV. Physical Institute – Solids and Nanostructures, University of Göttingen, Germany

The thermalization of photogenerated hot charge carriers in graphene leads to photoluminescence (PL) at wavelengths far away from that of the exciting pump laser [1,2]. Although a strongly anisotropic carrier distribution is created by linearly polarized optical excitation [3], the polarization properties of the emerging PL have not been reported yet.

In this contribution, we report the anisotropic polarization response of the hot carrier PL in graphene and discuss a possible coherent contribution to the incoherent emission. On the basis of spectral interferometry, we find that any coherent contribution to the emission must be smaller than 4% of the total PL signal. By comparing the experimentally measured degree of polarization to a microscopic model of the carrier dynamics based on Boltzmann rate equations, we are able to determine a time-scale of 12 ± 2 fs for the ultrafast momentum relaxation in graphene [4].

[1] C. H. Lui *et al.*, Phys. Rev. Lett. **105**, 127404 (2010)
[2] W. Liu *et al.*, Phys. Rev. B. **82**, 081408 (2010)
[3] E. Malic *et al.*, Appl. Phys. Lett. **101**, 213110 (2012)
[4] Th. Danz *et al.*, in preparation.

HL 14.3 Mon 14:00 P2-OG3

Modulation of the Optical Gas-Sensing Performance of Single-Layer MoS2 Transistors by Electric Gating — Philip Klement[1], Paula Neuderth[1], Sangam Chatterjee[1], and •Martin Eickhoff[1,2] — [1]Institute of Experimental Physics I, Justus Liebig University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany — [2]Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

Two-dimensional transition metal dichalcogenides such as MoS_2 are promising candidates for gas-sensing applications due to their large surface-to-volume ratio. They offer the possibility of an optical detection of the gas-sensing effect. However, the performance is limited due to a low response, slow recovery and a lack of selectivity [1]. The application of a perpendicular electric field modulates the adsorption of gas molecules and therefore may improve the performance [2]. Here, we detected the adsorption of different gas molecules to MoS_2 optically with a perpendicular electric field. We studied the optical response under different gate voltages and gas concentrations and found a systematic modulation of the optical emission and response.

[1] Ko, K. Y., et al., ACS Nano 10, 9287-9296 (2016). [2] Yue, Q., et al., Nanoscale Res Lett. 8, 425 (2013).

HL 14.4 Mon 14:00 P2-OG3

Charge transport in bottom-up synthesized graphene nanoribbon networks — •Nils Richter[1,2], Zongping Chen[3], Akimitsu Narita[3], Xinliang Feng[4], Mathias Kläui[1,2], and Klaus Müllen[2,3,5] — [1]Institut für Physik, Johannes Gutenberg Universität, Mainz, Germany — [2]Graduate School of Excellence Materials Science in Mainz, Mainz, Germany — [3]Max Planck Institute for Polymer Research, Mainz, Germany — [4]Center for Advancing Electronics Dresden & Department of Chemistry and Food Chemistry, Technische Universität, Dresden, Germany — [5]Institut für Physikalische Chemie, Johannes Gutenberg-Universität, Mainz, Germany

Graphene nanoribbons (GNRs) attract particular attention due to physical phenomena resulting from their geometrical confinement. GNRs with atomically perfect edge structures are synthesized on gold surfaces and transferred to insulating substrates [1, 2]. We determine the conductivity and mobility of chevron edged GNRs with a width of 9 carbon atoms (N=9) using GNR-FET devices. At room temperature the resistivity of such devices lies in the regime of approximately 1 GOhm and the mobility is in the order of 10^{-4} cm^2/Vs. We compare chevron GNRs and armchair GNRs with N=9 to demonstrate the influence of the edge structure. Secondly, armchair GNRs with N=7 and N=9 are studied to test for the influence of the ribbon width. Temperature dependent measurements reveal details of their band gaps [3].

[1] A. Narita et al., Nature Chem. 6, 126 (2014). [2] Z. Chen et al., J. Am. Chem. Soc. in press (2016). [3] N. Richter et al., (manuscript in preparation 2016).

HL 14.5 Mon 14:00 P2-OG3

G-factor determination of excitonic states in monolayer tungsten disulfide (WS_2) — •Jan Kuhnert, Simon Schmitt, Arash Rahimi-Iman, 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 (PL) 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 of the peak positions of each excitonic species. By fitting the measured PL spectra we determine the g-factors for the free excitonic transitions: exciton and trion; and for three bound exciton states that exhibit slightly different g-factors due to different localization lengths.

HL 14.6 Mon 14:00 P2-OG3

The effects of substrate and chemical treatment on the optical properties of 2D MoS_2 — •Oleg Gridenco, Genrietta Steingelb, Kathrin Sebald, and Jürgen Gutowski — Semiconductor Optics, Institute of Solid State Physics, University of Bremen, Germany

Two-dimensional transition metal dichalcogenide semiconductors are intriguing materials for the realization of quantum light sources due to their opto-electronic properties. We present a systematic study of the optical properties of ultra-thin molybdenum disulfide (MoS_2) layers deposited on different substrates (SiO_2, Si_3N_4, GaN and polymeric dielectric gel-films). It is observed that the optical properties are affected by the interaction with different substrates. These changes can be related to a substrate-induced variation of the doping level, altering the relative intensity of charged and neutral excitons. Along with this, we present the results of a comparative analysis of the influence of different chemical treatments on the optical properties. These results raise the prospect to tune the optical properties of 2D MoS_2 crystal by choosing suitable substrates and chemical treatment.

HL 14.7 Mon 14:00 P2-OG3

Excitonic phonon sidebands in monolayer transition metal dichalcogenides — •Dominik Christiansen[1], Malte Selig[1], Gunnar Berghäuser[2], Robert Schmidt[3], Iris Niehues[3], Robert Schneider[3], Ashish Arora[3], Steffen Michaelis de Vasconcellos[3], Rudolf Bratschitsch[3], Ermin Malic[2], and Andreas Knorr[1] — [1]Nichtlineare Optik und Quantenelektronik, Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Department of Physics, Chalmers University of Technology, SE-412 96 Gothenburg, Sweden — [3]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm Str. 10, 48149 Münster, Germany

Monolayer transition metal dichalcogenides (TMDs) are direct band gap semiconductors with an extraordinarily strong Coulomb interaction, leading to the formation of excitonic quasiparticles.

Here, we present a microscopic study of the influence of the exciton-phonon interaction on the absorption line shape of TMDs. A treatment of the exciton-phonon interaction beyond the Markov approximation predicts the appearance of phonon-induced sidebands that are accompanied by a pronounced polaron-red shift. In a joint theory-experiment study, we observe an asymmetry of the absorption line shape due to the interplay of phonon emission/absorption and dark intra- and intervalley excitonic states.

HL 14.8 Mon 14:00 P2-OG3

Optical Absorption and Darkfield Microscopy on Two-Dimensional Semiconductors — •Konstantin Neuhaus[1], Edward Leong[2], Thomas E. Murphy[2,3], Martin Mittendorff[3], and Sangam Chatterjee[4] — [1]Faculty of Physics, Philipps-Universität Marburg, D-35032 Marburg, Germany — [2]Department of Electrical & Computer Engineering, University of Maryland, College Park, MD, 20742, USA — [3]Institute for Research in Electronics & Applied Physics, University of Maryland, College Park, MD, 20742, USA — [4]Institute of Experimental Physics I, Justus-Liebig University Giessen, D-35392 Gießen, Germany

The optical properties of two-dimensional semiconductors offer a great potential in technological applications from FETs, gas sensors and solar cells to new optoelectronic devices. Furthermore, the potential is enhanced by the possibility of assembling heterostructures of different layers, thereby tuning the bandgap and other optoelectronic properties.

Here, we investigate the ability to locate and identify monolayer structures of molybdenum disulfide (MoS2) and black phosphorus by means of optical darkfield microscopy and high spatial resolution absorption measurements at room temperature. Especially MoS2 monolayers are easily identified in darkfield microscopy because of their characteristic triangular shapes.

HL 14.9 Mon 14:00 P2-OG3

Vibrational properties of metal phosphorus trichalcogenides from first principles — •Seyed Arsalan Hashemi Petrudi, Hannu-Pekka Komsa, Arkady Krasheninnikov, and Martti Puska — Finland, Espoo, Otakaari 1, floor 4, room Y427a

Recently, the family of 2D materials was further expanded following the fabrication of single-layer transition metal phosphorus trichalcogenides (TMTCs), with the general formula of MPX3 (where M = V, Mn, Fe, Co, Ni, Zn, Cd, Mg; X = S, Se and Te which are stacked in a X-P-M-P-X fashion). They offer a unique set of material properties that can open up new opportunities in optoelectronic and spintronic applications. Understanding the vibrational properties is critical in the material characterization. However, apart from the calculations on magnetic and electronic properties, a comprehensive ab-initio study of the vibrational properties of these 2D materials is still lacking. To reach this goal, we performed first-principles calculations for the phonon spectra, and Raman and IR intensities of MnPS3, MnPSe3, CdPS3, CdPSe3, ZnPS3 and ZnPSe3. To analyze the vibrational modes, we examine the ionic displacements and the contributions from different elements. Group theory is used to understand the Raman and IR activity of each mode. Finally, we also determined the elastic constants of these materials.

HL 14.10 Mon 14:00 P2-OG3

Transport measurements in high mobility hBN-graphene-WS2 stacks — •Tobias Rockinger[1], Tobias Völkl[1], Martin Drienovsky[1], Kenji Watanabe[2], Takashi Taniguchi[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, D-93053 Regensburg — [2]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

To induce spin-orbit coupling in graphene, heterostructures of graphene and tungsten disulfide (WS2) are investigated. To achieve high mobilities, we encapsulated graphene between hexagonal boron nitride (hBN) and WS2 via the van der Waals pickup method. Using Cr/Au edge contacts it is possible to achieve reliable, low resistance contacts. In this way we obtained carrier mobilities in graphene between 30.000 cm^2/Vs and 116.000 cm^2/Vs. We observed Shubnikov-de Haas oscillations in graphene sandwiched in between WS2 and hBN. While searching for weak localization and weak antilocalization we get results which are dominated by other effects. It seems that due to the small ($0,8$ μm) width of the hall bar geometry, propagation of electrons through the structure is mainly influenced by sample edges and ballistic effects. This leads to a peak in the magnetoresistance around 100 mT. With this value we calculated a cyclotron radius of $0,8$ μm and an effective sample width of $0,4$ μm which equates 50 percent of the measured width.

HL 14.11 Mon 14:00 P2-OG3

Possible topological insulator / superconductor interfaces for the investigation of Majorana excitations: $(Bi_{1-x}Sb_x)_2Te_3$ and FeSe — •Philipp Küppers[1], Jens Kellner[1], Markus Eschbach[2], Martin Lanius[3], Marcus Liebmann[1], Lukasz Plucinski[2], and Markus Morgenstern[1] — [1]II. Physikalisches Institut B RWTH Aachen University — [2]PGI 6 Forschungszentrum Jülich — [3]PGI 9 Forschungszentrum Jülich

Proximity induced s-type superconductivity (SC) in a topological insulator (TI) can lead to spinless, p-type superconductivity, which is the main ingredient for the creation of Majorana excitations (ME). To prove the existence of such quasi particles within the vortex of a type II SC grown on top of a TI with STS, two requirements have to be fulfilled. The Fermi energy E_F of the system has to be close to the Dirac point energy E_D of the TI and the superconducting gap has to be large in order to differentiate the ME from conventionally excited states within the vortex.

We present a method of tuning E_D with respect to E_F within 10 meV in the ternary TI $(Bi_{1-x}Sb_x)_2Te_3$ by variation of the Sb concentration x [1]. We show first ARPES measurements of the band structure of the SC FeSe grown on $SrTiO_3$. Methods of inducing high temperature SC in FeSe are also presented.

[1] Jens Kellner et al., Appl. Phys. Lett. **107**, 251603 (2015)

HL 14.12 Mon 14:00 P2-OG3

Long Wavelength Rayleigh Waves at the Surface of the Topological Insulator $BiSbTeSe_2$ — •Henning Kuhn, Matteo Montagnese, Jingyi Zhu, Zhiwei Wang, Yoichi Ando, and Paul H.M. van Loosdrecht — II. Physikalisches Institut, Universität zu Köln

Ultrafast transient grating measurements are performed on the topological insulator $BiSbTeSe_2$ in order to generate and investigate the properties of Rayleigh type surface acoustic waves (SAW) in the long wavelength (μm) regime, and their possible interactions with the topological surface states. The SAWs are observed as oscillations in the diffracted signal, with lifetimes exceeding 3 ns. The SAW dispersion and lifetime are measured as a function of temperature (10K to 300K) and for different azimuthal orientations of the SAW wave vector with respect to the crystallographic directions. No conclusive evidence for a coupling to the topological surface state is found.

HL 14.13 Mon 14:00 P2-OG3

Optimization of MBE growth of topological insulator thin films and device fabrication — •Andrea Bliesener, Patrick Janoschka, Fan Yang, Alexey Taskin, and Yoichi Ando — Institute of Physics II, University of Cologne

Topological insulators (TIs) belong to a new class of quantum materials in which a strong spin-orbit coupling leads to a band inversion and, as a consequence, to a gapless metallic state on the surface. The realization of many exciting theoretical predictions about the surface transport properties depends greatly on the sample quality and, first of all, on achieving a negligible bulk conductivity. The MBE growth technique is among the best suited for this challenge. Furthermore to observe the novel quantum phenomena, fabrications of thin-film devices are required which allows for tuning the Fermi level across the Dirac point. Here we show the results of growth of a $Bi_{2-x}Sb_xTe_3$ system, where the optimization of the composition between n-type Bi_2Te_3 and p-type Sb_2Te_3 can give almost perfect compensation. In combination with a greatly reduced bulk-to-surface ratio in the films, this approach allows to obtain TI samples where the surface transport is dominating. We also report a comprehensive method to fabricate a top-gated TI device consisting of a $Bi_{2-x}Sb_xTe_3$ Hall-bar using photo-lithography and e-beam lithography together with other techniques. With this device we are able to demonstrate the tuning of the chemical potential.

HL 14.14 Mon 14:00 P2-OG3

Puddles in compensated $Bi_{2-x}Sb_xTe_{3-y}Se_y$ — •Alessandro Revelli[1], Nick Borgwardt[1], Jonathan Lux[2], Zhiwei Wang[1], Malte Langenbach[1], Achim Rosch[2], Yoichi Ando[1], Paul van Loosdrecht[1], and Markus Grüninger[1] — [1]II, Physikalisches Institut, Universität zu Köln, Cologne, Germany — [2]Institut für theoretische Physik, Universität zu Köln

The topological insulator $Bi_{2-x}Sb_xTe_{3-y}Se_y$ shows bulk-insulating behaviour due to a low defect density and compensation of acceptors and donors. However, large fluctuations of the Coulomb potential give rise to strong local band bending even in fully compensated samples. This is demonstrated by the formation of electron and hole puddles which some of us have recently detected by infrared absorption measurements on $BiSbTeSe_2$ [1]. Puddles are important for both bulk and surface properties as they may e.g. yield a spatial variation of the surface charge density. According to Monte Carlo simulations [1], the temperature dependence of puddle formation depends on the Coulomb interaction between defects, while their spectral weight additionally depends on the size of the band gap. To test these predictions and to deepen our understanding of puddles, we performed infrared measurements on $Bi_{2-x}Sb_xTe_{3-y}Se_y$ as a function of x and y, varying the level of compensation, the defect density, and the band gap. The experimental results are in excellent agreement with the theoretical predictions for puddles in topological insulators.

[1] Borgwardt et al., Phys. Rev. B 93, 245149 (2016).

HL 14.15 Mon 14:00 P2-OG3

Towards one-dimensional topological Josephson junctions on molecular beam grown topological insulator thin films — •Tobias W. Schmitt, Daniel Rosenbach, Peter Schüffelgen, Martin Lanius, Michael Schleenvoigt, Gregor Mussler, Stefan Trellenkamp, Detlev Grützmacher, and Thomas Schäpers — Peter Grünberg Institute 9, Forschungszentrum Jülich & JARA-FIT, 52425 Jülich, Germany

Lateral topological Josephson junctions comprised of two superconducting leads on top of a topological insulator thin film are one way to probe possible Majorana excitations. These exotic quasiparticles are predicted to arise at the interface of a conventional s-wave superconductor to a topological non-trivial surface and possess similar properties as the long sought Majorana fermion. A current across such topological Josephson junctions however does not only contain information about possible Majorana assisted transport but also transport by conventional Andreev bound states.

The contribution of the conventional Andreev bound states to the supercurrent depends on the width of the junction. In a quasi one-dimensional system the width of the junction therefore is adjusted to the Fermi wavelength to allow for only two possible conducting modes, the Majorana bound states. In our recent work we focus on the realization of quasi one-dimensional topological Josephson junctions by selectively depositing topological insulator nanoribbons of reduced width and by increasing the Fermi wavelength by adjusting the Fermi level to the Dirac point of the linear disperse surface states.

HL 14.16 Mon 14:00 P2-OG3

Growth and transport measurements of gapless HgCdTe. — •Raimund Schlereth, Christoph Brüne, Hartmut Buhmann, and Laurens Molenkamp — Universität Würzburg, EP3

Three dimensional gapless semiconductors show promising new transport phenomena, due to their linear dispersion in all three momentum directions.

In this work we focus on HgTe/CdTe based compounds which crystalize in a zinc blende structure. Tensile strained HgTe is a three dimensional topological insulator [1] with an inverted band structure where the Γ8-bands lie above the Γ6-band. To get a linear dispersion, the band gap of the HgTe needs to be closed. Hg and Cd substitute each other in alloys of HgCdTe nearly randomly, making any Hg/Cd ratio possible. Therefore we can adjust the band structure in such a way, that the Γ8-band touches the Γ6-band, creating a linear dispersion. This linear dispersion however is not protected by symmetry or topology, but is achieved by fine-tuning of a system parameter (Hg/Cd ratio) [2]. We present magnetic field and gate voltage dependent transport data of HgCdTe with varying Hg concentration around the transitional point from the Cd rich to the Hg rich band structure.

HL 14.17 Mon 14:00 P2-OG3

Magnetotransport measurements on $Bi_4Br_xI_{4-x}$ bulk single crystals — •Marco Busch[1], Olivio Chiatti[1], Anna Isaeva[2], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Group Inorganic Chemistry II, Technische Universität Dresden, 01069 Dresden, Germany

Recent progress in the field of topological states of matter has largely been initiated by the discovery of bismuth chalcogenide bulk topological insulators, followed by closely related ternary compounds. Recently, Bi_4I_4 was found as a quasi-one-dimensional topological insulator with highly anisotropic surface-state Dirac fermions which suggests the possibility of combining topological order with other types of ordering characteristic to one-dimensional systems. Here, we present the results of our study on the mixed bismuth monohalides $Bi_4Br_xI_{4-x}$ with $x = 1, 2, 3, 4$, which were prepared by the reactions of bismuth metal with bismuth trihalides taken in stoichiometric amounts. The crystal composition was verified by electron-dispersive X-ray spectroscopy and the crystal structure was tested by X-ray diffraction. We investigated the magnetotransport properties of $Bi_4Br_xI_{4-x}$ bulk single crystals down to a temperature of $T = 0.3$ K for magnetic fields up to $B = 10$ T as previously for Bi_2Se_3 [2].

[1] G. Autès *et al.*, Nature Mater. **15**, 154 (2016)
[2] O. Chiatti *et al.*, Sci. Rep. **6**, 27483 (2016)

HL 14.18 Mon 14:00 P2-OG3

Influence of magnetic doping on the behavior of Bi_2Se_3 — •Jakub Sebesta, Pavel Balaz, and Karel Carva — Charles University, Faculty of Mathematics and Physics, Department of Condensed Matter Physics, Ke Karlovu 3 121 16 Praha 2, Czech Republic

Magnetic doping of topological insulators represents a way which enables us to control transport properties related to the presence of the conducting surface states in these materials. The conducting states are topologically protected while the time symmetry exists there. We can remove it by including a magnetic field that originates for instance from magnetically ordered impurities. In our work we focus on studying physical properties of topological insulators containing magnetic impurities or structural defects by using the ab-initio computations and the simulations of the magnetization dynamic. The basis of our research consists in computing of electronic structures by ab-initio TB-LMTO + CPA calculations, where we are interested in the influence of a doping or defects on the position of the Fermi level or on magnitudes of exchange interactions. In this contribution we show our results achieved in Bi_2Se_3 which contains Mn impurities or others structural defects. The obtained results are used to simulate a magnetic behavior of magnetic dopants in non-zero temperatures by the Monte-Carlo or spin dynamic simulations to obtain the ordering temperature etc. Also, we compare obtained results with an experiment.

HL 15: Focus Session: Two-dimensional materials II (joined session with TT)

Time: Monday 14:45–18:15 Location: POT 81

Invited Talk HL 15.1 Mon 14:45 POT 81

2D / 3D Heterostructures for Optoelectronis — •Max Lemme — University of Siegen, Germany

Broad spectral optical detection is of high interest for imaging, sensing, communication and spectroscopy. Two-dimensional (2D) materials are very promising for such applications due to their high optical absorption, potential wide detection range and material flexibility.

In this talk, graphene / silicon Schottky diodes made of chemical vapor deposited (CVD) graphene on n-type Si substrates will be discussed. Broad spectral response of 60 - 407 mA/W is measured from ultraviolet to near infrared light. In contrast to graphene, bulk molybdenum disulfide (MoS_2) is an n-type semiconducting 2D material with an indirect band gap of 1.3 eV. MoS_2/Si hybrid diodes made with multilayer, CVD grown MoS_2 yield a maximum spectral response of 8.6 mA/W.

Hybrid integration of large area CVD graphene as transparent conductive electrodes with amorphous silicon (a-Si) will be discussed for applications as multispectral photodetectors. A strong enhancement of the detectors' spectral response is observed in the ultraviolet region compared to reference devices with conventional aluminum doped zinc oxide electrodes. The maximum responsivity of these multispectral PDs can be tuned in their wavelength from 320 nm to 510 nm by external biasing, which allows single pixel detection of UV to visible light. The material combination of graphene and a-Si enables flexible diodes on polyimide substrates. Bilayer graphene boosts the maximum photoresponsivity of these flexible diodes up to 239 mA/W.

HL 15.2 Mon 15:15 POT 81

Optical properties of atomically thin MoS2 exposed to helium ions — •Anna Nolinder[1], Julian Klein[1,2], Agnieszka Kuc[4], Marcus Altzschner[1], Jakob Wierzbowski[1], Florian Sigger[1], Franz Kreupl[3], Thomas Heine[4], Jonathan Finley[1,2], Ursula Wurstbauer[1,2], Alexander Holleitner[1,2], and Michael Kaniber[1] — [1]Walter Schottky Institut und Physik Department, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany — [2]Nanosystems Initiative Munich (NIM), Schellingstr. 4, 80799 München, Germany — [3]Department of Hybrid Electronic Systems, Technische Universität München, Arcisstr. 21, 80333 Munich, Germany — [4]Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Linnéstr. 2, 04103 Leipzig, Germany

We present a spectroscopic study on atomically thin MoS2 exposed to helium ions. Distinct changes of the first-order Raman bands, additional defect luminescence and strong modification of the intrinsic valley spin relaxation properties are observed, shedding light on the effect of disorder on the optical properties and valley spin relaxation mechanisms. Moreover, our observations are in good qualitative agreement with Density Functional Theory calculations.

HL 15.3 Mon 15:30 POT 81

Coulomb Engineering of Excitonic Transitions in Transition

Metal Dichalcogenides for New Non-Classical Light Sources — •Sven Borghardt[1], Jhih-Sian Tu[1], Tim Flatten[2], Frank Matthes[2], Daniel Bürgler[2], Detlev Grützmacher[1], and Beata Kardynal[1] — [1]Peter Grünberg Institute 9 (PGI-9), Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]Peter Grünberg Institute 6 (PGI-6), Forschungszentrum Jülich, D-52425 Jülich, Germany

The spatial confinement of excitons is a key prerequisite for the creation of non-classical light sources. Since the dielectric environment of transition metal dichalcogenide monolayers (TMD-MLs) changes the screening of electrostatic fields and, thus, the interaction of charge carriers within the MLs, both the single particle band gap and the binding energy of exciton complexes in TMD-MLs can be tuned by modifying the dielectric properties of the environment.

In our experiments, we prepare TMD-MLs in different environments and apply optical spectroscopy methods in order to quantify the effects of the dielectric environment on the transition energies of exciton complexes. Furthermore, we correlate the results with single particle band gaps estimated from excited exciton states and single particle band gaps measured in scanning tunnelling spectroscopy experiments. This correlation gives access to the binding energy of exciton complexes.

In addition to TMD-MLs in laterally homogeneous environments, we examine lateral heterostructures of TMD-MLs in environments with laterally changing dielectric properties, paving the way towards controllable confinement of excitons within TMD-MLs.

HL 15.4 Mon 15:45 POT 81

Exciton-trion competition and single photon emission in III-V- monolayer hybrid architectures — •Oliver Iff[1], Yu-Ming He[1], Nils Lundt[1], Sebastian Stoll[1], Vasilij Baumann[1], Sven Hoefling[1,2], and Christian Schneider[1] — [1]Technische Physik and Wilhelm Conrad Roentgen Research Center for Complex Material Systems, Physikalisches Institut, Universitaet Wuerzburg, Am Hubland, D-97074 Wuerzburg, Germany — [2]SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, KY16 9SS, United Kingdom

Atomic monolayers represent a novel class of materials to study localized and free excitons in two dimensions and to engineer optoelectronic devices based on their significant optical features. Here, we investigate the role of epitaxially grown III-V substrates on the photoluminescense response from exfoliated MoSe2 and WSe2 monolayers in comparison to regular SiO2 substrates. In the case of MoSe2, we observe a significant qualitative modification of the emission spectrum, which is widely dominated by the trion resonance on InGaP substrates. Even more remarkably, in sheets of WSe2, we notice emission lines from localized excitons with linewidths down to 70 μeV, only limited by our system resolution. Furthermore, these spectral signatures are identified as single photon or even photon pair emitters without any sign of spectral jitter or blinking. Overall, the results outline the enormous potential of hybrid III-V- monolayer architectures in obtaining high quality emission signals from atomic monolayers, enhancing their optical properties.

HL 15.5 Mon 16:00 POT 81

The Influence of the Substrate Material on the Optical Properties of Tungsten-Diselendide Monolayers — Sina Lippert[1], •Lorenz Schneider[1], Dylan Renaud[1], Kyung Nam Kang[2], Obafunso Ajayi[3], Marc Halbich[1], Oday Abdulmunem[1], Xing Lin[1], Jan Kuhnert[1], Khaleel Hassoon[1], Saideh Edalati-Boostan[1], Young Duck Kim[3], Wolfram Heimbrodt[1], Eui-Hyeok Yang[2], James Hone[3], and Arash Rahimi-Iman[1] — [1]Faculty of Physics, Philipps-Universität, Marburg 35032, Germany — [2]Department of Mechanical Engineering, Stevens Institue of Technology, Hoboken, New Jersey, 07030, USA — [3]Department of Mechanical Engineering, Columbia University, New York, New York, 10027, USA

In recent years 2D materials based on transition metal dichalogenides (TMDs) have come up as an interesting material system mainly due to their remarkable properties in the monolayer regime after the successful exploration of graphene. While the main optical properties of these materials have been studied and understood well, the influence of the substrate material on the energy levels and the recombination dynamics are not yet sufficiently discussed. Here, we present a systematic comparison of the optical properties of monolayered WSe_2 on different substrates including SiO_2, sapphire, Si_3N_4-hBN and MgF_2. In addition to the exfoliated monolayers, a CVD grown monolayer on sapphire is included. While similarities have been found for the Raman signal and PL of these samples, small differences regarding excitonic features, emission characteristics and decay dynamics have been observed in dependence on the substrate.

Coffee Break

Invited Talk HL 15.6 Mon 16:45 POT 81

Excitons in colloidal 2D-CdSe nanocrystals — •Ulrike Woggon — Institut für Optik und Atomare Physik, TU Berlin, Str. des 17. Juni 135, 10623 Berlin, Germany

Two-dimensional II-VI semiconductor nanoplatelets (NPLs) gained increasing interest because of their unique electronic and optical properties, such as the Giant Oscillator Strength, strong electroabsorption response, low exciton-phonon interaction and high impact of dielectric confinement on exciton binding energies [1]. CdSe platelets are of special importance since they combine large particle volumes with ultrastrong confinement. We present a comprehensive study of the influence of dimensionality, size and shape on excitons in CdSe NPLs. They are an attractive system allowing to control not only the exciton energy states by thickness (z-direction) but also with lateral size variation the LO-phonon coupling (x,y-direction) [2]. The larger the particles' aspect ratio, the greater is the confinement related electronic contribution to the increased two-photon absorption and CdSe NPLs are ideally suited for two-photon imaging and non-linear opto-electronics [3-5]. [1] A.W. Achtstein et al., Nano Letters 12, 3151 (2012); [2] A.W. Achtstein et al., Phys. Rev. Lett. 116, 116802 (2016); [3] A.W. Achtstein et al., J. Phys. Chem. C 119, 20156 (2015); [4] R. Scott et al., Nano Lett. 15, 4985 (2015); [5] A.W. Achtstein et al., ACS Nano 8, 7678 (2014)

HL 15.7 Mon 17:15 POT 81

Controlled MoS2 deposition by metal-organic vapour phase epitaxy — Matthias Marx[1], Dominik Andrzejewski[2], Annika Grundmann[1], You-Ron Lin[1,3], Gerd Bacher[2], Holger Kalisch[1], Andrei Vescan[1], and •Michael Heuken[1,3] — [1]GaN Device Technology, RWTH Aachen University — [2]WET, University Duisburg-Essen — [3]AIXTRON SE

Recently, layered transition metal dichalcogenides (TMDC) have attracted a lot of attention. Their thermodynamically stable 2D form and their unique electrical and optical properties are very promising for integration in future electronic devices. For systematic scientific studies and in particular for implementation in commercial devices, it will be necessary to achieve a reproducible, homogeneous and scalable deposition on wafer scale. A promising option to achieve this goal is to use metal-organic vapour phase epitaxy (MOVPE) processes employing MO precursors for the TMDC constituents. All deposition experiments reported here are carried out in an AIXTRON horizontal hot-wall reactor. Molybdenum hexacarbonyl (MCO) and Di-tert-butyl sulfide (DTBS) are used as Mo and S sources, respectively. The samples are characterized via Raman spectroscopy, photoluminescence (PL) spectroscopy, atomic force microscopy (AFM) and scanning electron microscopy (SEM) to investigate their optical and structural properties. To reduce and control the nucleation density and to promote a layer-by-layer growth mode, the growth parameters such as DTBS and MCO precursor flows are optimized and temperature treatment was adjusted.

HL 15.8 Mon 17:30 POT 81

Ion implantation of 2D transition metal dichalcogenides monolayers — •Jhih-Sian Tu[1], Sven Borghardt[1], Hans Hofsass[2], Ursel Bangert[3], Quentin Ramasse[4], Detlev Grützmacher[1], and Beata Kardynał[1] — [1]PGI 9, Forschungszentrum Jülich, Jülich, Germany — [2]II. Physikalisches Institut, Georg-August-University Göttingen, Göttingen, Germany — [3]Department of Physics, Univsity of Limerick, Limerick, Ireland — [4]SuperSTEM Laboratory, Daresbury, UK

Monolayer transition metal dichalcogenides (TMDs) have gained interest as material for optoelectronics. In order to realise the technological potential of the TMDs semiconductors, it is desirable to be able to form heterostructures and introduce dopants in the monolayers. In this study, we examine the possibility to do so using ion implantation. We show that chalcogen atoms of the monolayer MoS2 can be substituted using very low energy ion beams (<50 eV) as verified using Raman spectroscopy and scanning transmission electron microscopy. Implantation levels of a few percent are realised with no structural damage visible in Raman spectra. Significant changes of the photoluminescence compared with pristine MoS2 monolayers are observed at cryogenic temperature. The technique under development is to be

applied for forming lateral heterostructures of 2D TMDs.

HL 15.9 Mon 17:45 POT 81

synthesis of bismuth/reduced graphene oxide composites and their electrochemical properties for Na-ion batteries — •Benrong Hai[1,2], Yang Xu[1], Min Zhou[1], Liying Liang[1], and Yong Lei[1] — [1]TU-ilmenau, Ilmenau, Germany — [2]Northeastern University, Shenyang, P. R. China

Recently, Na-ion batteries have been considered as a desirable alternative to Li-ion batteries, because of the greater abundance and lower cost of sodium-containing precursors. Even though Na-ion batteries have attracted great attention, more research is needed to enhance their performance. Reduced graphene oxide sheets have extraordinary electronic transport properties, large surface area and mechanical flexibility. Therefore, reduced graphene oxide sheets have been considered as a matrix material to improve electrochemical performance of metal nanoparticles. Here, we demonstrate a facile strategy to prepare bismuth/reduced graphene oxide composites. Such composites exhibit high specific capacity and enhanced cycling performance as anode. Compared to pure bismuth nanoparticles, the enhancement of sodium storage could be attributed to the introduction of reduced graphene oxide sheets that not only buffer the large volume changes during the reaction of sodium and bismuth, but also provide a highly conductive network for rapid electron transport in electrochemical reaction.

HL 15.10 Mon 18:00 POT 81

Optical properties of boron vacancies and boron vacancy complexes in hexagonal boron nitride — •Mažena Mackoit and Audrius Alkauskas — Center for Physical Sciences and Technology, Vilnius, Lithuania

In this work we perform density functional theory calculations of boron vacancies and boron vacancy complexes with oxygen in hexagonal boron nitride. It is shown that interaction with oxygen significantly lowers the formation energy of boron vacancies. Therefore, when oxygen is present, complexes are more likely to occur that bare vacancies. We find that electronic defect states can be of both σ and π type. This gives rise to various possible configurations of ground and excited states. In particular, it is suggested that intra-defect luminescence can be polarized both in- and out-of-plane. We also provide estimates of intra-defect excitation energies and associated Franck-Condon shifts, making the connection with recent experimental observations of single photon emitters in this material.

HL 16: Ultrafast Phenoma II

Time: Monday 14:45–17:30 Location: POT 51

Invited Talk HL 16.1 Mon 14:45 POT 51

The role of phonons for the optical control of semiconductor quantum dots — •Doris Reiter — Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Semiconductor quantum dots are a versatile source of single or entangled photons, hence a high fidelity control of the quantum dot states is required. For semiconductor quantum dots, which are embedded in a crystal matrix, the optical control is greatly influenced by the electron-phonon interaction. Here, I will discuss the phonon influence for different types of excitation mechanisms. For an excitation with pulses having a constant frequency, Rabi oscillations of the electronic system occur, which are damped due to the electron-phonon interaction. Fascinatingly, the phonon influence depends non-trivially on the excitation power. At sufficiently high pulse intensity, phonons become less influential and a reappearance of Rabi rotations has been predicted. Experimentally this reappearance has not been observed, yet. Using an excitation with chirped laser pulses, the electron-phonon interaction can also deteriorate the state preparation. Again, for sufficiently high pulse intensity a decoupling of the phonons takes place, but in contrast to Rabi rotations at lower excitation power. Therefore it has been recently possible to experimentally enter the reappearance regime in excellent agreement with theoretical predictions. In my talk, I will present the latest results on phonon effects on optical control of quantum dots comparing the two excitation scenarios.

HL 16.2 Mon 15:15 POT 51

Impact of the electronic band structure in high-harmonic generation spectra of solids — •Nicolas Tancogne-Dejean[1], Oliver D. Mucke[2,3], Franz X. Kartner[2,3,4,5], and Angel Rubio[1,2,4] — [1]Max Planck Institute for the Structure and Dynamics of Matter and ETSF, Luruper Chaussee 149, 22761 Hambourg, Germany — [2]Center of Free-Electron Laser Science, DESY, Notkestrasse 85, 22607 Hamburg, Germany — [3]The Hamburg Center of Ultrafast Imaging, Luruper Chaussee 149, 22761 Hambourg, Germany — [4]Physics Department, University of Hamburg, Luruper Chaussee 149, 22761 Hambourg, Germany — [5]Research Laboratory of Electronics, Massachusetts Institute of Thechnology, 77 Massachusetts Avenue, Cambridge, MA 02139, USA

An accurate analytic model describing high-harmonic generation (HHG) in solids is derived. Extensive first-principles simulations within a time-dependent density-functional framework corroborate the conclusions of the model. Our results reveal that: (i) the emitted HHG spectra are highly anisotropic and laser-polarization dependent even for cubic crystals, (ii) the harmonic emission is enhanced by the inhomogeneity of the electron-nuclei potential, the yield is increased for heavier atoms, and (iii) the cutoff photon energy is driver-wavelength independent. Moreover, we show that it is possible to predict the laser polarization for optimal HHG in bulk crystals solely from the knowledge of their electronic band structure. Our results pave the way to better control and optimize HHG in solids by engineering their band structure.

HL 16.3 Mon 15:30 POT 51

Electron transport in small CdSe Quantum Dots coupled with Methyl Viologen — •Mona Rafipoor[1,2], Jan-Philip Merkl[1], Zhi Wang[1], Gabriel Bester[1,2], and Holger Lange[1,2] — [1]Physikalische chemie, Uni Hamburg, Germany — [2]center of ultrfas imaging, Hamburg, Germany

Semiconductor nanocrystals have drawn significant interest due to their light absorption and electron transport properties which are mostly used for solar cells materials. Electron transfer and light absorption in very small CdSe quantum rods (QRs) (diameter of 1.8 nm) coupled with electron acceptors Methyl Viologen (MV+2) were investigated by Transient Absorption spectroscopy.

HL 16.4 Mon 15:45 POT 51

Quantum descriptions of spatio-temporal dynamics in carrier-capture processes: comparison between approaches — •Roberto Rosati, Doris E. Reiter, and Tilmann Kuhn — Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Due to the ultrashort spatial and temporal scales involved, carrier capture processes in nanostructures are genuine quantum processes. While a density matrix-based quantum kinetik (QK) approach has been successfully applied to describe phonon-induced carrier capture from a GaAs quantum wire into an embedded quantum dot [1], due to the numerical complexity extensions of this approach to higher dimensional systems, to longer times and to phenomena involving different interaction mechanisms remain difficult. By properly tailoring a recently proposed nonlinear density matrix equation based on a Lindblad superoperator [2], here we present an approach which, thanks to additional approximations, is computationally less demanding and inherently stable. By comparing the two approaches we show that the essential features of the capture dynamics are well reproduced by the Lindblad-based approach.

[1] Glanemann et al., Phys. Rev. B 72, 045354 (2005)
[2] Rosati et al., Phys. Rev. B 90, 125140 (2014)

Coffee Break

HL 16.5 Mon 16:30 POT 51

Material Science applications at ELI Beamlines: VUV transient ellipsometry — •Shirly Espinoza[1], Michael Rübhausen[1,2], and Jakob Andreasson[3] — [1]ELI Beamlines, Institute of Physics, Czech Academy of Science, Na Slovance 2, 182 21 Prague, Czech

Republic — [2]Condensed Matter Physics, Department of Physics, Chalmers University of Technology, Kemigården 1, SE-412 96 Göteborg, Sweden — [3]Institute for Nanostructures and Solid State Physics, University of Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany

In this talk, an introduction to the ELI Beamlines User Facility, to the material science end stations, and to the VUV transient ellipsometry technique will be presented. ELI Beamlines (ELI-BL) is a user facility being built in Prague, Czech Republic, as one of the three pillars of the transnational European Extreme Light Infrastructure (ELI) project that will hold some of the most intense lasers in the world. At EL-BL, high power lasers drive secondary sources (Plasma X-ray and High Harmonic Generation) that allow the study of transient processes in solid state materials. The planned end stations include Transient X-ray Diffraction, X-ray Absorption Spectroscopy, VUV ellipsometry and Transient Optical Spectroscopy (absorption and Raman). Time-resolved transient measurements are possible in the range of a few femtoseconds to hundred of picoseconds. Currently, experiments with transient absorption and transient ellipsometry in the UV-Visible range are being performed on semiconductor materials. Using these results, the advantages of the time-resolved techniques will be explained.

HL 16.6 Mon 16:45 POT 51

Towards fs-time-resolved spectroscopic ellipsometry — •Oliver Herrfurth[1], Steffen Richter[1], Mateusz Rebarz[2], Miroslav Kloz[2], Shirly Espinoza[2], Jakob Andreasson[2,3], Marius Grundmann[1], and Rüdiger Schmidt-Grund[1] — [1]Universität Leipzig, Institut für Experimentelle Physik II, Linnéstraße 5, 04103 Leipzig — [2]ELI Beamlines, Institute of Physics, Czech Academy of Science, Na Slovance 2, 182 21 Prague, Czech Republic — [3]Condensed Matter Physics, Department of Physics, Chalmers University of Technology, Gothenburg, Sweden

We report on recent progress in developing a spectroscopic ellipsometer with femtosecond time-resolution, which can be realised employing a pump-probe technique. The third harmonic of an amplified Ti:Sa laser (6 mJ,35 fs) is used as pump pulse and its fundamental wavelength is used to create a supercontinuum white light probe by focussing onto CaF_2. This method allows to probe a spectral range from 340 nm to 1000 nm with a single shot. The time resolution is set by the temporal width of the probe pulse. Pump-probe reflectometry measurements on a *c*-plane ZnO thin film were successfully conducted yielding first insight in the ultrafast carrier dynamics, which is particularly interesting for understanding the physical processes ruling lasing operation. First results on the respective temporal evolution of the dielectric function will be discussed.

HL 16.7 Mon 17:00 POT 51

Long-life pulse states of exciton polariton condensates in GaAs QWs — •Bernd Berger[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

A ring-shaped CW laser is used to non-resonantly excite exciton polaritons in a two dimensional DBR microcavity. Due to phonon scattering and polariton-polariton scattering the exciton polaritons undergo relaxation and a condensate of polaritons is formed. An additional non-resonant pulsed laser is used to perturb the formed condensate. By performing a series of time resolved measurements the spatial and temporal dynamics are studied. In a comprehensive analysis we find an unexpected long living polariton signal after pulsed excitation. Its duration exceeds the polariton lifetime by more than one order of magnitude and could potentially store information for several hundreds of picoseconds.

HL 16.8 Mon 17:15 POT 51

Nonspherical atomic effective pseudopotentials for surface passivation — •Anastasia Karpulevich[1,2], Hanh Bui[1,2], Denis Antonov[3], Peng Han[1], and Gabriel Bester[1,2] — [1]Institute of Physical Chemistry, Hamburg University, Grindelallee 117, D-20146 Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, D-22761 Hamburg, Germany — [3]Physics Institute, Stuttgart University, Pfaffenwaldring 57, D-70569 Stuttgart, Germany

The quantum mechanical atomistic calculation of the electronic properties of experimental-size colloidal semiconductor nanostructures remains a challenging task. We present a method to extract accurate pseudopotentials for surface passivants, within the framework of the atomic effective pseudopotential (AEP) method [1]. AEPs are constructed by extracting the local part of the self-consistent effective pseudopotentials from DFT calculations using an analytic connection. For the passivant atoms we retain the imaginary part of the pseudopotential in the construction procedure [2]. This imaginary part reproduces an asphericity of the passivant pseudopotential and allows to model surface dipoles and corresponding band offsets. We show that these surface effects need to be taken into account to model electronic properties of quantum dots accurately. The good level of transferability, without additional computational costs, is demonstrated. The results are directly compared to large-scale DFT calculations.

[1] Cardenas J.R. et al., Physical Review B, 86(11), 115332 (2012)
[2] Karpulevich A. et al., Physical Review B, 94, 205417 (2016)

HL 17: Spintronics II (joined session with TT)

Time: Monday 14:45–17:00 Location: POT 151

HL 17.1 Mon 14:45 POT 151

Observation of suppressed electron giant-Zeeman splitting in a (Cd,Mn)Te/(Cd,Mg)Te quantum well — •Janina J. Schindler[1], Jörg Debus[1], Victor F. Sapega[2], Dmitri R. Yakovlev[1,2], Grzegorz Karczewski[3], Tomasz Wojtowicz[3], and Manfred Bayer[1,2] — [1]Experimental Physics 2, TU Dortmund University, Dortmund, Germany — [2]Ioffe Institute, Russian Academy of Sciences, St. Petersburg, Russia — [3]Institute of Physics, Polish Academy of Sciences, Warsaw, Poland

We have studied the electron spin properties in a (Cd,Mn)Te/(Cd,Mg)Te quantum well modulation-doped with a high-mobile, highly concentrated two-dimensional electron gas by means of resonant spin-flip Raman scattering (SFRS). Resonant SFRS is a spin manipulating optical tool that also provides insight in spin interaction processes and spin-level structures. Two electron-SFRS signals with sharp resonance profiles at about 1.594eV and 1.599eV are observed, both showing no exciton-exchange energy offset at 0 T. The Mn-ion interactions with carriers in diluted magnetic semiconductors (DMS) lead typically to the giant Zeeman splitting of the electron and hole spin states with effective g-factors in the range of 10 to 80. However, the electron-SFRS signals demonstrate an effective g-factor of -1.7, which is characteristic for non-magnetic II-VI quantum wells. The optical selection rules derived from the circular polarization features let us assume that the SFRS processes involve a negative trion with componensated electron spins or a highly localized exciton bound to an impurity in the (Cd,Mn)Te quantum well.

HL 17.2 Mon 15:00 POT 151

Optical control of a strongly coupled spin-spin system in ZnO — Jan Heye Buss[1], Jörg Rudolph[1], Thomas A. Wassner[2], Martin Eickhoff[3], and •Daniel Hägele[1] — [1]Spektroskopie der kondensierten Materie, Ruhr-Universität Bochum, D-44780 Bochum — [2]Walter Schottky Institut, Technische Universität München, D-85748 Garching — [3]Justus-Liebig-Universität Gießen, I. Physikalisches Institut, D-35392 Gießen

The electron spin of the indium donor in ZnO couples strongly to the 9/2 nuclear spin of indium providing a non-trivial quantum system that can be optically manipulated and read out. Time-resolved Kerr-rotation measurements show directly a complex beating behavior of the electron spin under the application of an external magnetic field. The beat-structure provides a fingerprint of the 10 nuclear spin levels. We find evidence for an efficient optical pumping of the nuclear spin state via the optically pumped donor electron. A modulated pump pulse po-

larization reduces the nuclear spin polarization starting at frequencies above 100 kHz reaching zero polarization at 8 MHz. A full quantum mechanical modeling of the system including spin relaxation, optical pumping, and electron hopping exhibits excellent agreement with experiment [1]. Prospects for creating non-classical nuclear spin states will be discussed.
[1] J. H. Buß, J. Rudolph, T. A. Wassner, M. Eickhoff, and D. Hägele, Phys. Rev. B 93, 155204 (2016)

HL 17.3 Mon 15:15 POT 151

Design of polarization degenerate photonic nanocavities for cavity-enhanced optical spin-pumping — •Tobias M. Petzak[1], Sebastian Hammer[1,2], and Hubert J. Krenner[1,2] — [1]Lehrstuhl für Experimentalphysik 1, Institut für Physik, Universität Augsburg, Universitätsstr. 1 86159 Augsburg, Germany — [2]Nanosystem Initiative Munich (NIM), Schellingstraße 4, 80339 München, Germany

Defect cavities in photonic crystal membranes exhibit high quality factors and enable the efficient confinement of light within small volumes. Therefore, these nanoscale optical cavities can enhance the light-matter interaction between cavity photons and optical excitations of embedded semiconductor nanosystems.
Here, we propose and demonstrate by finite-difference-time-domain (FDTD) simulations, that a crossed-beam cavity design [1] allows to obtain polarization-degenerate photonic modes. This is achieved by varying the geometry of the two perpendicular cavities. The resulting tunable superposition of two linear polarized modes permits for the formation of a single and completely unpolarized mode. Such polarization properties are highly desirable for optically addressing spin- and valley degrees of freedom e.g. in monolayer transition metal dichalcogenides [2]. We show that our design can be implemented on thermally grown SiO_2 for which our FDTD simulations predict quality factors exceeding 300 for cavities resonant with the exciton transition of WS_2.
References:
[1] K. Riviore et al., *Appl. Phys. Lett.* **99**, 013114 (2011)
[2] K. F. Mak et al., *Nature Nanotechnology* **4**, 494-498 (2012)

HL 17.4 Mon 15:30 POT 151

Anisotropy of the spin diffusion in GaAs-based two-dimensional electron gases — •Markus Schwemmer[1], Andreas Hanninger[1], Dieter Schuh[1], Werner Wegscheider[2], Tobias Korn[1], and Christian Schüller[1] — [1]Institute of Experimental and Applied Physics, Faculty of Physics, University of Regensburg, Germany — [2]ETH Zurich, Switzerland

The combination of a femtosecond pulsed TiSa-Laser system with a magneto-optical Kerr effect microscope setup allows us to study time- and space-resolved propagation of an optically injected electron spin packet in a two-dimensional electron system (2DES) based on a modulation-doped AlGaAs/GaAs quantum well. The electron spin dynamics, and thus the electron spin diffusion, is determined by the interplay between Dresselhaus and Rashba fields. 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 symmetrically modulation-doped, (110)-grown GaAs quantum well, optically injected electron spins align parallel or antiparallel to the spin-orbit field. Therefore, D'yakonov-Perel spin dephasing is suppressed and a long spin coherence time can be attained. For such a system one would expect naively isotropic electron spin diffusion in the quantum well plane. Nevertheless a strongly direction-dependent behaviour of the electron spin diffusion is observed.

Coffee Break

HL 17.5 Mon 16:15 POT 151

Higher-order quantum theory of spin noise spectroscopy — •Daniel Hägele — Spektroskopie der kondensierten Materie, Ruhr-Universität Bochum, D-44780 Bochum

Spin noise spectroscopy has recently evolved into a versatile tool for studying spin dynamics in atoms and solids with minimal perturbation of the quantum system. A fully quantum mechanical theory of the detector output $z(t)$ is highly desirable for calculating higher order spectra of complex spin systems taking into account measurement back-action and relaxation. Treating spin noise spectroscopy within a stochastic master equation approach we find $z(t)$ in all orders of the measurement strength β [1]. This continuous quantum noise formula (CQNF) depends non-linearly on the equilibrium density matrix ρ_0 and contains as further ingredients the system propagator $G(t)$, the measurement operator σ_z, and multiple convolutions with white Gaussian noise $\Gamma(t)$. The CQNF allows for a systematic derivation of the spin noise spectrum $S_{\mathrm{q}}(\omega) = \frac{1}{2}\left(\mathrm{Tr}\left[(\sigma_z - \mathrm{Tr}(\sigma_z\rho_0))G(\omega)(\sigma_z\rho_0 + \rho_0\sigma_z)\right] + \mathrm{c.c.}\right)$ and higher order spectra such as the bispectum and trispectrum. The CQNF may also be applied to transport theory and measurement theory in general.
[1] D. Hägele, https://arxiv.org/abs/1611.02077

HL 17.6 Mon 16:30 POT 151

Off-diagonal g-tensor components in [113]-grown two-dimensional hole systems — •Christian Gradl[1], Michael Kempf[1], Johannes Holler[1], Roland Winkler[2], Dieter Schuh[1], Dominique Bougeard[1], Christian Schüller[1], and Tobias Korn[1] — [1]Universität Regensburg, 93040 Regensburg, Germany — [2]Department of Physics, Northern Illinois University, DeKalb, Illinois 60115, USA

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, off-diagonal components of the hole g-tensor are 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. By varying the direction of the applied magnetic field, we observe a non-diagonal hole g-tensor and quantify the individual tensor components, which are in very good agreement with our theoretical calculations.

HL 17.7 Mon 16:45 POT 151

An origin of large spin accumulation voltage in non-degenerate Si MOSFET at room temperature — •Masashi Shiraishi[1], Yuichiro Ando[1], Takayuki Tahara[1], and Hayato Koike[2] — [1]Kyoto University, Japan — [2]TDK Corporation, Japan

Si spintronics has been attracting much attention in a decade, and recent success of room temperature operation of Si spin MOSFET [1] can accelerate its progress. In this presentation, a large spin accumulation voltage of more than 1.5 mV at 1 mA measured in non-degenerate Si-based lateral spin valves (LSVs) at room temperature is introduced [2]. The notable is that this is the largest spin accumulation voltage measured in semiconductor-based LSVs in our best knowledge. The modified spin drift-diffusion model, which successfully accounts for the spin drift effect, explains the large spin accumulation voltage and significant bias-current-polarity dependence. The model also shows that the spin drift effect enhances the spin-dependent magnetoresistance in the electric two-terminal scheme. This finding provides a useful guiding principle for spin metal-oxide-semiconductor field-effect transistor operations. The detail of experiments and theoretical considerations will be introduced in the presentation. Reference:[1] T. Tahara, M. Shiraishi et al., APEX8, 113004 (2015). [2] T. Tahara, M. Shiraishi et al., Phys. Rev. B93, 214406 (2016).

HL 18: Semiconductor Lasers II

Time: Monday 14:45–17:30 Location: POT 06

HL 18.1 Mon 14:45 POT 06

Pump-power-driven mode switching in quantum-dot microlasers — •Heinrich A.M. Leymann[1,2], Daniel Vorberg[2], Thomas Lettau[1], Caspar Hopfmann[3], Christian Schneider[4], Martin Kamp[4], Sven Höfling[4], Roland Ketzmerick[2,5], Jan Wiersig[1], Stephan Reitzenstein[3], and André Eckardt[2] — [1]OvG Universität Magdeburg — [2]MPI PKS Dresden — [3]Technische Universität Berlin — [4]Universität Würzburg — [5]Technische Universität Dresden

We investigate the switching of the steady-state lasing mode of a high-β quantum-dot microlaser, occurring in bimodal lasers when varying the pump power. Comparing experiment to theory, we identify the underlying mechanism to be based on the competition between the effective gain on the one hand and the inter-mode kinetics on the other. We show that, while the largest effective gain determines the laser mode for weak pumping (just above the lasing threshold), it is the inter-mode kinetics that selects the laser mode in the limit of strong pumping. We point out that the latter mechanism is akin to (non-equilibrium) condensation of massive bosons. This similarity allows us to describe the mode switching by generalizing the theory of Bose selection and to obtain an analytical criterion for the mode selection. Within this framework, we find that the excitation-power-dependent switching from one laser mode to the other occurs via an intermediate phase, where both modes are lasing. Finally, we employ exact numerical simulations to investigate the origin of the experimentally observed super-thermal intensity fluctuations of the non-lasing mode.

HL 18.2 Mon 15:00 POT 06

First order coherence of semiconductor nanowire lasers — •Franz Langrieger, Michael Kaniber, Thomas Stettner, Philipp Zimmermann, Gregor Koblmüller, and Jonathan J. Finley — Walter Schottky Institut and Physik Department, Technische Universität München, Garching b. München, Germany

We experimentally probe the temporal coherence of the emission from individual GaAs-AlGaAs core-shell nanowire lasers dispersed onto Al_2O_3 substrates. Excitation power dependent photoluminescence spectroscopy shows continuous wave lasing from individual nanowires with threshold power densities of 11.3 ± 0.8 kW/cm2 and lasing persists from cryogenic temperatures up to T=140K. By measuring the first order coherence using a Michelson interferometer we obtain coherence times τ_c of a few ps. Our results are compared with spectral linewidth measurements of the lasing mode. The mechanism that lead to a limitation of the coherence times in nanowire lasers will be discussed.

HL 18.3 Mon 15:15 POT 06

Controlling the influence of background emitters on lasing in quantum dot micropillars — •Fabian Gericke[1], Mawussey Segnon[3], Martin von Helversen[1], Tobias Heindel[1], Christian Schneider[2], Frank Jahnke[3], Sven Höfling[2], Anna Musial[2], Xavier Porte[2], Martin Kamp[2], Christopher Gies[3], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Germany — [2]Technische Physik, Universität Würzburg, Germany — [3]Institut für Theoretische Physik, Universität Bremen, Germany

In case of microlasers with a low number of quantum dots (QDs) acting as gain material, it is important to consider the relative gain contribution from individual QDs. In particular, in the single QD lasing regime one has to distinguish between the gain contribution of a single QD in resonance with the cavity mode and that of additional off-resonant emitters. In this regime, we control and study the relative gain contribution of the resonant QD and a small ensemble of non-resonant QDs by using a two-color excitation scheme. The experiments are supported by a theoretical description in which we describe the system using a microscopic semiconductor model. This enables us to discriminate a truly single QD laser from a device where lasing threshold is enabled by additional background emitters. We show that a single QD in the spontaneous emission regime contributes with up to 70% to the laser output. Interestingly, increasing the number of contributing off-resonant emitters changes the effective beta-factor and lowers the laser threshold.

HL 18.4 Mon 15:30 POT 06

Gain compression induced polarization mode competition in quantum-dot micropillar lasers: Effects of coherent feedback on multi-mode rate equations — •Benjamin Kurt Miller, Christoph Redlich, Lina Jaurigue, Benjamin Lingnau, and Kathy Lüdge — Institut f. Theo. Physik, Sekr. EW 7-1, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Quantum-dot (QD) high-Q micropillar lasers are promising optoelectronic devices for data communication. The effects of feedback on QD lasers has profound consequences on stability and behavior, as seen in our previous work on single-mode QD micropillar lasers [1]. We investigated bimodal systems without feedback [2] and our preliminary results found that introducing feedback would induce novel dynamics. We present a bifurcation analysis of two-mode light emission from QD semiconductor micropillar VCSEL lasers subjected to optical feedback. Our model includes multi-mode rate equations with phenomenological gain compression parameters; a deterministic spontaneous emission parameter; and delayed, optical feedback. In this presentation, we consider the effects of tuning feedback phase, time delay, and intensity on the stability and output of a QD micropillar VCSEL. Our results offer optimization data for future experimental implementation.

References: [1]C. Otto, B. Globisch, K. Lüdge, E. Schöll and T. Erneux, Int. J. Bifurcation Chaos **22**, 1250246 (2012). [2]C. Redlich, B. Lingnau, S. Holzinger, E. Schlottmann, S. Kreinberg, C. Schneider, M. Kamp, S. Höfling, J. Wolters, S. Reitzenstein, and K. Lüdge, New J. Phys. **18**, 063011 (2016).

HL 18.5 Mon 15:45 POT 06

Non-markovian delay in the formation of coherence in a pulsed quantum-dot crytal laser — •Mawussey Segnon[1], Galan Moody[2], Frank Jahnke[1], Marty Stevens[2] und Christopher Gies[1] — [1]Institute for Theoretical Physics, University of Bremen, P.O. Box 330 440, 28334 Bremen, Germany — [2]Departement of Physics, University of Colorado and National Institute of Standards and Technology, Boulder, Colorado 80309-04440 USA

Photonic crystal (PC) cavities represent one way of tailoring the electromagnetic environment of an emitter and constitute an important structure for studying quantum electrodynamic phenomena. Within this work, we present results for time-resolved photon-correlation spectroscopy and its interpretation in terms of theory of InAsP/InP quantum dots (QDs) coupled to L3 cavity of a PC structure. The theoretical model, having its basis on a microscopic Hamiltonian of the QD and the quantum mechanical light field, allows us to access the output intensity and the second-order correlation function $g^{(2)}(t, \tau = 0)$. When using pulsed excitation, the time evolution of the photon number crosses different regimes of thermal and coherent light, together making up the emitted pulse. We find systematic shifts between the time-resolved intensity pulse maximum and the coherence maximum revealed in $g^{(2)}(t, \tau = 0)$. It is demonstrated that this stems from non-Markovian effects in the correlation dynamics. Our findings point out the possibility of using such devices as thermal light sources with unconventionally large output power.

Coffee Break

HL 18.6 Mon 16:30 POT 06

Stability in Optically Injected Two-State Quantum Dot Lasers — •Stefan Meinecke, Benjamin Lingnau, André Röhm, and Kathy Lüdge — Technische Universtität Berlin, Berlin, Germany

Semiconductor lasers based upon self-assembled quantum-dots (QDs) are promising sources for applications in optical networks used e.g. for data transmission via optical fibers. Recently, their ability to show simultaneous two-state lasing became the focus of diverse investigations.

We theoretically study a two-state quantum-dot laser subjected to optical injection into the ground state from a master laser. Our modeling approach is based on microscopically based rate-equations and goes beyond the constant alpha-factor approximation by including carrier dependent frequency shifts obtained from a full Bloch-equation approach.

Our results nicely reproduce recent experimental results on optical bistability. Furthermore, we show an increase of the dynamical stability of the two-state QD laser if compared to a single-color QD laser.

We find that the chaotic dynamics, predicted for single-color QD lasers under strong and detuned injection, completely vanish, if excited state lasing is possible [1]. This phenomenon is surprising, as an increase in the dynamical complexity, i.e. the degrees of freedom, leads to a stabilization of the device.

[1] S. Meinecke, B. Lingnau, A. Röhm, K. Lüdge, Ann. d. Physik (2017)

HL 18.7 Mon 16:45 POT 06

Towards self-mode locking of VECSELs in the red spectral range — •Marius Grossmann[1], Roman Bek[1], Max Vaupel[2], Hermann Kahle[1], Thomas Schwarzbäck[1], Arash Rahimi-Iman[2], Michael Jetter[1], Martin Koch[2], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen and Research Centers SCoPE and IQST, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]Department of Physics and Materials Sciences Center, Philipps-Universität Marburg, Renthof 5, 35032 Marburg, Germany

The introduction of mode-locked vertical external-cavity surface-emitting lasers (VECSELs) in 2000 was followed by tremendous progress in laser performance, especially for mode locking within the IR spectral range. Such devices facilitate a compact realization of ultrafast and -short pulse generation and are certainly desirable over a wide wavelength range. The recently demonstrated self-mode locking technique simplifies these devices even more, bypassing the intrinsic non-saturable losses of semiconductor saturable absorber mirrors.

We present the characterization of pulsed VECSELs with repetition rates in the GHz regime with focus on self-mode locking in the red spectral range. Our semiconductor structures are fabricated by metal-organic vapor-phase epitaxy. The active regions consist of quantum wells or dots based on the AlGaInP material system. Current research includes the investigation of hard and soft aperture modulation initiating the pulsed operation as well as the effect of the gain chip characteristics on the mode locking behavior.

HL 18.8 Mon 17:00 POT 06

Optical losses in intra-cavity heat spreaders for GaSb based VECSELs — •Chiara Lindner, Steffen Adler, Peter Holl, Andreas Bächle, Elke Diwo-Emmer, Rolf Aidam, and Marcel Rattunde — Fraunhofer-Institut für Angewandte Festkörperphysik IAF, Tullastr. 72, D-79108 Freiburg, Germany

Semiconductor disk lasers, also known as vertical-external-cavity surface-emitting lasers (VECSEL), exhibit the wavelength versatility of semiconductor lasers in combination with the capability of a nearly diffraction-limited high-power output. In order to achieve this, an efficient heat extraction from the active medium is needed. For GaSb (and also InP) based VECSEL, heat extraction through the distributed Bragg reflector is inefficient and thus has to be realized with an intra-cavity heat spreader. Due to their transparency at emission and pump wavelength and high thermal conductivity, silicon carbide (SiC) and diamond are most often applied.

Using a diamond heat spreader, a GaSb based VECSEL with up to 20 W output power at room temperature at 2 μm emission wavelength has been reported recently. However, the quality of the optical grade diamond still differs significantly from sample to sample.

In this presentation, we report on the results of a new experimental setup designed to determine the optical intra-cavity losses and the homogeneity of heat spreaders. We will compare different SiC and diamond based samples and discuss their influence on power scaling of VECSEL with an intra-cavity heat spreader.

HL 18.9 Mon 17:15 POT 06

Measuring the Photon Number Distribution of a Bimodal Quantum Dot Microlaser — •Elisabeth Schlottmann[1], Martin von Helversen[1], Marco Schmidt[1,2], Felix Krüger[1], Heinrich A.M. Leymann[3], Thomas Lettau[4], Alexander Foerster[4], Mikayel Khanbekyan[4], Christian Schneider[5], Sven Höfling[5], Martin Kamp[5], Jörn Beyer[2], Jan Wiersig[4], and Stephan Reitzenstein[1] — [1]Technische Universität Berlin — [2]Physikalisch Technische Bundesanstalt — [3]MPIPKS Dresden — [4]Universität Magdeburg — [5]Universität Würzburg

Microlasers operating in the regime of cavity quantum electrodynamics (cQED) exhibit enhanced coupling of spontaneous emission into the cavity mode. This leads to a smooth transition from thermal to coherent emission at threshold which makes it difficult to prove lasing solely by the input-output behavior. Against this background, measuring the second order auto-correlation function $g^{(2)}(\tau)$ has become a valuable tool to identify laser action. Beyond that, $g^{(2)}(\tau)$ is also indicative for superradiance, mode-switching or thermal emission.
Here, we apply for the first time a photon number resolving transition edge sensor (TES) to directly access the photon number distribution of quantum dot microlasers. Our combined experimental and theoretical study demonstrates that TES detectors can be used to differentiate between mode-switching and thermal emission of bimodal microlasers. Both show a $g^{(2)}(0) \approx 2$, but in the case of switching, a linear combination of a thermal and a coherent distribution appears in the photon number distribution.

HL 19: Transport: Graphene and Carbon Nanostructures (jointly with DY, DS, HL, MA, O)

Time: Monday 15:00–18:15 Location: HSZ 204

HL 19.1 Mon 15:00 HSZ 204

Creating and steering highly directional electron beams in graphene — Ming-Hao Liu[1,2], •Cosimo Gorini[1], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg, Regensburg, Germany — [2]Department of Physics, National Cheng Kung University, Tainan, Taiwan

We put forward a concept to create highly collimated, non-dispersive electron beams in pseudo-relativistic Dirac materials such as graphene or topological insulator surfaces [1]. Combining negative refraction and Klein collimation at a parabolic *pn* junction, the proposed lens generates beams, as narrow as a few Fermi wave lengths, that stay focused over scales of several microns and can be steered by a magnetic field without losing collimation. We demonstrate the lens capabilities by applying it to two paradigmatic settings of graphene electron optics: We propose a setup for observing high-resolution angle-dependent Klein tunneling, and, exploiting the intimate quantum-to-classical correspondence of these focused electron waves, we consider high-fidelity transverse magnetic focusing accompanied by simulations for current mapping through scanning gate microscopy. Our proposal opens up new perspectives for next-generation graphene electron optics experiments.

[1] M.-H. Liu, C. Gorini, K. Richter, arXiv:1608.01730.

HL 19.2 Mon 15:15 HSZ 204

Graphene *p-n* junction in a magnetic field as a valley switch — •Tibor Sekera, Rakesh P. Tiwari, and Christoph Bruder — Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

Low-energy excitations in graphene exhibit relativistic properties due to the linear dispersion relation close to the Dirac points in the first Brillouin zone. Two of the cones located at opposite corners of the first Brillouin zone can be chosen as inequivalent, representing a new *valley* degree of freedom, in addition to the charge and spin of an electron. Using the valley degree of freedom to encode information aroused significant interest, both theoretically and experimentally, and gave rise to the field of *valleytronics*.

We study a graphene *p-n* junction in an out-of-plane magnetic field as a platform to generate and controllably manipulate the valley polarization of electrons. We show that by tuning the external potential giving rise to the *p-n* junction we can switch the current from one valley polarization to the other. We also consider the effect of different types of edge terminations and present a setup, where we can partition an incoming valley-unpolarized current into two branches of valley-polarized currents. The branching ratio can be chosen by changing the location of the *p-n* junction.

HL 19.3 Mon 15:30 HSZ 204

Probing electronic wave functions in a nanotube quantum dot via conductance in a magnetic field — Magdalena Marganska[1], Alois Dirnaichner[1,2], Daniel R. Schmid[2], Peter L. Stiller[2], Christoph Strunk[2], Milena Grifoni[1], and •Andreas K. Hüttel[2] — [1]Institute for Theoretical Physics, Uni-

versität Regensburg, Regensburg, Germany — [2]Institute for Experimental and Applied Physics, Universität Regensburg, Regensburg, Germany

The tunneling of electrons through a contact between two systems depends on the overlap of their electronic wave functions. In quantum dots the overlap is often tuned via the height of tunneling barriers. Conversely, in carbon nanotubes the unique combination of cylindrical topology and honeycomb atomic lattice allows for a manipulation of the longitudinal component of the electronic wave function via a parallel magnetic field. The amplitude of the wave function at the point of contact with the leads is directly reflected in the coupling strength. Experimentally, we detect the changes in the electronic wave function through the evolution of conductance resonances corresponding to single particle quantum states with magnetic field. The magnitude of the magnetic field in our experiment, up to 17 T, allows us to confirm our prediction of the very different behaviour of the two valley states. The K' valley states experience a strengthening of the tunnel coupling at low magnetic field, followed by subsequent decoupling. In contrast, the K valley states decouple from the leads monotonically, and coupling becomes unmeasurably small already for moderate magnetic fields.

HL 19.4 Mon 15:45 HSZ 204

Electron-electron interaction correction to tunneling in graphene-graphene nanojunctions — •Matthias Popp, Ferdinand Kisslinger, and Heiko B. Weber — Lehrstuhl für Angewandte Physik, FAU Erlangen-Nürnberg (FAU), Erlangen, Germany.

In weakly disordered conductors, electron-electron interaction is expected to provide a zero-bias anomaly in tunneling characteristics [1]. This purely electronic effect is seemingly suppressed in scanning tunneling spectroscopy experiments on graphene due to momentum mismatch, which requires phonon assisted tunneling. [2,3]. In order to overcome this limitation, we fabricate in-plane graphene-graphene nanojunctions by an electro burning process using epitaxial graphene on SiC as starting material. In some junctions with an overall conductance of about e^2/h we indeed observed a zero-bias anomaly at low temperatures which follows the logarithmic scaling characteristics predicted by *Altshuler* and *Aronov*. These experiments offer the opportunity to study the nonlocal aspects of electron tunneling via manipulation of the environment.

[1] Altshuler, B. L. and Aronov, A. G., *Electron-Electron Interaction in Disordered Conductors*, 1985
[2] Brar, V. W. et al., Applied Physics Letters, 2007, 91, 122102
[3] Zhang, Y. et al., Nature Physics, 2008, 4, 627-630

HL 19.5 Mon 16:00 HSZ 204

Electroluminescence of Graphene Nanojunctions — •Christian Ott, Konrad Ullmann, and Heiko B. Weber — Lehrstuhl für Angewandte Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Staudtstr. 7/A3, D-91058 Erlangen, Germany

We report on electroluminescence (EL) detected at graphene nanojunctions, the latter being formed by electroburning of epitaxial graphene ribbons on silicon carbide [1]. The EL shows a broad spectrum with emphasis on the near infrared regime. Its intensity scales with applied current and is temperature independent down to liquid helium temperatures. Surprisingly, we find a weak voltage dependence. The spectrum is similar to blackbody radiation with apparent temperatures well above the damage threshold of graphene and the silicon carbide substrate. A similar phenomenon has already been observed in single atom point contacts [2] and island metal films [3]. There a model was proposed based on hot electron luminescence which goes along with a large mismatch between electron gas temperature and lattice temperature due to a reduced electron-phonon interaction in nanoscopic structures. A critical discussion of the underlying mechanism is provided.

[1] Ullmann et al, Nano Letters 15, 5 (2015)
[2] Downes et al., Applied Physics Letters 81, 7 (2002)
[3] Fedorovich et al., Physics Reports 328 (2000)

HL 19.6 Mon 16:15 HSZ 204

Reversible Photochemical Control of Doping Levels in Supported Graphene — •Marie-Luise Braatz[1,2], Nils Richter[1,2], Hai I. Wang[1], Axel Binder[3], Mischa Bonn[4], and Mathias Kläui[1,2] — [1]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany — [2]Graduate School of Excellence Materials Science in Mainz (MAINZ), 55128 Mainz, Germany — [3]BASF SE, 67056 Ludwigshafen, Germany — [4]Max Planck Institute for Polymer Research, 55128 Mainz, Germany

The type and density of carriers in graphene are important parameters to control its properties. Based on Terahertz (THz)-spectroscopy and electrical characterization of Nitrogen-doped graphene, we show that the doping level can be optically tuned between the p-type and intrinsic n-type regime [1]. This is achieved photochemically by controlling the dynamical equilibrium between the oxygen adsorption and desorption process via UV laser pulse irradiation treatment [2]. This approach is reversible, easy to use and contact free. This simple method can be used to write doping structures with spatial control by a focused laser beam, not requiring sophisticated nanostructuring to generate doping for instance by gate electrodes that need to be defined at the time of device fabrication.

[1] H. I. Wang, M.-L. Braatz et al., submitted (2016)
[2] S. M. Hornett et al., Phys Rev B 90 (2014)

15 min. break.

HL 19.7 Mon 16:45 HSZ 204

Time evolution of Floquet states in graphene — •Matteo Puviani[1], Francesco Lenzini[1], and Franca Manghi[1,2] — [1]Dipartimento FIM, Università di Modena e Reggio Emilia — [2]CNR - Institute of NanoSciences - S3, Modena

When a time-periodic field is applied to electrons in a lattice the Bloch theorem can be applied twice, both in space and in time, to describe the photon-dressed quasiparticles which are formed. This is the essence of Floquet theory, which has recently attracted a large renewed interest for its ability to describe topological phases in driven quantum systems. The discovery that circularly polarized light may induce nontrivial topological behavior in materials which would be standard in static condition has opened the way to the realization of the so-called Floquet Topological Insulators. In these systems, the topological phases may be engineered and manipulated by tunable controls such as polarization, periodicity and amplitude of the external perturbation.

In the presence of a continuous time-periodic driving, electrons are in a non-equilibrium steady state characterized by a time-periodic dependence of the wave function, and therefore of the expectation values of any observable. In this talk we will consider the prototypical case of graphene that, under the influence of circularly polarized light, exhibits in its Floquet band structure the distinctive features of a topological insulator, namely a gap in 2D and linear dispersive edge states in 1D (graphene nanoribbon). In particular, we will discuss how these characteristics affect the time behavior of some relevant observables such as energy, charge and current density.

HL 19.8 Mon 17:00 HSZ 204

Quantum chaos and out-of-time order correlation functions in graphene — •Markus Klug, Mathias Scheurer, and Jörg Schmalian — Institute for Theoretical Condensed Matter Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe, Deutschland

Out-of-time order correlation functions of type $C = \langle A(t)B(0)A(t)B(0)\rangle_\beta$ are believed to be a reasonable measure of quantum chaos which manifests in an exponential growth of C with a certain Lyapunov exponent determined by the microscopic model under considerations. Recently, it was conjectured hat this Lyapunov exponent is be bounded by $\lambda \leq 2\pi k_B T/\hbar$ [1].

In this work we investigate the out-of-time order correlation functions in graphene subject to the long range Coulomb interaction. To this end we develop a formalism to capture the relevant effects which determines the dominant time dependence of C. We demonstrate that the critical Dirac fluid graphene is a good candidate for saturating the bound mentioned above.

[1] J. Maldacena, S.H. Shenker and D. J. Stanford, High Energ. Phys. (2016) 2016: 106.

HL 19.9 Mon 17:15 HSZ 204

Interaction induced Dirac fermions from quadratic band touching in bilayer graphene — •Thomas C. Lang[1], Sumiran Pujari[2], Ganpathy Murthy[2], and Ribhu K. Kaul[2] — [1]Institute for Theoretical Physics, University of Innsbruck, Austria — [2]Department of Physics & Astronomy, University of Kentucky, Lexington, KY

We revisit the effect of local interactions on the quadratic band touching (QBT) of Bernal stacked bilayer graphene models using renormalization group (RG) arguments and quantum Monte Carlo simulations of the Hubbard model. We present an RG argument which predicts,

contrary to previous studies, that weak interactions do not flow to strong coupling even if the free dispersion has a QBT. Instead they generate a linear term in the dispersion, which causes the interactions to flow back to weak coupling. Consistent with this RG scenario, in unbiased quantum Monte Carlo simulations of the Hubbard model we find compelling evidence that antiferromagnetism turns on at a finite U/t, despite the $U = 0$ hopping problem having a QBT. The onset of antiferromagnetism takes place at a continuous transition which is consistent with $z = 1$ as expected for Gross-Neveu criticality. We conclude that generically in models of bilayer graphene, even if the free dispersion has a QBT, small local interactions generate a Dirac phase with no symmetry breaking and there is a finite-coupling phase transition out of this phase to a symmetry-broken state.

HL 19.10 Mon 17:30 HSZ 204

Dynamical charge and pseudospin currents in graphene and possible Cooper pair formation — •Klaus Morawetz — Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics (IIP) Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany

With the quantum kinetic equations for systems with SU(2) structure, regularization-free density and pseudospin currents are calculated in graphene realized as the infinite mass-limit of electrons with quadratic dispersion and a proper spin-orbit coupling. The intraband and interband conductivities are discussed with respect to magnetic fields and magnetic domain puddles. The optical conductivity agrees well with the experimental values using screened impurity scattering and an effective Zeeman field. The universal value of Hall conductivity is shown to be modified due to this Zeeman field. The pseudospin current reveals an anomaly since a quasiparticle part appears though it vanishes for particle currents. The density and pseudospin response functions to an external electric field are calculated and the dielectric function is discussed with respect to collective excitations. A frequency and wave-vector range is identified where the dielectric function changes sign and the repulsive Coulomb potential becomes effectively attractive allowing for Cooper pairing.

[1] Phys. Rev. **B 94** (2016) 165415

HL 19.11 Mon 17:45 HSZ 204

Interplay between the long-range Coulomb interaction and edge-state magnetism in zigzag graphene nanoribbons — •Marcin Raczkowski and Fakher Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Quasi-one-dimensional graphene nanoribbons terminated by zigzag edges host partially flat bands at the Fermi energy. Theoretical studies of the Hubbard model with the effective on-site interaction only predict spontaneously induced spin polarizations at the zigzag edges and the associated finite dispersion of the low-energy band. Here, we revisit the stability and dynamical signatures of spin-polarized edge states by performing projective quantum Monte Carlo simulations of a more realistic model with long-range Coulomb interactions. On the one hand, increasing the relative strength of nonlocal interactions with respect to the on-site repulsion reduces noticeably the spin correlation length along the zigzag edge; nevertheless the tendency towards the extended spin polarization along the edges remains dominant over the competing short-range charge correlations. On the other hand, growing charge fluctuations are responsible for the emergence of incoherent low-energy excitations in the dynamical charge structure factor. In addition, we resolve a systematic shift of the dominant low-energy peak in single-particle spectral function on the edge towards higher frequencies that we attribute to quasiparticle scattering from charge excitations.

HL 19.12 Mon 18:00 HSZ 204

Quantum phase transition in effective spin ladders derived from graphene nanoribbons — •Cornelie Koop and Stefan Wessel — Institut für Theoretische Festkörperphysik, RWTH Aachen University

Zigzag edges of graphene nanoribbons host localized edge states, which show a ferromagnetic coupling along each edge and an antiferromagnetic one to the opposite edge. Using an effective model that treats the edge-bulk interaction as a perturbation to the edge-edge interaction, we can drastically reduce the numerical effort needed for this system, and we eventually find a rather general spin ladder model.

We examine this model at low, but finite temperatures by means of Monte-Carlo techniques using the stochastic series expansion method. Susceptibilities and correlation functions can be investigated. We find a quantum-phase transition (QPT), as a function of the antiferromagnetic inter-leg coupling strength, between a weak-coupling phase with long-range ferromagnetic order along each leg, which does not have a spin excitation gap, and a disordered, gapped singlet-phase. The location and estimates for the critical exponents are assessed by numerical methods and compared to known results from renormalization group calculations.

HL 20: Fundamentals of Perovskite Photovoltaics II (joint session CPP/DS/HL)

Time: Monday 15:00–18:15 Location: ZEU 222

Invited Talk HL 20.1 Mon 15:00 ZEU 222

Visualizing Charge Carrier Diffusion In Hybrid Halide Perovskite Thin Films — •Achim Hartschuh, Kathrin Handloser, Irene Grill, Nicolai Hartmann, Nadja Giesbrecht, Meltem Aygüler, Mathhias Handloser, Thomas Bein, and Pablo Docampo — Department of Chemistry and CeNS, LMU Munich, 81377 Munich, Germany

Organic-inorganic metal halide perovskites represent one of the most promising classes of absorber materials for future photovoltaic applications [1]. A prerequisite for the efficient extraction of photo-generated carriers is the combination of low non-radiative relaxation rates and rapid diffusive transport. We study the excited state dynamics and charge carrier transport properties in different perovskite thin films using time-resolved photoluminescence microscopy. By scanning the confocal detection with respect to the excitation spot, we visualize diffusive transport on micrometer length scales and determine the charge carrier diffusion constants and mobilities [2]. We complement these studies by transient photocurrent measurements on the same films and derived devices [3,4].

Invited Talk HL 20.2 Mon 15:30 ZEU 222

Photon recycling in hybrid lead-halide perovskite semiconductors — •Felix Deschler — University of Cambridge, Cambridge, UK

We discuss the effect of photon recycling on the externally measured radiative recombination rates in hybrid perovskites. By combining transient absorption with transient photoluminescence (PL) data, we distinguish radiative from non-radiative processes and find that the PL originates from a bimolecular process for all investigated carrier densities. We measure external photoluminescence quantum efficiencies (PLQEs) under continuous-wave and pulsed excitation. Taking into account photon recycling, we connect the externally measured radiative efficiencies with the actual internal values, and derive internal PLQEs exceeding 80%.

We map the propagation of photo-generated luminescence and charges from a local photo-excitation spot in thin films of lead triiodide perovskites using a confocal microscopy setup. We observed regenerated PL emission at distances as far as 50 micrometers away from photo-excitation. We map the internal photon distribution in the film and find that, over these distances, the peak of the internal photon spectrum red-shifts from 765 to >800 nanometers. We build a lateral-contact solar cell with selective electron- and hole-collecting contacts, using a combination of photo-lithography and electro-deposition. We used these devices as a platform to study photocurrent propagation and found that charge extraction can be achieved well beyond 50 micrometers away from the excitation.

HL 20.3 Mon 16:00 ZEU 222

Coherent Dynamics of Free Exciton Dissociation in Lead-iodide Perovskites observed by 2D Electronic Spectroscopy — •Ajay Jha[1], Hong-Guang Duan[1,2,3], Vandana Tiwari[1], Pabitra Nayak[4], Michael Thorwart[2,3], Henry J. Snaith[4], and R. J. Dwayne Miller[1,3,5] — [1]MPI-Structure & Dynamics of Matter, Ham-

burg, Germany — [2]Universität Hamburg,Germany — [3]CUI Hamburg, Germany — [4]University of Oxford, UK — [5]University of Toronto, Canada

Hybrid organolead halide perovskites with high carrier mobility and large dielectric constant have received considerable attention as an excellent material for low-cost efficient photovoltaics. The power conversion efficiency of perovskite based solar cells has meteorically advanced to 22.1% with excitonic dye-sensitization concept and ~15% for planar heterojunction configuration. The unprecedented success of this material demands the fundamental understanding of underlying microscopic mechanisms for photoinduced charge generation. Recent studies suggest that most photoexcitations in perovskite are free charge carriers behaving like III-V inorganic semiconductors, but the contribution of excitons has been a matter of debate. We have employed ultrafast 2D electronic spectroscopy to probe elementary optical excitation of CH3NH3PbI3 thin films. We distinctly observe the electronically coupled excitonic and free carrier transitions at room temperature. We captured an ultrafast exciton dissociation favored by low exciton binding energy of ~40 meV. The interplay of strongly coupled dominant vibrational mode to exciton dynamics will also be discussed.

HL 20.4 Mon 16:15 ZEU 222

Time Resolved Microwave Conductivity on Perovskites — •Marvin Grüne[1], Andreas Sperlich[1], Andreas Baumann[2], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

Organo-metal halide perovskites continue to be the star of thin film solar cells exhibiting rapidly rising power conversion efficiencies. For further improvement of these solar cells it is essential to understand the fundamental intrinsic properties like photoconductivity, recombination and charge carrier mobility. Therefore, we investigate the mixed halide perovskite layers of $CH_3NH_3PbX_3$ (X: I^-, Br^- and Cl^-) using time-resolved microwave conductivity. With this contactless measurement technique we address the charge carrier lifetime, decay kinetics and intrinsic mobility of perovskite structures with different halide substituents X. The mobility increases more than a factor of 2 in this order of substituents up to 8 cm^2/Vs. Furthermore, the influence of solvent annealing on the crystallization process of the $CH_3NH_3PbI_3$ film has been investigated, now considering temperature dependence. This crystallization method generates e.g. bigger crystal domain sizes and almost one order of magnitude higher mobilities. Due to the absence of transport layers, we can relate differences in the results to intrinsic properties of the perovskite layers. Solar cells with the investigated layer achieve up to 16% efficiency in our labs.

15 min break

Invited Talk HL 20.5 Mon 16:45 ZEU 222

Interface engineering: the route towards high efficiency and stable hybrid perovskite solar cells — •Giulia Grancini — Group for Molecular Engineering of Functional Materials, EPFL Valais Wallis, CH-1951 Sion, Switzerland

Hybrid perovskite solar cells are undoubtedly leading the photovoltaic scene with their power conversion efficiency (PCE) >22%. Tuning the material composition, i.e. by cations and anions substitution (e.g. introducing a small amount of Br) and the interfacial properties, optimizing the structural and chemical interactions and the optoelectronic processes therein have been the successful routes for a real breakthrough in device efficiency and reproducibility. However, despite the impressive PCE reported, hybrid perovskite suffer of severe instability mainly due to material degradation upon exposure to water and moisture further accelerated under local heating and UV irradiation. Diverse technological approaches have been proposed delivering appreciable improvements, but still failing by far the market requirements. Recently, we pioneered a new concept by interface engineering a multi-dimensional composite of two dimensional (2D) (HOOC(CH2)2NH3)2PbI4 / 3D-CH3NH3PbI3 perovskite molecular junction. The composite forms an exceptional gradually organized structure that yields up to 12.9% PCE. Aiming at the up-scaling of this technology, we realize 10x10 cm2 large-area solar modules by a fully printable, industrial-scale process delivering 11.2% stable devices for 9,000 hours under accelerated testing conditions, leading to a record one-year stability.

HL 20.6 Mon 17:15 ZEU 222

Characterization of perovskite solar cells: Towards a reliable measurement protocol — •Eugen Zimmermann[1], Ka Kan Wong[1], Michael Müller[1], Hao Hu[1], Philipp Ehrenreich[1], Markus Kohlstädt[2,3], Uli Würfel[2,3], Simone Mastroianni[2], Gayathri Mathiazhagan[2], Andreas Hinsch[2], Tanaji P. Gujar[4], Mukundan Thelakkat[4], Thomas Pfadler[1], and Lukas Schmidt-Mende[1] — [1]Universität Konstanz, Konstanz, Germany — [2]Fraunhofer Institute for Solar Energy Systems ISE, Freiburg, Germany — [3]Freiburg Materials Research Center FMF, University of Freiburg, Freiburg, Germany — [4]Applied Functional Polymers, Department of Macromolecular Chemistry I, University of Bayreuth, Bayreuth, Germany

Tremendous progress on power conversion efficiency of lead halide perovskite solar cells during the last few years drastically increased the interest in research on this material. However, a so called "hysteretic" behaviour during current density-voltage (J-V) measurements is differently severe for differently prepared solar cells and strongly depends on scan parameters like scan rate, and measurement history. This challenges reliable results across different laboratories and hinders the aspect of commercialization. Here, we propose a reliable measurement protocol by introducing stabilized device characteristics obtained from an adaptive tracking of the maximum power point and the open circuit voltage, and compare such obtained values to device characteristics derived from standard and time resolved J-V measurements for varying solar cells fabricated in different laboratories.

HL 20.7 Mon 17:30 ZEU 222

Removing leakage recombination current in planar perovskite solar cells — •Kristofer Tvingstedt[1], Lidon Gil-Escrig[2], Christina Momblona[2], Philipp Rieder[1], David Kiermasch[1], Andreas Baumann[3], Henk J. Bolink[2], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximillian University of Würzburg, 97074 Würzburg — [2]Instituto de Ciencia Molecular, Universidad de Valencia, C/Catedrático J. Beltrán 2, 46980 Paterna, Spain — [3]Bavarian Center for Applied Energy Research 97074 Würzburg

All solar cells, including perovskites, suffer from recombination mechanisms of various types out of which leakage current usually dominates at lower voltages. Herein, we demonstrate a three order reduction of this recombination loss mechanism in planar perovskite solar cells by replacing the commonly used hole selective electrode PEDOT:PSS with a polymer arylamine hole transporting semiconductor. This renders these solar cells more useful under lower light intensity, such as end of the day and indoor conditions which we demonstrate via the extreme case of moon lighting conditions, where the cells still generates open circuit voltages of 530 mV. By this substantial leakage reduction we can be able to confirm charges to also remain in the photovoltaic device for up to 2 hours after the light has been switched off. We discuss the mechanisms behind this feature and explain why the arylamine is a superior hole selective electrode.

HL 20.8 Mon 17:45 ZEU 222

Double-layer charge selective contacts in perovskite solar cells as a key to improved efficiency and reduced hysteresis effects — •Lukas Kegelmann[1], Christian Wolff[3], Celline Awino Omondi[1], Lars Korte[1], Thomas Dittrich[1], Dieter Neher[3], Bernd Rech[1], and Steve Albrecht[2] — [1]Helmholtz-Zentrum Berlin, Inst. for Silicon Photovoltaics, Berlin, 12489, Germany. — [2]Helmholtz-Zentrum Berlin, Young Investigator Group Perovskite Tandem Solar Cells, Berlin, 12489, Germany. — [3]University of Potsdam, Soft Matter Physics, Potsdam, 14476, Germany.

Planar low-temperature processed perovskite solar cells without a mesoscopic scaffold are advantageous for a possible large-scale production but often suffer from photocurrent hysteresis, especially in the regular 'n-i-p'-structure. Here, we systematically study the influence of different low-temperature deposited electron transport materials (ETM) on planar regular solar cell characteristics. We further show that an elaborately chosen metal oxide interlayer in an ITO/metal oxide/PCBM double-layer ETM can significantly improve the device performance. J-V measurements reveal substantial reductions of hysteresis effects and enhanced power conversion efficiencies up to a champion stabilized value of 18.0 % for TiO2 interlayers. Surface photovoltage spectroscopy is used to show comparable absorber qualities on all ETMs for the fabrication process used here. Additionally, improved hole blocking for the double-layer structure is suggested by UPS and the metal oxide interlayer is considered to reduce shunt paths as it hampers direct contact between perovskite and the ITO electrode.

HL 20.9 Mon 18:00 ZEU 222

Electrical impedance spectroscopy on perovskite solar cells — •Fischer Mathias[1], David Kiermasch[1], Vladimir Dyakonov[1,2], and Andreas Baumann[2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research, 97074 Würzburg

Electrical impedance spectroscopy has shown to be a powerful technique to obtain informations about key parameters of a solar cell, like series and recombination resistance, build-in potential and the dielectric constant. Here, we performed impedance measurements over a wide temperature range from 300K down to 150K on solution processed $CH_3NH_3PbI_3$ perovskite solar cells. We compared the impedance spectra of n-i-p and p-i-n device configuration which is FTO/TiO_2/Perovskite/Spiro-MeOTAD/Au and ITO/PEDOT:PSS/Perovskite/$PC_{60}BM$/C_{60}/BCP/Au, respectively. We fit the impedance spectra by using corresponding equivalent circuits to investigate the dielectric behavior depending on the cell layout and preparation technique. We compare the extracted time constants at different frequency domains to reveal the influence from the p- and n-layer materials on the photovoltaic properties of the perovskite absorber material itself and examined charge carrier recombination behavior in dependency of illumination intensity.

HL 21: Fundamentals of Perovskite Photovoltaics II (joint session CPP/DS/HL)

Time: Monday 15:00–18:15 Location: ZEU 222

Invited Talk HL 21.1 Mon 15:00 ZEU 222

Visualizing Charge Carrier Diffusion In Hybrid Halide Perovskite Thin Films — •Achim Hartschuh, Kathrin Handloser, Irene Grill, Nicolai Hartmann, Nadja Giesbrecht, Meltem Aygüler, Mathhias Handloser, Thomas Bein, and Pablo Docampo — Department of Chemistry and CeNS, LMU Munich, 81377 Munich, Germany

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Invited Talk HL 21.2 Mon 15:30 ZEU 222

Photon recycling in hybrid lead-halide perovskite semiconductors — •Felix Deschler — University of Cambridge, Cambridge, UK

We discuss the effect of photon recycling on the externally measured radiative recombination rates in hybrid perovskites. By combining transient absorption with transient photoluminescence (PL) data, we distinguish radiative from non-radiative processes and find that the PL originates from a bimolecular process for all investigated carrier densities. We measure external photoluminescence quantum efficiencies (PLQEs) under continuous-wave and pulsed excitation. Taking into account photon recycling, we connect the externally measured radiative efficiencies with the actual internal values, and derive internal PLQEs exceeding 80%.

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HL 21.3 Mon 16:00 ZEU 222

Coherent Dynamics of Free Exciton Dissociation in Lead-iodide Perovskites observed by 2D Electronic Spectroscopy — •Ajay Jha[1], Hong-Guang Duan[1,2,3], Vandana Tiwari[1], Pabitra Nayak[4], Michael Thorwart[2,3], Henry J. Snaith[4], and R. J. Dwayne Miller[1,3,5] — [1]MPI-Structure & Dynamics of Matter, Hamburg, Germany — [2]Universität Hamburg,Germany — [3]CUI Hamburg, Germany — [4]University of Oxford, UK — [5]University of Toronto, Canada

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HL 21.4 Mon 16:15 ZEU 222

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15 min break

Invited Talk HL 21.5 Mon 16:45 ZEU 222

Interface engineering: the route towards high efficiency and stable hybrid perovskite solar cells — •Giulia Grancini — Group for Molecular Engineering of Functional Materials, EPFL Valais Wallis, CH-1951 Sion, Switzerland

Hybrid perovskite solar cells are undoubtedly leading the photovoltaic scene with their power conversion efficiency (PCE) >22%. Tuning the material composition, i.e. by cations and anions substitution (e.g. introducing a small amount of Br) and the interfacial properties, optimizing the structural and chemical interactions and the optoelectronic processes therein have been the successful routes for a real breakthrough in device efficiency and reproducibility. However, despite the impressive PCE reported, hybrid perovskite suffer of severe instability mainly due to material degradation upon exposure to water and moisture further accelerated under local heating and UV irradiation. Diverse techno-

logical approaches have been proposed delivering appreciable improvements, but still failing by far the market requirements. Recently, we pioneered a new concept by interface engineering a multi-dimensional composite of two dimensional (2D) (HOOC(CH2)2NH3)2PbI4 / 3D-CH3NH3PbI3 perovskite molecular junction. The composite forms an exceptional gradually organized structure that yields up to 12.9% PCE. Aiming at the up-scaling of this technology, we realize 10x10 cm2 large-area solar modules by a fully printable, industrial-scale process delivering 11.2% stable devices for 9,000 hours under accelerated testing conditions, leading to a record one-year stability.

HL 21.6 Mon 17:15 ZEU 222

Characterization of perovskite solar cells: Towards a reliable measurement protocol — •Eugen Zimmermann[1], Ka Kan Wong[1], Michael Müller[1], Hao Hu[1], Philipp Ehrenreich[1], Markus Kohlstädt[2,3], Uli Würfel[2,3], Simone Mastroianni[2], Gayathri Mathiazhagan[2], Andreas Hinsch[2], Tanaji P. Gujar[4], Mukundan Thelakkat[4], Thomas Pfadler[1], and Lukas Schmidt-Mende[1] — [1]Universität Konstanz, Konstanz, Germany — [2]Fraunhofer Institute for Solar Energy Systems ISE, Freiburg, Germany — [3]Freiburg Materials Research Center FMF, University of Freiburg, Freiburg, Germany — [4]Applied Functional Polymers, Department of Macromolecular Chemistry I, University of Bayreuth, Bayreuth, Germany

Tremendous progress on power conversion efficiency of lead halide perovskite solar cells during the last few years drastically increased the interest in research on this material. However, a so called "hysteretic" behaviour during current density-voltage (J-V) measurements is differently severe for differently prepared solar cells and strongly depends on scan parameters like scan rate, and measurement history. This challenges reliable results across different laboratories and hinders the aspect of commercialization. Here, we propose a reliable measurement protocol by introducing stabilized device characteristics obtained from an adaptive tracking of the maximum power point and the open circuit voltage, and compare such obtained values to device characteristics derived from standard and time resolved J-V measurements for varying solar cells fabricated in different laboratories.

HL 21.7 Mon 17:30 ZEU 222

Removing leakage recombination current in planar perovskite solar cells — •Kristofer Tvingstedt[1], Lidon Gil-Escrig[2], Christina Momblona[2], Philipp Rieder[1], David Kiermasch[1], Andreas Baumann[3], Henk J. Bolink[2], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximillian University of Würzburg, 97074 Würzburg — [2]Instituto de Ciencia Molecular, Universidad de Valencia, C/Catedrático J. Beltrán 2, 46980 Paterna, Spain — [3]Bavarian Center for Applied Energy Research 97074 Würzburg

All solar cells, including perovskites, suffer from recombination mechanisms of various types out of which leakage current usually dominates at lower voltages. Herein, we demonstrate a three order reduction of this recombination loss mechanism in planar perovskite solar cells by replacing the commonly used hole selective electrode PEDOT:PSS with a polymer arylamine hole transporting semiconductor. This renders these solar cells more useful under lower light intensity, such as end of the day and indoor conditions which we demonstrate via the extreme case of moon lighting conditions, where the cells still generates open circuit voltages of 530 mV. By this substantial leakage reduction we can be able to confirm charges to also remain in the photovoltaic device for up to 2 hours after the light has been switched off. We discuss the mechanisms behind this feature and explain why the arylamine is a superior hole selective electrode.

HL 21.8 Mon 17:45 ZEU 222

Double-layer charge selective contacts in perovskite solar cells as a key to improved efficiency and reduced hysteresis effects — •Lukas Kegelmann[1], Christian Wolff[3], Celline Awino Omondi[1], Lars Korte[1], Thomas Dittrich[1], Dieter Neher[3], Bernd Rech[1], and Steve Albrecht[2] — [1]Helmholtz-Zentrum Berlin, Inst. for Silicon Photovoltaics, Berlin, 12489, Germany. — [2]Helmholtz-Zentrum Berlin, Young Investigator Group Perovskite Tandem Solar Cells, Berlin, 12489, Germany. — [3]University of Potsdam, Soft Matter Physics, Potsdam, 14476, Germany.

Planar low-temperature processed perovskite solar cells without a mesoscopic scaffold are advantageous for a possible large-scale production but often suffer from photocurrent hysteresis, especially in the regular 'n-i-p'-structure. Here, we systematically study the influence of different low-temperature deposited electron transport materials (ETM) on planar regular solar cell characteristics. We further show that an elaborately chosen metal oxide interlayer in an ITO/metal oxide/PCBM double-layer ETM can significantly improve the device performance. J-V measurements reveal substantial reductions of hysteresis effects and enhanced power conversion efficiencies up to a champion stabilized value of 18.0 % for TiO2 interlayers. Surface photovoltage spectroscopy is used to show comparable absorber qualities on all ETMs for the fabrication process used here. Additionally, improved hole blocking for the double-layer structure is suggested by UPS and the metal oxide interlayer is considered to reduce shunt paths as it hampers direct contact between perovskite and the ITO electrode.

HL 21.9 Mon 18:00 ZEU 222

Electrical impedance spectroscopy on perovskite solar cells — •Fischer Mathias[1], David Kiermasch[1], Vladimir Dyakonov[1,2], and Andreas Baumann[2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research, 97074 Würzburg

Electrical impedance spectroscopy has shown to be a powerful technique to obtain informations about key parameters of a solar cell, like series and recombination resistance, build-in potential and the dielectric constant. Here, we performed impedance measurements over a wide temperature range from 300K down to 150K on solution processed $CH_3NH_3PbI_3$ perovskite solar cells. We compared the impedance spectra of n-i-p and p-i-n device configuration which is FTO/TiO_2/Perovskite/Spiro-MeOTAD/Au and ITO/PEDOT:PSS/Perovskite/$PC_{60}BM$/C_{60}/BCP/Au, respectively. We fit the impedance spectra by using corresponding equivalent circuits to investigate the dielectric behavior depending on the cell layout and preparation technique. We compare the extracted time constants at different frequency domains to reveal the influence from the p- and n-layer materials on the photovoltaic properties of the perovskite absorber material itself and examined charge carrier recombination behavior in dependency of illumination intensity.

HL 22: Organic Electronics and Photovoltaics II: Doping

Time: Monday 15:00–18:15 Location: ZEU 260

Invited Talk HL 22.1 Mon 15:00 ZEU 260

Molecular Electrical Doping of Organic Semiconductors — •Ingo Salzmann — Humboldt Universität zu Berlin, Berlin, Germany

In contrast to inorganic semiconductors, the potential of doping organic semiconductors (OSCs) for enabling new functionality and improving opto-electronic device performance has only recently been established. Here, the broad range of phenomena observed upon molecularly doping conjugated polymers (CPs) and molecules (COMs) is discussed, from which, finally, two different competing scenarios emerge [1]: (i) the formation of both OSC and dopant ions through integer-charge transfer, i.e., an ion pair (IPA), and (ii), the emergence of OSC/dopant ground-state charge transfer complexes (CPXs). In particular, the doping of poly(3-hexylthiophene) (P3HT) will be juxtaposed with that of quaterthiophene (4T) where, for both systems, an increase in thin-film conductivity by several orders of magnitude is observed. The underlying doping mechanisms at work are, however, fundamentally different [2]: IPA formation occurs for the polymer while CPX formation is found for the chemically and structurally similar oligomer. For both cases (i) and (ii), the doping-induced modification of the OSC density of states (DOS) is generally discussed for both p- and n-doping and its Fermi-Dirac occupation is modelled by numerical simulations. Therefrom finally emerges that engineering the DOS of doped OSCs, the occupation of which ultimately determines the doping efficiency, represents a key challenge in dopant design.

[1] I. Salzmann et al., Acc. Chem. Res. 49, 370 (2016)
[2] H. Méndez et al., Nature Commun. 6, 8560 (2015)

HL 22.2 Mon 15:30 ZEU 260

Inter-facial charge transfer studied in organic hetero-structure field-effect transistors. — •Eduard Meister, Stefan Schmidt, and Wolfgang Brütting — Institut für Physik, Universität Augsburg, Germany

In this work we studied inter-facial morphology dependent charge transfer (CT) happening in hetero-structure FETs based on vapour deposited small molecules. Therefore we used alpha-sexithiophene (α-6T) as donor and hexafluorotetracyanonaphthoquinodimethane (F_6TCNNQ) as acceptor. The lowest unoccupied molecular orbital of F_6TCNNQ is placed below of the highest occupied molecular orbital of α-6T, so that from an energetic point of view CT from α-6T to F_6TCNNQ molecules should occur. As evidence of CT we observed strong reduction of the switch-on voltage.

In order to get more information about morphology dependent CT and charge transport we produced devices with different gate insulator surfaces acting as template: blank SiO_2, as well as additional PMMA and thermally smoothed tetratetracontane [1] passivation layers. The morphology of α-6T layers was studied by atomic force microscopy and X-ray diffraction measurements. We employed also morphology dependent contact doping by application of tetrathiafulvalene tetracyanoquinodimethane salt contacts in contrast to mostly used gold electrodes. For the study of the transport mechanisms we performed temperature dependent measurements and calculated an upper limit of the activation energy for all the used configurations.

[1] L. Pithan et al., *J. Chem. Phys.* **143** (2015) 164707.

HL 22.3 Mon 15:45 ZEU 260

Frontier orbital energy levels and exciton binding energies in organic charge transfer complexes — •Paul Beyer[1], Stefan Krause[2], Timo Florian[1], Eduard Meister[3], Lutz Grubert[4], Wolfgang Brütting[3], Norbert Koch[1,2], and Andreas Opitz[1] — [1]Dep. of Physics, Humboldt-Universität zu Berlin — [2]Helmholtz-Zentrum Berlin — [3]Institute of Physics, University of Augsburg — [4]Dep. of Chemistry, Humboldt-Universität zu Berlin

The frontier π-orbitals of planar molecules tend to overlap upon contact and hybridization takes place resulting in charge transfer complexes (CTC) with modified energy levels [1]. We characterize the energy levels for the materials diindenoperylene (DIP) and hexafluorotetracyanonaphthoquinodimethane (F6TCNNQ) in solution by cyclic voltammetry as well as in thin films and in planar heterojunction geometry by photoelectron spectroscopy. Optical transitions were measured by UV/Vis/NIR absorption and X-ray transitions by near edge X-ray absorption fine structure spectroscopy.

At the planar DIP/F6TCNNQ interface CTC formation occurs. Due to the energy level alignment at the interface, which will be shown in detail for standing and lying molecular orientations, and the lower gap of the CTC in contrast to the semiconductor DIP, doping is present and DIP field-effect transistors with F6TCNNQ deposited on top are showing a strongly reduced threshold voltage. Furthermore, the exciton binding energies, which are much larger for X-ray than for optical excitations, will be discussed together with the energy levels.

[1] H. Méndez et al., *Nat. Commun.* **6** (2015) 8560.

HL 22.4 Mon 16:00 ZEU 260

Conical Intersection Dynamics of F4TCNQ Anion Radical doped Conducting Polymer Observed by 2D Electronic Spectroscopy — Ajay Jha[1], Hong-Guang Duan[1,2,3], •Vandana Tiwari[1], Michael Thorwart[2,3], and R. J. Dwayne Miller[1,3,4] — [1]MPI-Structure & Dynamics of Matter, Hamburg, Germany — [2]Universität Hamburg, Germany — [3]CUI Hamburg, Germany — [4]University of Toronto, Canada

Quinones are well celebrated electron acceptors which are even employed by nature for their impressive ability to retain electrons e.g. ubiquinone and plastoquinone. Quinone derivatives like tetrafluorotetracyano-quinodimethane (F4TCNQ) are popularly used as a p-type dopant to obtain high conducting polymer blend. To achieve higher conductivity, there has been a constant empirical effort to obtain different derivatives of quinones. In order to develop a molecular basis for rational tailoring F4TCNQ unit, understanding the electronic structure and relaxation dynamics of the TCNQ doped within a polymer framework is paramount. We have employed two-dimensional electronic spectroscopy to probe the coherent dynamics of F4TCNQ with the semiconducting polymer forming a charge transfer complex. We captured an ultrafast decay of F4TCNQ- mediated by conical intersection which is in agreement with the photoelectron spectroscopic studies in gas-phase. Additionally, we also observe that electronic transitions in F4TCNQ- are strongly coupled to polymer cation electronic structure. Our results open up new perspectives for tailoring intermolecular interactions to obtain high electrical conductivities.

HL 22.5 Mon 16:15 ZEU 260

Electronic structure of charge transfer compounds using Fermi- Löwdin orbital self-interaction corrected DFT — •Torsten Hahn[1], Martin Knupfer[2], and Florian Rückerl[2] — [1]Institute for Theoretical Physics, TU Freiberg, Freiberg, Germany — [2]Institute for Solid State Research, IFW Dresden, Germany

We present experimental and theoretical results on novel Picene/F4TCNQ and related donor / acceptor systems [1,2]. The recently developed Fermi-Löwdin orbital based approach for self-interaction corrected density functional theory (FLO-SIC DFT [3,4]) is used to investigate the electronic structure of these materials. The theoretical results are compared to standard DFT calculations and experimental data obtained by photoemission spectroscopy. We focus our analysis on the description of the magnitude of the ground state charge transfer and on the details of the formed hybrid orbitals. Further, we show that for weakly bound donor / acceptor systems the FLO-SIC approach delivers a more realistic description of the electronic structure compared to standard DFT approaches.

[1] B. Mahns, et al., Cryst. Growth Des. 14, 1338 (2014).
[2] F. Rückerl et al., JCP 145, (2016).
[3] M. R. Pederson et al., JCP 140, 121103 (2014).
[4] M. R. Pederson, JCP 142, 064112 (2015).

15 min break

HL 22.6 Mon 16:45 ZEU 260

UV-Vis-NIR spectroscopy studies on molecularly doped semiconducting polymers — •Malavika Arvind[1], Patrick Pingel[2], Silvia Janietz[2], and Dieter Neher[1] — [1]University of Potsdam, Soft Matter Physics, Germany — [2]Fraunhofer Institute for Applied Polymer Research, Potsdam, Germany

In recent years, significant efforts have been devoted towards understanding the fundamental processes involved in the doping of organic semiconductors with small molecules. Nevertheless, there is still a large degree of ambiguity in the field, which has prevented us from being able to truly exploit this method to better our organic devices. In this work, we utilize UV-Vis-NIR spectroscopy to study the sub-band gap optical transitions that occur in the well known semiconducting polymer poly(3-hexylthiophene) (P3HT) when doped with tris(pentafluorophenyl)borane (BCF), a strong Lewis acid, and compare it to the more commonly studied p-dopant, tetrafluorotetracyanoquinodimethane (F4TCNQ). In spite of the dissimilarity in their structures, both dopants are found to efficiently create positive polarons in P3HT, in solutions as well as in films. Here we investigate the influence of various parameters such as polymer/dopant concentration, solvent, temperature on the nature and efficiency of molecular doping, and also address the question of whether pre-aggregation of the polymer in solution assists or suppresses polaron-formation in P3HT.

HL 22.7 Mon 17:00 ZEU 260

Redox-Potentials Outperform Ionization Energy / Electron Affinity for Predicting Ion Pair Formation in Molecular Electrical Doping — •Berthold Wegner[1], Lutz Grubert[2], Dennis Chercka[3], Andreas Opitz[4], Stefan Hecht[2], Klaus Müllen[3], and Norbert Koch[1,4] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [2]Institut für Chemie, Humboldt-Universität zu Berlin, Berlin, Germany — [3]Max-Planck-Institut für Polymerforschung, Mainz, Germany — [4]Institut für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

Electrical doping with strong molecular donors and acceptors is a key technological component to control the charge carrier density and Fermi level of organic semiconductors. While commonly ionization energy / electron affinity values (measured on thin films via ultraviolet / inverse photoelectron spectroscopy) are employed to guide the selection of molecular dopants for organic hosts, we find strong indications that redox-potentials (measured in solution via cyclic voltammetry) are indeed better suited. A set of donor-acceptor systems, both in solution and in thin films, is studied using structurally similar molecules. Our results show that redox-potentials provide a useful basis to predict ion pair formation in the studied systems, while ionization energies /

electron affinities fail to provide such a basis. This is ascribed to the molecular length scale dopant-host interaction well described by local redox events at the molecule-electrode interface, whereas thin film ionization and affinity level measurements include collective and long-range solid state properties.

HL 22.8 Mon 17:15 ZEU 260

Effective work function reduction of practical electrodes using an organometallic dimer — Kouki Akaike[1], Marco V. Nardi[1], Martin Oehzelt[2,1], Johannes Frisch[2,1], •Andreas Opitz[1], Christos Christodoulou[1], Giovanni Ligorio[1], Paul Beyer[1], Melanie Timpel[1], Igor Pis[3], Federica Bondino[4], Karttikay Moudgil[5], Stephen Barlow[5], Seth R. Marder[5], and Norbert Koch[1,2] — [1]Humboldt-Universität zu Berlin, Germany — [2]Helmholtz-Zentrum Berlin, Germany — [3]Elettra-Sincrotrone Trieste, Italy — [4]IOM CNR Laboratorio TASC, Italy — [5]Georgia Institute of Technology, USA

The control of the cathode work function (WF) is essential to enable efficient electron injection and extraction at organic semiconductor/cathode interfaces in organic electronic devices. Here, ultraviolet photoelectron spectroscopy is used to determine the work function reduction by moderately air-stable pentamethylrhodocene dimer onto various conducting electrodes, by either vacuum deposition or drop casting from solution, to less than 3.6 eV, with 2.7 eV being the lowest attainable value. Electron transfer from the molecule to the respective substrates is responsible for the appreciable WF reduction. Notably, even after air exposure, the WF of the donor-covered electrodes remains below those of typically used clean cathode metals, such as Al and Ag. This demonstrates the ability of the pentamethylrhodocene dimer to reduce the WF for a wide range of electrodes used in all-organic or organic-inorganic hybrid devices.

K. Akaike et al., *Adv. Funct. Mater.* **26** (2016) 2493-2502.

HL 22.9 Mon 17:30 ZEU 260

Temperature-induced F4TCNQ desorption from p-doped P3HT films — •Hannes Hase[1], Andreas Opitz[1], Norbert Koch[1,2,3], and Ingo Salzmann[1] — [1]Humboldt-Universität zu Berlin, Supramolekulare Systeme, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Bereich Solarenergieforschung, Germany — [3]Jiangsu Key Laboratory for Carbon-Based Functional Materials & Devices, Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou 215123, P.R. China

Thermal post-fabrication annealing is common practice for functional conjugated polymer (CP) films in organic photovoltaic cells, which is also applied to p-doped CPs in a number of studies. However, the typically small molecular-weight dopants, like, e.g., tetrafluorotetracyanoquinodimethane (F4TCNQ), can be expected to be prone to diffusion upon thermal treatment, which has been largely disregarded in pertinent literature. Here, we explore to which extent the annealing temperature impacts films of poly(3-hexylthiophene-2,5-diyl) (P3HT) doped with F4TCNQ. For temperatures beyond 60 °C, we find a reduction in conductivity with a concomitantly lowered dopant concentration, as deduced from optical and Fourier-transform infrared spectroscopy. While atomic force microscopy indicates the morphology to be essentially retained, grazing-incidence X-ray diffraction confirms the transition from a P3HT/F4TCNQ mixed crystal structure to pure P3HT and points towards F4TCNQ desorption. We conclude that, upon thermal annealing, dopant loss needs to be accounted for by adjusting the dopant concentration.

HL 22.10 Mon 17:45 ZEU 260

Molecular drift of p-type dopants in doped organic semiconductors driven by an external electric field and studied by spectroscopic IR-microscopy — •Sebastian Beck[1,2], Vipilan Sivanesan[1,2], Lars Müller[2,3], Seon-Young Rhim[1,2], Jakob Bernhardt[1,2], and Annemarie Pucci[1,2] — [1]Universität Heidelberg, Kirchhoff-Institut für Physik — [2]InnovationLab GmbH, Heidelberg — [3]TU Braunschweig, Institut für Hochfrequenztechnik

A homogeneous dopant distribution is known to be important for efficient charge transfer (CT) in doped organic semiconductors as well as the functionality of organic electronic devices. Therefore, a lot of effort is made to control the molecular composition in devices throughout the deposition process. However, during device operation an unintentional movement of charged molecules such as dopants through the layers can occur and can reduce or even destroy device performance. To further improve the understanding of these effects the implementation of new analytical methods is advised. In this study, the motion of the p-type dopant Mo(tfdCO2Me)3 in highly regioregular P3HT induced by an external electric field was studied with spectroscopic IR-microscopy. The molecular drift was identified by measuring laterally resolved IR spectra of doped layers between two electrodes before and after applying a dc field of about 2 V/micron. An analysis of the changes of the vibrational modes of the dopant molecule as well as the spectral features of the charged P3HT chains enabled an estimate of the mobility of the dopant molecules. Our results are in agreement with electrical measurements and clarify underlying processes of device fatigue.

HL 22.11 Mon 18:00 ZEU 260

Drift of Dopants in Organic Semiconductors — •Lars Mueller[1,2,3], Seon-Young Rhim[1,3], Vipilan Sivanesan[1,3], Dongxiang Wang[1], Sebastian Beck[1,3], Annemarie Pucci[1,3], Wolfgang Kowalsky[1,2,3], and Robert Lovrincic[1,2] — [1]InnovationLab, Heidelberg, Germany — [2]Institute for High-Frequency Technology, TU Braunschweig, Germany — [3]Kirchhoff Institute for Physics, Heidelberg University, Germany

Electrical doping of organic semiconductors is widely applied to fabricate high performance organic electronic devices. The usually unwanted but still prevalent effect of dopant mobility in organic semiconductors is known for various dopant molecules in terms of diffusion towards a stable equilibrium. A mostly neglected effect is the influence of operating conditions that can cause a drift of dopants additionally to the known diffusion. We study this drift behavior and compare different dopant-host combinations, starting from Poly(3-hexylthiophen-2,5-diyl) (P3HT) doped with 2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ) to larger dopant molecules and different host materials. We find a dynamic drift-process that can be utilized to deliberately create highly doped and almost undoped regions within one thin film, resulting in a spatially altered conductivity. To demonstrate the applicability, we show first data of a proof-of-principle memory device that is based on a spatially controlled dopant distribution.

HL 23: Plasmonics and Nanooptics II: Light-Matter Interaction

Time: Monday 15:00–16:45 Location: TRE Ma

HL 23.1 Mon 15:00 TRE Ma

Three-electron photon interaction mediated by localized plasmons — Peter-Jan Peters and •Richard Berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel

The light emission from a scanning tunneling microscope operated on Ag(111) surfaces at 5 K is analyzed from low conductances G to values approaching the conductance quantum. Optical spectra reveal emission due to localized plasmons with photon energies exceeding the applied bias more than twice ($h\nu > 3eV$). The emission intensity varies in a non-monotonic fashion with G. An empirical model reproduces the scaling of the photon yield and the optical spectra near the thresholds for two-electron and three-electron processes. While some heating of the electron gas occurs, the predominat part of the light emission is due to coherent processes.

HL 23.2 Mon 15:15 TRE Ma

AlN/GaN multilayer interface phonons studied with mid-IR second-harmonic phonon spectroscopy — •Christopher J. Winta[1], Nikolai Passler[1], Ilya Razdolski[1], D. Scott Katzer[2], Ioannis Chatzakis[3], Neeraj Nepal[2], David J. Meyer[2], Chase T. Ellis[2], Joseph G. Tischler[2], Alexander J. Giles[2], Sandy Gewinner[1], Wieland Schöllkopf[1], Martin Wolf[1], Joshua D. Caldwell[2], and Alexander Paarmann[1] — [1]Fritz-Haber-Institut der MPG, Faradayweg 4–6, 14195 Berlin — [2]U.S. Naval Research Laboratory, Washington, D.C. 20375 — [3]NRC Postdoctoral Fellow (residing at NRL, Washington D.C. 20375)

Combining multiple atomic-scale layers of polar crystals allows for active modification of phonon lifetimes, frequencies and hence engineering of Reststrahlen band spectral positions. Specifically, new interface optical phonon modes emerge in these so-called crystalline hybrids (XHs). The atomic-scale layer thicknesses allow for tuning of these modes, opening up a new class of engineered materials [1].

In our experiments, we study the nonlinear response of an AlN/GaN 27-layer superlattice material on a SiC substrate with varying layer thicknesses ranging from ∼2 to 4 nm independently for both constituents by means of mid-IR second-harmonic phonon spectroscopy [2]. The higher spectral resolution of SHG as compared to reflectivity allows us to uniquely assign peaks to specific modes. In consequence, we are able to identify interface phonons by their layer thickness dependent behavior. [1] Caldwell et al., Nat. Nanotechnol. **11**, 9–15 (2016); [2] Paarmann et al., Phys. Rev. B **94**, 134312 (2016)

HL 23.3 Mon 15:30 TRE Ma

Second Harmonic Generation from Surface Phonon Polaritons in Silicon Carbide — •Nikolai Christian Passler, Ilya Razdolski, Martin Wolf, and Alexander Paarmann — Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin

Surface Phonon Polaritons (SPhP) have recently emerged as novel building block for mid-infrared (MIR) nanophotonic applications, promising to possibly overcome the intrinsic loss problem of plasmonics [1]. SPhPs arise in polar dielectrics due to optical phonon resonances leading to negative permittivity between transverse and longitudinal optical phonon frequencies. Furthermore, SPhPs exhibit tremendous field enhancements, driving the lattice atoms into a strongly nonlinear regime. Hence, SPhPs might grant a frequency-tunable access to vibrational-driven transient transitions of material phases.

Here, we use linear and nonlinear MIR spectroscopy [2], revealing the resonant second harmonic generation (SHG) arising from propagating SPhPs in SiC in the Otto geometry. Our experiments employ intense, tunable and narrowband MIR pulses from a free-electron laser. Corresponding to the absorption dip in our reflectivity spectra, we observe a strongly enhanced SHG yield at the SPhP resonance. Furthermore, we develop a matrix formalism for anisotropic multilayer wave propagation, allowing for precise prediction of the linear and non-linear properties of SPhPs.

[1] Caldwell et al., Nano Letters (2014) [2] Paarmann et al., APL (2015)

HL 23.4 Mon 15:45 TRE Ma

Charge dynamics in organic materials imaged with nanosecond and nanometer resolution. — •Anna Rosławska[1], Pablo Merino[1], Christoph Grosse[1,2], Markus Etzkorn[1], Klaus Kuhnke[1], and Klaus Kern[1,3] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — [2]NanoPhotonics Centre, Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK — [3]École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

The dynamics of charges and bound pairs of charge carriers (excitons) determines the performance of organic optoelectronic devices, such as light emitting diodes or solar cells. Precise nanoscale characterization of light emission at the nanosecond timescale can help to improve the efficiency of such devices. Here, by using low-temperature Scanning Tunneling Microscopy-induced Luminescence (STML) we probe the charge dynamics on defect-related light emission centers in C_{60} thin films. We apply 100 ns long square voltage pulses [1] to the tunnel junction and record transients of the emitted light with subnanosecond resolution as a function of injection current and lateral distance from the emission center. Analysis of luminescence transients discloses time constants ranging from 5 ns to 50 ns depending on the position in space. They can be attributed to hole and electron injection rates to the defect state. Our approach allows mapping the transients on a grid and therefore obtaining light intensity videos with sub-nanosecond time resolution at the ultimate molecular scale.
[1] C. Große, *et al.*, Appl. Phys. Lett., 103, 183108 (2013)

HL 23.5 Mon 16:00 TRE Ma

Single solid state quantum emitter coupled to a resonant plasmonic antenna array — •Markus Pfeiffer[1,2,3], Paola Atkinson[4], Armando Rastelli[4], Oliver G. Schmidt[4], Harald Giessen[3], Markus Lippitz[5,2,3], and Klas Lindfors[1,2,3] — [1]Department of Chemistry, University of Cologne, Luxemburger Str. 116, 50939 Köln, Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [3]Fourth Physics Institute and Research Center SCOPE, University of Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — [4]Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany — [5]Experimental Physics III, University of Bayreuth, Universitätsstrasse 30, 95447 Bayreuth, Germany

Plasmon resonant arrays or meta-surfaces shape optical fields and the local density of states. They provide large regions of enhanced emission from emitters and greater design flexibility than single nanoantennas. This makes them of great interest for engineering optical absorption and emission. Here we study the coupling of single self-assembled semiconductor quantum dots to plasmonic meta-surfaces. We investigate the influence of spectral properties of the nanoantenna array and the position of the emitter in the unit cell of the structure. We observe a resonant enhancement due to emitter-array coupling in the far-field regime and find a clear difference from the interaction of an emitter with a single antenna.

HL 23.6 Mon 16:15 TRE Ma

Plasmon-exciton coupling in microcavities — •Igor Shavrin[1], Mario Hentschel[2], Daniel E. Gómez[3,4], Dirk Hertel[1], Klaus Meerholz[1], Timothy J. Davis[3,4], Harald Giessen[2], and Klas Lindfors[1] — [1]Department of Chemistry, University of Cologne, Luxemburger Str. 116, 50939 Köln, Germany — [2]4^{th} Physics Institute and Research Center SCOPE, University of Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — [3]CSIRO, Materials Science and Engineering, Private Bag 33, Clayton, Victoria, 3168, Australia — [4]Melbourne Centre for Nanofabrication, Australian National Fabrication Facility, Clayton VIC 3168, Australia

Strong interactions between plasmons and excitonic states are interesting due to the extreme field confinement in plasmon resonant structures [1]. So far strong plasmon-exciton coupling has been achieved by placing the excitonic material in the near-field of a metal nanostructure. This however results in strong quenching of fluorescence.

Here we study the plasmon-exciton coupling mediated by a microcavity mode. We fabricate gold nanorod antennas in a wavelength-thick thin-film microcavity with the antennas positioned at one of the field anti-nodes using dielectric spacer layers. At the other anti-node we deposit a thin film of merocyanine molecules. These molecules form large J-aggregates that exhibit excitons with a strong dipole moment and therefore resulting in enhanced light-matter coupling. We observe three avoided crossings in reflection spectra that are well explained by a model with three coupled oscillators.

[1] J. Bellessa *et al.*, Phys. Rev. Lett. **93**, 036404 (2004).

HL 23.7 Mon 16:30 TRE Ma

Double Modematching for Metal Nanoantennas — •Thorsten Feichtner[1], Silke Christiansen[2,3], and Bert Hecht[1] — [1]Nano-Optics & Biophotonics Group, Department of Experimental Physics 5, Röntgen Research Center for Complex Material Research (RCCM), Physics Institute, University of Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Freie Universität Berlin, Arnimallee 14, 14195 Berlin — [3]Max Planck Institute for the Science of Light, Günther-Scharowsky-Straße 1, 91058 Erlangen, Germany

The efficient coupling of photons from propagating far-fields to nanoscale volumes is a fundamental problem in quantum optics and at the heart of light-matter interaction. A common model system is the coupling between a point-like two-level quantum emitter (QE) and the continuum of radiative modes, which can be expressed in terms of the frequency-dependent partial local density of states (LDOS) at the QE position. Resonant plasmonic nanoantennas can be designed to strongly localize fields into a small volume leading to a LDOS enhanced by a factor of 10^5 and possibly beyond.

Here a description of power transfer between a QE and an optical antenna resembling a three-dimensional mode matching formalism is developed[1]. After introducing a second dipole in the far-field, another mode-matching step leads to a set of novel optical antenna design guidelines for QE emission enhancement. Accordingly a plasmonic cavity antenna (PCA) geometries is devised and compared to an established dipolar two-wire antenna geometry.

[1] T. Feichtner, S.H. Christiansen, and B. Hecht; arXiv:1611.05399

HL 24: Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - II

Time: Monday 15:00–18:15 Location: GER 38

Invited Talk HL 24.1 Mon 15:00 GER 38

Towards efficient orbital-dependent density functionals for weak and strong correlation — •Igor Ying Zhang[1], Patrick Rinke[1,2], John P. Perdew[3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut, Berlin, Germany — [2]Aalto University, Finland — [3]Temple University, USA

We present a new paradigm for the design of exchange-correlation functionals in density-functional theory [1]. Electron pairs are correlated explicitly by means of the recently developed second order Bethe-Goldstone equation (BGE2) approach [2]. Here we propose a screened BGE2 (sBGE2) variant that efficiently regulates the coupling of a given electron pair. sBGE2 correctly dissociates H_2 and H_2^+, a problem that has been regarded as a great challenge in density-functional theory for a long time [3]. The sBGE2 functional is then taken as a building block for an orbital-dependent functional, termed ZRPS, which is a natural extension of the PBE0 hybrid functional. While worsening the good performance of sBGE2 in H_2 and H_2^+, ZRPS yields a remarkable and consistent improvement over other density functionals across various chemical environments from weak to strong correlation. [1] IY Zhang et al., Phys. Rev. Lett. 117, 133002 (2016); [2] IY Zhang et al., New J. Phys. 18 073026 (2016); [3] AJ Cohen et al., Chem. Rev. 112 289 (2011).

HL 24.2 Mon 15:30 GER 38

Towards a functional for strong correlation via semiclassical model for the indirect energy and local interpolation along the adiabatic connection — •Stefan Vuckovic and Paola Gori-Giorgi — Department of Theoretical Chemistry and Amsterdam Center for Multiscale Modeling, FEW, Vrije Universiteit, De Boelelaan 1083, 1081HV Amsterdam, The Netherlands

Finding an approximate XC functional that is able to capture strong correlation effects is a big, unsolved DFT challenge. Even a bigger challenge is to find a functional able to treat any correlation regime successfully. We attempt to construct an XC functional that has no bias towards a particular correlation regime by using a local interpolation along the adiabatic connection between the weak and the strong coupling limit of DFT. [1] In addition to this approach, I will also present our semiclassical model for accurate indirect energies. I will discuss how this model can be used for a construction of XC functionals, exploiting its XC energy density in the conventional gauge, the one of the electrostatic potential of the XC hole.

1. Stefan Vuckovic, Tom J. P. Irons, Andreas Savin, Andrew M. Teale, and Paola Gori-Giorgi, Journal of Chemical Theory and Computation 2016, 12 (6), 2598-2610

HL 24.3 Mon 15:45 GER 38

Benchmark of *GW* approaches for the *GW*100 test set — •Patrick Rinke[1], Matthias Dauth[2], Fabio Caruso[3], and Michiel van Setten[4] — [1]COMP Centre of Excellence, Aalto University, Finland — [2]University of Bayreuth, Germany — [3]University of Oxford, England — [4]Université Catholique de Louvain, Belgium

Many-body theory in the *GW* approach has become the method of choice for calculating charged excitations in solids. Now it is increasingly being applied to molecules, but fundamental questions regarding its *modus operandi* and its accuracy remain. To address both of these aspects, we present a comprehensive assessment of different *GW* methodologies for the recent *GW*100 test set [1] of molecular ionization energies [2]. We compare our *GW* calculations to coupled-cluster singles, doubles, and perturbative triples [CCSD(T)] reference data for *GW*100. We find ionization energies of fully self-consistent *GW* and quasiparticle self-consistent *GW* in excellent agreement with CCSD(T), with discrepancies typically smaller than 0.3 eV and 0.2 eV, respectively. For partially self-consistent and perturbative *GW* the deviation from CCSD(T) is strongly dependent on the starting point. An optimal starting point is found by minimizing the deviation from the straight-line error [3], which concomitantly yields a systematic improvement of the ionization energies. [1] M. J. van Setten, P. Rinke, *et al.*, J. Chem. Theory Comput. **11**, 5665 (2015), [2] F. Caruso, M. Dauth, M. J. van Setten, and P. Rinke, J. Chem. Theory Comput. **12**, 5076 (2016), [3] M. Dauth, F. Caruso, S. Kümmel, and P. Rinke, Phys. Rev. B **93**, 121115(R) (2016).

HL 24.4 Mon 16:00 GER 38

Addressing electron-hole correlation in core excitations of solids: A first-principles all-electron approach based on many-body perturbation theory — •Christian Vorwerk, Caterina Cocchi, and Claudia Draxl — Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

In the framework of an all-electron implementation of many-body perturbation theory, we investigate K, $L_{2,3}$, and M_4 absorption edges of three exemplary solids, spanning a broad range of transition energies from a few hundred to several thousands eV. We find that transitions from deep core states, such as the Ti 1*s* states in TiO_2 and the Pb 3*d* states in PbI_2, are ruled by the long-range electron-hole attraction. Spin-orbit coupling and local fields play only a minor role for these excitations, which occur at several keV. The exchange interaction between the excited electron and the core hole becomes more relevant for smaller transition energies, as exemplified with the Ca $L_{2,3}$ edge in CaO. The overlap between Ca 2*p* and 3*d* states calls for a careful treatment of local field effects in order to describe these excitations. Our results, in good agreement with the available experimental data, are thoughtfully analyzed with advanced visualization tools in order to further gain insight into the electronic contributions and the spatial extension of the resulting electron-hole pairs.

HL 24.5 Mon 16:15 GER 38

Non-linear-screening contributions to photoemission spectra — •Marilena Tzavala[1,2], Claudia Rödl[1,2,3], and Lucia Reining[1,2] — [1]Laboratoire des Solides Irradiés, École polytechnique, CNRS, CEA, Université Paris-Saclay, 91128 Palaiseau, France — [2]European Theoretical Spectroscopy Facility (ETSF) — [3]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

The state-of-the-art approach to calculate photoemission spectra of a broad range of materials is many-body perturbation theory in the *GW* approximation, sometimes combined with a cumulant expansion. The effective interaction that appears in these approaches is screened within the linear-response approximation. However, the photoemission of a core electron or a localized valence electron may be a strong perturbation, which suggests that non-linear screening effects could be important. We propose a formulation of the functional relations between the one-body Green's function and the screened interaction which is an alternative to Hedin's equations and which explicitly displays non-linear screening. Using a simple model, we show that exchange-correlation contributions are crucial in order to capture the non-linear effects. We also discuss how to apply the scheme to real materials using time-dependent density-functional theory (TDDFT).

HL 24.6 Mon 16:30 GER 38

Dynamic LDA for electronic excitations — •Marco Vanzini[1,2], Matteo Gatti[1,2,3], and Lucia Reining[1,2] — [1]Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA, Université Paris-Saclay, 91128 Palaiseau, France — [2]European Theoretical Spectroscopy Facility (ETSF) — [3]Synchrotron SOLEIL, L'Orme des Merisiers, BP 48 Saint-Aubin, 91192 Gif sur Yvette, France

Density Functional Theory is an extremely useful tool for dealing with ground state properties such as the density or total energy. Kohn–Sham eigenvalues are often considered as approximated electronic excitations, but the resulting spectra are poor.

We propose a generalization of the Kohn–Sham approach to address in an exact framework electron addition and removal spectra. They can be measured by photoemission experiments, and can be evaluated using a computationally expensive non–local Self Energy. Our method is instead based on a frequency–dependent *local* potential [1], which significantly reduces the computing time of an ab–initio calculation.

To find this spectral potential in practice, we propose a jellium–based *dynamical* local density approximation (dynLDA): it relates the unknown potential to its homogeneous counterpart, via a non–trivial connector in space and frequency, which is based on physical insight.

In this talk, I will discuss the achievements and the limits of dynLDA, using models and real solids.

[1] M. Gatti et al., Phys. Rev. Lett. **99**, 057401 (2007).

HL 24.7 Mon 16:45 GER 38

Recent developments of the Sternheimer-GW method — •Martin Schlipf[1], Henry Lambert[1,2], and Feliciano Giustino[1] — [1]Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom — [2]Department of Physics, King's College London, London WC2R 2LS, United Kingdom

The GW many-body perturbation method is an important tool to access accurate band gaps from first principles calculations. The conventional implementation determines the Green's function and the screened Coulomb interaction by a summation over unoccupied states tedious to converge. Giustino et al. demonstrated an alternative method to obtain these quantities by solving Sternheimer linear response equations. In this poster, we present our Sternheimer-GW software implemented in the Quantum Espresso framework and highlight some recent advances regarding the precision and stability of the method. We present our results for a small set of semiconducting materials and compare these to results obtained with conventional GW codes. We illustrate on selected examples the complete frequency dependent self energy, which is a natural product of the Sternheimer-GW method, and can be directly compared to experimental angle-resolved photoemission spectroscopy (ARPES) experiments.

HL 24.8 Mon 17:00 GER 38

Calculating electronic correlations in the CASTEP ab initio code — •Vincent Sacksteder[1] and Evgeny Plekhanov[2] — [1]W155 Wilson Building, Royal Holloway University of London, Egham Hill, Egham, TW20 0EX, — [2]Kings College London

We present new DMFT and GW features in the CASTEP DFT code. These features are designed to provide more accurate treatment of correlations between localized orbitals, of electronic screening, and of excited states. In present benchmarks on Cerium Oxide, the gamma phase of Cerium, and Silicon. We discuss the calculation of atomic forces within the GW framework.

HL 24.9 Mon 17:15 GER 38

Efficient G_0W_0 using localized basis sets: a benchmark for molecules — •Peter Koval[1,2], Mathias Per Ljungberg[1], and Daniel Sánchez Portal[1,2] — [1]Donostia International Physic Center, San Sebastian, Spain — [2]Centro de Fisica de Materiales, San Sebastian, Spain

Electronic structure calculations within Hedin's *GW* approximation are becoming increasingly accessible to the community. In particular, as it has been shown earlier and we confirm by calculations using our **MBPT_LCAO** package [1], the computational cost of the so-called G_0W_0 can be made comparable to the cost of a regular Hartree-Fock calculation. In this work, we study the performance of our new G_0W_0 implementation based on a contour deformation technique to reproduce the ionization potentials of all 117 closed-shell molecules belonging to the G2/97 test set, using a pseudo-potential starting point provided by the popular density-functional package **SIESTA** [2]. Moreover, the ionization potentials and electron affinities of a set of 24 acceptor molecules [3] are compared to experiment and to reference all-electron calculations.

[1] `http://mbpt-domiprod.wikidot.com`; [2] Soler J. M., *etal* J. Phys.: Condens. Matter **14** (2002) 2745; [3] Knight J. W., *etal* J. Chem. Theory Comput., **12** (2016) 615.

HL 24.10 Mon 17:30 GER 38

A dynamic exchange correlation kernel derived from recent results for the homogeneous electron gas — •Martin Panholzer, Matteo Gatti, and Lucia Reining — Laboratoire des Solides Irradies UMR 7642, CNRS-CEA/DSM, Ecole Polytechnique, Palaiseau, France

Time-Dependent Density Functional Theory (TDDFT) is a method of choice to calculate the dynamic structure factor of a wide range of materials. Even in the simplest Adiabatic Local Density Approximation (ALDA), plasmon spectra are generally well described. However, several shortcomings remain. In particular, the onset energy of the spectrum is underestimated [1], and dynamical effects such as lifetime damping and double plasmon excitations are absent [2].

In this work we investigate recent results for the dynamic response of the homogeneous electron gas (HEG)[3] to extract an exchange correlation kernel for TDDFT. In order to get an estimate of the validity of such an approach we compare our results for the dynamic kernel $f_{xc}(q,\omega)$ for the HEG with different kernels and known exact properties. We implemented this kernel with the simplest connection between the HEG and the real material, the mean density approximation. We compare results on simple metals, such as Na and Al, with experiments and ALDA. In order to explore the validity of such an approach we also applied the kernel to Si.

[1] G. Onida et al., Rev. Mod. Phys. 74, 601 (2002)
[2] M. Cazzaniga et al., Phys. Rev. B 84, 075109 (2011)
[3] H. M. Böhm et al., Phys. Rev. B 82, 224505 (2010)

HL 24.11 Mon 17:45 GER 38

Benchmark calculations of the electronic structure for molecules from the second-Born self-energy — •Michael Schüler[1] and Yaroslav Pavlyukh[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle, Germany — [2]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, P.O. Box 3049, 67653 Kaiserslautern, Germany

The non-equilbrium Green's function (NEGF) formalism provides a state-of-the-art tool for modeling modern spectroscopic experiments. In particular, time-dependent problems can be treated based on the Kadanoff-Baym equations. The underlying approximation to the self-energy has to be consistent with the treatment of the initial state - as captured by the Matsubara formalism - in order to guarentee the basic conservation laws. One of simplest non-trivial approximation to the self-energy is the second-Born approximation (2BA), which has been employed in numerous time-dependent studies. Systematic tests on the accuracy of the 2BA for various molecules has, however, been lacking so far. In our contribution we fill this gap by benchmark calculations for the 2BA for small molecules from the well established G2 test set. We demonstrate that the accuracy of the 2BA for predicting ionization potentials and electron affinities can compete with accurate quantum chemistry methods such as the Møller-Plesset perturbation theory and the coupled-cluster method. We also apply our method to a class of larger molecules, the diamonoids, which are in the focus of recent experiments and theoretical studies.

HL 24.12 Mon 18:00 GER 38

Performance of the GW approximation at reproducing key features in exact Kohn-Sham potentials — •Jack Wetherell[1], Leopold Talirz[1], Matt Hodgson[2], and Rex Godby[1] — [1]University of York, York, United Kingdom — [2]Max Planck Institute of Microstructure Physics, Halle, Germany

One of the major goals of the GW method is to improve the accuracy of charge densities produced by density functional theory (DFT). In this work we test the applicability of one-shot GW from various DFT starting Kohn-Sham orbitals. Also we implement and test the fully self-consistent GW method. We test the applicability of these methods by using them to compute densities for simple model 1D systems from which the exact density can be obtained by the direct solution of the Schrodinger Equation. We choose a set of test systems that are either dominated by exchange or correlation, or contain non-local steps in the exact exchange-correlation potential. Also we analyse systems dominated by electronic interaction. We can also investigate how accurate the exchange-correlation potentials associated with the GW densities are, using our reverse-engineering algorithm.

HL 25: Poster: Nitrides

Time: Monday 15:00–19:00 Location: P2-OG2

HL 25.1 Mon 15:00 P2-OG2

In-situ metal deposition for low contact resistance on n-type ZnSe — •Johanna Janssen[1], Torsten Rieger[1], Arne Hollmann[2], Lars Schreiber[2], and Alexander Pawlis[1] — [1]Peter Grünberg Institute 9 and JARA-FIT, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA Institute for Quantum Information, RWTH Aachen University, 52056 Aachen, Germany

As promising for quantum computing, electron spin qubits realized in electrostatically-defined quantum dots (QDs) were studied in GaAs and Si systems. Our goal is to define QDs in the 2D electron gas of ZnSe/(ZnMg)Se quantum wells, as ZnSe combines the advantages of both systems, a direct band gap and nuclear spin-free host lattice. An important parameter is the n-doping profile of ZnSe. We use ex-situ implantation of Fluorine donors to provide quantitative and spatial control of the doping concentration. However, the main challenge is to fabricate ohmic contacts on n-ZnSe. Low contact resistance and a linear current/voltage characteristic even at low temperatures (100 mK) are crucial for charge-based read-out of the QDs. In the context of studies on ZnSe for optoelectronics, the contact metals Al, Mg and In have shown to be suitable candidates for contact fabrication.

Here, we report our studies on the transport characteristics through as-grown ZnSe layers for different doping concentrations, contact metals, and processing techniques such as surface etching or thermal activation. Additional to the mostly performed ex-situ metallization processes, we deposited the metal in-situ to avoid surface oxidation, thus reducing the contact resistance.

HL 25.2 Mon 15:00 P2-OG2

Optoelectronic coupling between colloidal quantum dots and quantum wells — •Mikko Wilhelm, Maria Steiger, Ruichan Lyu, Wolfgang Parak, and Wolfram Heimbrodt — Philipps-Universität Marburg

The interaction between colloidal CdS/ZnS core-shell quantum dots on a semiconductor substrate with buried quantum well is studied. The MBE grown quantum well structures consist of a 5nm thick ZnSe quantum well with a (Zn,Mn)Se barrier of different Mn concentrations. Quantum dots of different sizes have been deposited via spin coating on the surface of the quantum well structure. In order to investigate the energy transfer between the excitons in the quantum dots and the excitons in the quantum wells, cw- and time resolved luminescence measurements as well as photoluminescence excitation measurements have been performed at low temperatures (10K) and external magnetic fields up to 7 Tesla. To reveal the transfer properties the results of the hybrid system will be compared to the separated systems and discussed in detail.

HL 25.3 Mon 15:00 P2-OG2

Optical and magnetic studies of MBE-grown ferromagnetic CrSe and CrS layers in zincblende structure — •Johannes Röder[1], Richard T Moug[2], Kevin A Prior[2], Dana Vieweg[3], Hans-Albrecht Krug von Nidda[3], Alois Loidl[3], and Wolfram Heinbrodt[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 , United Kingdom — [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 time resolved photoluminescence measurements. Ferromagnetic phase transitions have been found. The highest yet observed Curie temperature was at 255 K. Optical measurements revealed excitonic transitions of ZnSe, CrSe as well as the type-II CrSe-ZnSe interlayer transition.

HL 25.4 Mon 15:00 P2-OG2

Characterization of epitaxial graphene nanoribbons (GNR) — •Jantje Schommartz[1,2], Talieh Ghiasi[2], Alexey Kaverzin[2], Johannes Aprojanz[1], Christoph Tegenkamp[1], and Bart J. van Wees[2] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Deutschland — [2]Physics of Nanodevices, University of Groningen, Netherlands

Epitaxially grown graphene nanoribbons (GNR) self-assembled on prestructured SiC nanofacets are recently shown to be single channel ballistic conductor even at room temperature on a length scale greater than ten micrometers [1]. The reported long mean free path, as well as the presence of topologically protected edge states, makes the GNR a subject of intense interest at present. In contrast to GNR, patterned lithographically by etching graphene, epitaxially grown GNR on SiC mesas shows well-defined edge states. In this study, Conductive Atomic Force Microscopy (CAFM) and PeakForce TUNA (PF-TUNA) probe techniques are applied to study the current profile and height profile of both sidewall and natural-step GNR. Compared with the CAFM measurements where the sample and tip are in contact, in the PF-TUNA measurements the sample is oscillating and the tip-sample position is controlled via monitoring the maximum force on the tip which eliminates the lateral forces on the sample. Detection of the electrical current only on the sidewalls and natural steps of the SiC mesa pattern confirms the selective growth of freestanding GNR on SiC nanofacets. [1] Baringhaus et al., Nature 506, 349 (2014)

HL 25.5 Mon 15:00 P2-OG2

***Ab initio* metal-insulator transition in doped silicon** — Edoardo G. Carnio[1], Nicholas D. M. Hine[1], 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 sulfur-doped silicon (Si:S) when the concentration of the dopants is increased. We use linear-scaling DFT, as implemented in the ONETEP code, to study model Si:S systems at realistic concentrations (i.e. a few impurities, in a large simulation cell). We then use the resulting *ab initio* Hamiltonian to build an effective tight-binding Hamiltonian for larger systems close to the critical concentration of the MIT. We finally use multifractal finite-size scaling to characterise the MIT in Si:S, including the *ab-initio*-determined possible interactions between the donated electrons.

HL 25.6 Mon 15:00 P2-OG2

In-situ monitoring of opto-coupler degradation during high energy proton irradiation — •Heinz-Christoph Neitzert[1], Carmine Pellegrino[1], Giovanni Landi[1], Sophie Seidel[2], Jürgen Bundesmann[2], and Andrea Denker[2] — [1]Dept. of Industrial Engineering (DIIn), Salerno University, Via Giovanni Paolo II 132, 84084 Fisciano (SA), Italy — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Protons for Therapy, Hahn-Meitner Platz 1, 14109 Berlin, Germany

The degradation under a high energy proton beam of a series of industrial opto-couplers, consisting of GaAs based LEDs and Silicon phototransistors, has been tested by monitoring ex-situ typical parameters, like current-transfer-ratio, receiver photo-current and -voltage, transistor gain and LED current-voltage characteristics. The devices have been irradiated with a 68 MeV proton beam with different fluences between 10^{11} p+/cm^2 and 10^{13} p+/cm^2. These are typical conditions that are relevant for space missions. In order to distinguish between GaAs emitter degradation and Silicon receiver degradation, the photocurrents of both emitter and receiver diodes have been monitored in-situ during the irradiation. In this way we could verify that the emitter degradation saturates for intermediate irradiation levels of 10^{12} p+/cm^2, while the receiver degradation is continuous and for 10^{13} p+/cm^2 a photocurrent decrease of about 5 orders of magnitude has been found. A beneficial effect of the irradiation in terms of switching speed has been observed, which may be interesting for low-level irradiated devices.

HL 25.7 Mon 15:00 P2-OG2

CW and Pulsed mode Characterization of LED — •Laveen P. Selvaraj, Thomas Hünnerkopf, Matthias Wachs, and Ulrich T. Schwarz — Chemnitz University of Technology, Experimental Sensor Science, Reichenhainer str. 70, 09126 Chemnitz, Germany

Lambertian source LEDs are most commonly used for lighting applications, with an angular intensity distribution following a cosine law with respect to the viewing angle of the emitting surface [1]. The current investigation deals with the characterization of standard Lambertian LED sources using Continuous Wave (CW) and Pulsed mode. In CW mode, a DC bias current was applied to measure the low current range with long source-on time (>0.2 s) with high sensitivity. For high currents, the pulsed mode was used at a low duty cycle to limit heat generation. The total flux emitted was calculated by integrating the peak intensity with Lambert's cosine law. The emission rate in normal direction was determined by a photodiode. We use this setup to measure the standard current-voltage (IV) and current-optical output power (IP) characteristics as reference for other measurements. Non-thermal efficiency droop of LEDs at high currents densities, which is caused by non-radiative recombinations, is observed as well as thermal droop [2]. The effect of heat generation on the IP and IV characteristics can be observed by varying the duty cycle of the pulsed mode at high currents. References: [1] A. Ryer, Light Measurement Handbook. International Light Inc., Technical Publications Department, 1997. [2] E. F. Schubert, Light emitting diodes. Cambridge University Press, 2003.

HL 25.8 Mon 15:00 P2-OG2

Ohmic V-based contacts on n-Al0:8Ga0:2N for deep UV LEDs — •Luca Sulmoni[1], Martin Guttmann[1], Johannes Enslin[1], Christian Kuhn[1], Frank Mehnke[1], Tim Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institut für Festkörperphysik — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Berlin

Minimizing the contact resistance on both p- and n-layers in deep ultraviolet (UV) light emitting diodes (LEDs) is essential for improving the efficiency of these devices suffering from the high operating voltages and resistive heating. Ohmic contacts to n-$Al_xGa_{1-x}N$ are challenging especially for high AlN mole fractions mainly due to the low electron affinity. Standard metal schemes such as Ti/Al/Ti/Au can form ohmic n-contacts only up to about 40% AlN mole fraction. In this study, we investigated the influence of vanadium as first-layer metal in a four-metal electrode V/Al/Ni/Au.

We evaluated the contact characteristics under various annealing conditions. The V/Al/Ni/Au contacts on n-$Al_{0.8}Ga_{0.2}N$ annealed at 800°C under N_2 atmosphere exhibit ohmic characteristics with contact resistivities as low as $8{\cdot}10^{-5}$ Ωcm^2 at a current density of 0.1 kA/cm^2. In contrast, Ti/Al/Ti/Au contacts form rectifying Schottky barriers of about 6 V. We finally demonstrate the fabrication of UVC LEDs emitting at 265 nm using both electrodes. A significant reduction of the operating voltage compared to the standard Ti/Al/Ti/Au electrodes was observed with V_{op} 11 V instead of 21 V at a current of 50 mA.

HL 25.9 Mon 15:00 P2-OG2

Influence of p-AlGaN superlattice and quantum barrier composition on electro-optical characteristics of UVC-LEDs — •Pascal Röder[1], Christian Kuhn[1], Sylvia Hagedorn[2], Arne Knauer[2], Tim Wernicke[1], Markus Weyers[2], and Michael Kneissl[1] — [1]Technische Universität Berlin, Institute of Solid State Physics — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Berlin

Ultraviolet light emitters can be used for the disinfection of water, sterilizing surfaces, and detecting gases such as NO_x and SO_2. However, the external quantum efficiency (EQE) of AlGaN-based LEDs in the UVC wavelength range (200 nm to 280 nm) is still relatively low. In this paper, we investigate the effect of carrier confinement on the EQE of UVC-LEDs emitting near 270 nm.

Electron leakage into the p-side of UVC-LEDs is a major contributor to the low efficiency. In order to investigate the carrier confinement we varied the aluminum content of the quantum barriers and the Mg-doped AlGaN short period superlattice (p-SPSL). The results indicate an intricate interplay of the band offsets of all interfaces. This includes the confinement of electrons in the quantum wells and the electron leakage from the last barrier into p-SPSL.

By improving the carrier confinement UVC-LEDs emitting at 270 nm with an output power of 0.9 mW at 20 mA (EQE 0.95 %, measured on wafer) have been fabricated.

HL 25.10 Mon 15:00 P2-OG2

Simulation of the temporal behavior of LEDs during fast modulation — •Dominic Kunzmann and Ulrich T. Schwarz — Chemnitz University of Technology, Experimental Sensor Science, Reichenhainer Str. 70, 09126 Chemnitz

In blue and green light emitting diodes (LEDs) based on InGaN quantum wells, the strain induced piezoelectric field and the field due to the built-in potential of the p-n junction causes a tilt of the band profile. The consequence is a red-shift of the emission (quantum confined Stark effect, QCSE) and reduction of the wave function overlap and consequently of the radiative recombination rate. Because the field of the p-n junction depends on the bias voltage, the radiative recombination rate can be modulated by the bias. In particular, a faster recombination is observed for zero or reverse bias [1]. This results to a rapid increase in light intensity at the trailing edge of a driving pulse. Here we simulate the temporal behavior of the light emission during modulation with a rectangular driving current. We are interested in the time averaged internal quantum efficiency (IQE). We observe an increase of the IQE for a standard set of LED parameters. The maximum gain of several percent points was observed for driving frequencies of 0.2 GHz to 1 GHz for the chosen parameters.

References: [1] U. T. Schwarz et al., Interplay of built-in potential and piezoelectric field on carrier recombination in green light emitting InGaN quantum wells, Appl. Phys. Lett. 91, 123503 (2007).

HL 25.11 Mon 15:00 P2-OG2

Continuous wave(CW) and Pulsed Characterization of LED — •Laveen Prabhu Selvaraj — Chemnitz University of Technology, 09107 Chemnitz, Germany, Experimental Sensor Science

Lambertian source LED is most commonly used for which states that radiation depends on the viewing angle of the emitting surface [1]. The current investigation deals with the characterization of standard Lambertian sources using CW and pulsed mode. CW mode was used to observe the small changes in low currents by sourcing continuously without switching it off (>0.2 s). To avoid heat generation on high current, source was switched on in regular intervals of time which is between 1 microsecs to 0.25 secs. The DC bias current was applied in two different modes for the characterization of the LED source. The continuous wave mode was used to sweep the LED on low current from 0 to 15 mA. On high currents more than 15 mA, the pulsed mode was used. The total flux emitted can be calculated by integrating the peak intensity with cosine law. The current from the photodiode placed normal to the emitter was used to calculate the peak intensity. The droop in efficiency of LEDs on high currents are caused by non-radiative recombinations [2]. These recombinations result in the heat generation in the LED. The heat generation cause electrical and optical power drop in the LED system. This effect of heat generation can be observed by varying the duty cycle of the Pulsed mode on high currents. References: [1]A. Ryer, Light Measurement Handbook. Newburyport: International Light Inc., Technical Publications Department, 1997. [2]E. F. Schubert, Light emitting diodes.Cambridge University Press, 2003.

HL 25.12 Mon 15:00 P2-OG2

Investigation of crystal properties of epitaxially grown BAlN layers with boron content in the lower percentage range — •Jan-Patrick Scholz[1], Sebastian Bauer[1], Oliver Rettig[2], Yueliang Li[3], Haoyuan Qi[3], Johannes Biskupek[3], Ute Kaiser[3], Ferdinand Scholz[2], and Klaus Thonke[1] — [1]Institute of Quantum Matter / Semiconductor Physics Group, Ulm University, 89081 Ulm, Germany — [2]Institute of Optoelectronics, Ulm University, 89081 Ulm, Germany — [3]Central Facility of Electron Microscopy, Ulm University, 89081 Ulm, Germany

AlGaN based UV-LEDs development is currently in progress. These LEDs still suffer from low external quantum efficiencies. One of the major problems is the high amount of threading dislocations, which emerge mostly due to the lattice mismatch of AlGaN layers on AlN.

Wurtzite BN is expected to have a smaller lattice constant than AlN, what helps to compensate the increase of the lattice constant when adding gallium to AlN.

First samples of AlBN layers on AlN substrate show a big change in surface morphology and luminescence properties: Typically columnar growth is found, and the surface roughness increases. We show cross section TEM micrographs to reveal details about the growth mode. According to SIMS, ~5% boron are incorporated in the AlBN layers.

HL 25.13 Mon 15:00 P2-OG2

Photoluminescence Pumping Characteristics in Ga(N,As,P)/(B,Ga)(As,P) Heterostructures — •Florian Dobener[1], Robin C. Döring[1], Peter Ludewig[2], Wolfgang Stolz[1,2], and Sangam Chatterjee[3] — [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 — [3]Institute of Experimental Physics I, Justus-Liebig-University Giessen, D-35392 Gießen, 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 to the one of Si through the control of nitrogen and phosphorous incorporation, potentially covering the near-infrared regime as well as the telecom wavelength.

Here, we investigate a series of Ga(N,As,P) multiple quantum well samples grown by MOVPE. The well thickness is varied between 1.5 and 9.9 nm. The bandgaps of the quantum-well material and of the barriers are determined by means of wavelength-modulation spectroscopy. Furthermore, photoluminescence excitation experiments reveal which of the layer contributes to the optical emission process. Thereby, some restrictions to the excited carrier injection from the (B,Ga)(As,P) barrier to the Ga(N,As,P) quantum well layer are found depending on the quantum well thickness.

HL 25.14 Mon 15:00 P2-OG2

Conoscopic Investigation of Birefringence in GaN Samples — •Lukas Uhlig, Ines Trenkmann, Matthias Wachs, and Ulrich T. Schwarz — Chemnitz University of Technology, Experimental Sensor Science, Reichenhainer Str. 70, 09126 Chemnitz, Germany

The propagation of light through GaN layers is influenced by birefringence. That means the refractive indices of the ordinary and extraordinary rays are different and depend in the case of the extraordinary one on the angle between the extraordinary ray and the c-axis. Superposition of these both rays leads to a change of the state of polarization compared to the initial ray. This effect can be observed well using the introduced conoscopic experimental setup, where the sample is located between a polarizer and an analyzer, that is rotated by 90°. For uniaxial crystals, like GaN, with the c-axis orientate parallel to the optical axis the observed conoscopic images show concentric rings and a dark "maltese" cross in the middle, wich is called isogyre. We describe a method for the evaluation of the resulting conoscopic pattern and compare these with simulated images using refractive indices $\Delta n = n_e - n_o$ from various studies [1-3].

References: [1] S. Shokhovets, R. Goldhahn and W. Richter, J. Appl. Phys. 94, 307 (2003). [2] G. Yu, H. Ishikawa and M. Umeno, Jpn. J. Appl. Phys. 36, L1029 (1997). [3] S. Ghosh, P. Waltereit and K. H. Ploog, Appl. Phys. Lett. 80, 413 (2002).

HL 25.15 Mon 15:00 P2-OG2

Investigation of electrical conduction mechanisms in Si-doped GaN — •Stefan Kammer[1], Klaus Irmscher[2], Frank Mehnke[1], Tim Wernicke[1], Johannes Enslin[1], Norman Susilo[1], Martin Guttmann[1], Luca Sulmoni[1], Matthias Bickermann[2], and Michael Kneissl[1,3] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Germany — [3]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Gustav-Kirchhoff-Str. 4, 12480 Berlin, Germany

The electronic properties of Si-doped GaN grown by metal-organic vapor phase epitaxy with various doping concentrations were investigated by temperature dependent Hall-effect measurements. In contrast to the commonly described behavior of $n \propto \exp(-E_A/k_B T)$, the data show an increase of the Hall carrier density below 50 K. This implies the presence of multiple conduction mechanisms, requiring a more complex evaluation of the Hall carrier density. For this reason, a model considering carrier densities and mobilities from different conduction mechanisms has been applied in order to extract donor and acceptor concentrations as well as ionization energies from the Hall data. To determine the concentrations of Si and background impurities SIMS measurements have been performed. The influence of donor concentration and the effects of impurity conduction and interface charges on the temperature dependent charge carrier density will be discussed.

HL 25.16 Mon 15:00 P2-OG2

Determination of threading dislocation density of AlN on sapphire substrates by X-ray diffraction — •Daniel Pacak[1], Johannes Enslin[1], Tim Wernicke[1], Sylvia Hagedorn[2], Arne Knauer[2], Carsten Hartmann[3], Heike Oppermann[3], Markus Weyers[2], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik — [3]Leibniz-Institut für Kristallzüchtung, Berlin

AlN on sapphire substrates with low threading dislocation density (TDD) is essential for the growth of efficient UV light emitting diodes. The TDDs of a series of AlN layers on sapphire with different dislocation densities, ranging from $1{\cdot}10^9 \mathrm{cm}^{-2}$ to $2{\cdot}10^{10} \mathrm{cm}^{-2}$ were determined by X-ray diffraction (XRD) by measuring the FWHM of ω-scans for different reflections. For this, we first separated the broadening of the XRD peaks due to finite coherent length and wafer curvature from the broadening by tilt and twist. Then the tilt and twist contributions were determined by two different approaches. One method was based on obtaining the tilt value by measuring a reflection in asymmetric geometry and calculating the corresponding twist value. In a second approach the tilt and twist components were determined by extrapolating the FWHM against the χ-angle. From these tilt and twist values we calculated the TDDs for correlated and randomly distributed dislocations, based on the models of Chierchia et al. and Dunn & Kogh. Finally we compared the TDD obtained by XRD with the results from defect selective etching.

HL 25.17 Mon 15:00 P2-OG2

Light extraction in UVC LEDs grown on ELO AlN/sapphire templates — •Sarina Graupeter[1], Martin Guttmann[1], Frank Mehnke[1], Christian Kuhn[1], Tim Wernicke[1], Mickael Lapeyrade[2], Arne Knauer[2], Sven Einfeldt[2], Markus Weyers[2], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Berlin

Light emitting diodes (LEDs) in the UVC spectral range have various promising applications, e.g. gas sensing and water disinfection. However, the external quantum efficiency strongly decreases with decreasing emission wavelength. This can be partly explained by a reduced light extraction efficiency (LEE) due to an increasingly transverse magnetic polarized emission, with increasing Al content and total reflection at the AlN/sapphire interface. In this contribution, we investigate UVC LEDs using epitaxially laterally overgrown (ELO) AlN on patterned sapphire substrates, which can potentially increase the LEE due to photon redirection. The emission wavelength and the optical polarization has been varied by adjusting the aluminium content in the quantum wells, thus changing the optical polarization. Using ray tracing simulations and measurements of the far field pattern the emission has been studied in dependence of the optical polarization and the ELO geometry. Both, simulation and experiment, show that the influence of the optical polarization on the far field is negligible. However, the ELO geometry has significant influence on the far-field pattern enabling new pathways for the improvement of light extraction.

HL 25.18 Mon 15:00 P2-OG2

Investigation of AlGaN multiple quantum wells for deep ultraviolet emission using temperature and excitation power density dependent photoluminescence spectroscopy — Christoph Reich, •Baran Avinc, Johannes Enslin, Norman Susilo, Christian Kuhn, Tim Wernicke, and Michael Kneissl — Technische Universität Berlin, Institute of Solid State Physics

Light emitting diodes in the deep UV spectral region have various interesting applications, e.g. gas sensing or water disinfection. However, the output power and performance of devices emitting in the UVC (200 nm - 280 nm) spectral region are poor compared to devices emitting at longer wavelenghts. This low external quantum efficiency in the UVC spectral region can be explained by the challenging carrier injection and lower internal quantum efficiency as well as a reduced light extraction due to a switching of the optical polarization from TE (transverse electric) to TM (transverse magnetic) for decreasing emission wavelengths. Using temperature and excitation power density dependent photoluminescence spectroscopy, we investigated the influence of the AlGaN-based multiple quantum well (QW) active region design on the internal quantum efficiency, the quantum confined Stark effect, and the radiative recombination processes. In a systematic study, the QW width as well as the aluminum contents in the QWs and barriers have been varied. The measured photoluminescence results will be compared with simulations based on $\mathbf{k} \cdot \mathbf{p}$-perturbation

theory including a discussion of the influence of the QW design on the optical polarization.

HL 25.19 Mon 15:00 P2-OG2

Impact of a SiN surface layer on the core-shell growth of InGaN quantum wells around GaN microrods — •Christian Tessarek[1,2], Stefanie Rechberger[3], Christel Dieker[3], Martin Heilmann[2], Erdmann Spiecker[3], and Silke Christiansen[1,2,4] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH — [2]Max-Planck-Institut für die Physik des Lichts, Erlangen — [3]Friedrich-Alexander-Universität Erlangen-Nürnberg, Institut für Mikro- und Nanostrukturforschung & Center for Nanoanalysis and Electron Microscopy (CENEM) — [4]Physics Department, Freie Universität Berlin

GaN microrods were grown by metal-organic vapor phase epitaxy (MOVPE) using a self-catalyzed and Si-induced growth mode [1]. Spontaneous formation of SiN on the surface of microrods leads to enhanced vertical growth due to the antisurfactant and stabilization effect of SiN [2]. Core-shell growth of InGaN multiple quantum wells with GaN barriers is carried out on microrods with different growth times and thus different heights. Microrods with a short growth time are completely covered with an InGaN shell. For microrods with an extended height the InGaN shell only forms at the upper part leaving the lower part free of any deposition. Based on structural investigations including transmission electron microscopy a growth model will be proposed to explain this behaviour. Furthermore, optical properties of the different core-shell structures will be discussed.

[1] C. Tessarek et al., J. Appl. Phys. **114**, 144304 (2013).
[2] C. Tessarek et al., Cryst. Growth Des. **14**, 1486 (2014).

HL 25.20 Mon 15:00 P2-OG2

The effective potential energy drop as a control parameter for the sheet carrier density of two-dimensional electron gases in AlGaN/GaN heterostructures — •Dennis Mauch, Heiko Bremers, Uwe Rossow, and Andreas Hangleiter — Institut für Angewandte Physik, TU Braunschweig, Germany

We introduce the effective potential energy drop in AlGaN/GaN heterostructures as a control parameter for the sheet carrier density of two-dimensional electron gases (2DEG). As a consequence of the non-centrosymmetry of the wurtzite structure in group-III nitrides and the large ionicity factor of the covalent metal-nitrogen bond, a large spontaneous polarization is oriented along the hexagonal c-axis. In addition, group-III nitrides are highly piezoelectric. Hence, in AlGaN/GaN heterostructures, where the AlGaN layer is grown pseudomorphically on top of GaN, strain leads to piezoelectric polarization in the AlGaN epitaxial layer. Under certain conditions, the induced electric fields, due to polarization discontinuity at the heterointerface, give rise to the formation of a 2DEG. We also investigated the influence of an additional AlN-interlayer at the AlGaN/GaN interface in order to reduce alloy disorder scattering and thus to reach higher 2DEG mobilities. The samples were grown in our commercial MOVPE system/reactor on c-oriented sapphire substrates. The electrical properties were obtained via Hall effect measurements at room temperature using the van der Pauw configuration, and the structural details via HR-XRD. Our aim is to optimize these structures to highest mobilities and small sheet carrier densities down to the quantum Hall regime.

HL 25.21 Mon 15:00 P2-OG2

Formation of I2-type basal-plane stacking faults in In0.25Ga0.75N multiple quantum wells grown on a (10-11) semipolar GaN template — •yueliang li[1], haoyuan qi[1], tobias meisch[2], matthias hocker[3], klaus thonke[3], ferdinand scholz[2], and ute kaiser[1] — [1]Central Facility of Electron Microscopy, Electron Microscopy Group of Materials Science, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany — [2]Institute of Optoelectronics, Ulm University, Albert-Einstein-Allee 45, 89081 Ulm, Germany — [3]Institute of Quantum Matter, Ulm University, Albert-Einstein-Allee 45, 89081 Ulm, Germany

InGaN/GaN heterostructures grown on semipolar GaN templates have received considerable attention over the past years for the fabrication of LEDs operating in the green spectral range. However, the quantum efficiency is still substantially lower than that of their blue counterparts due to the defects such as dislocations and stacking faults, which appear during the growing process.

In this work, I2-type basal stacking faults were observed in In0.25Ga0.75N multiple quantum wells grown on a (10-11) GaN template by HRTEM. The structure and formation mechanism of the I2-type stacking faults were investigated. The relationship between the In content in the InGaN layer and the density of the I2-type stacking faults is discussed.

HL 25.22 Mon 15:00 P2-OG2

Epitaxial growth and characterization of thin AlBGaN layers with low boron content — •Natja Steiger[1], Jan-Patrick Scholz[1], Sebastian Bauer[1], Oliver Rettig[2], Tomáš Hubáček[2], Haoyuan Qi[3], Yueliang Li[3], Johannes Biskupek[3], Ute Kaiser[3], Ferdinand Scholz[2], and Klaus Thonke[1] — [1]Institut of Quantum Matter/ Semiconductor Physics Group, Ulm University, 89081 Ulm, Germany — [2]Institute of Optoelectronics, Ulm University, 89081 Ulm, Germany — [3]Central Facility of Electron Microscopy, Ulm University, 89081 Ulm, Germany

The development and design of efficient LEDs for the ultraviolet regime is of great interest, aiming at applications like water purification and sterilization. Using AlGaN as material for such an ultraviolet solid-state light source, the desired emitted wavelength can be chosen by variation of relative Al/Ga content. We try to incorporate boron into this material to reduce the lattice mismatch between the optically active AlBGaN layer and AlN barrier layer of the QWs. Lattice matching leads to a reduction of QCSE caused by strain.

Our AlBGaN thin layers are grown by MOVPE on AlN templates with sapphire as substrate at growth temperatures up to 1400°C. To examine the crystal structure and quality X-ray diffraction, scanning- and transmission electron microscopy and atomic force microscopy are performed. By exciting the samples with an ArF-laser, photoluminescence spectroscopy is used for further characterization of the samples.

HL 25.23 Mon 15:00 P2-OG2

Angular dependence of the Raman scattering intensity of optical phonons in wz-GaN — •Simon Brehm, Christian Röder, Cameliu Himcinschi, and Jens Kortus — TU Bergakademie Freiberg, Institute of Theoretical Physics, Leipziger Str. 23, D-09599 Freiberg, Germany

Gallium nitride (GaN) as one of the most promising wide-bandgap semiconductors has been studied intensively over the two last decades due to its numerous opto- and microelectronic applications. In this work, the angular dependence of the Raman scattering intensity of optical phonon modes was investigated in backscattering geometry using an a-plane oriented GaN thin film. For this purpose, two experimental approaches were realized as the observed Raman scattering intensity is connected with the scattering geometry by the so-called Raman tensor elements. At first the GaN sample was turned in-plane with respect to the laboratory coordinate system while the polarization directions of exciting and scattered light remained the same. Secondly, sample and position of the analyzer were fixed with respect to the laboratory coordinate system and the polarization direction of the incident laser beam was rotated. Using relative Raman scattering cross sections [1] the experimental results were found to be in an excellent agreement with theoretical simulations.

This work is financially supported by the European Union (European Social Fund) and by the Saxonian Government (grant no. 100231954).
[1] Irmer et al. J. Appl. Phys. **116** (2014) 245702

HL 25.24 Mon 15:00 P2-OG2

Optical biosensing with InGaN/GaN quantum wells — •Benedikt Hörbrand[1], Sabyasachi Chakrabortty[2], Martin Schneidereit[3], Dominik Heinz[3], Sebastian Bauer[1], Florian Huber[1], Tanja Weil[2], Ferdinand Scholz[3], and Klaus Thonke[1] — [1]Institute of Quantum Matter / Semiconductor Physics Group, Ulm University, 89081 Ulm, Germany — [2]Institute of Organic Chemistry III, Ulm University, 89081 Ulm, Germany — [3]Institute of Optoelectronics, Ulm University, 89081 Ulm, Germany

Sensing biomolecules is essential in the fields of medicine, pharmacy and biotechnology. Normally it goes along with previous preparation steps like labelling of the molecules. To avoid these complex preparation processes we are aiming at a detection of such molecules using pre-treated semiconductor surfaces. The optical emission of surface-near polar InGaN/GaN quantum well layers reacts on the attachment of biomolecules to the surface.

The surface-near band bending is changed by the deposition of biomolecules like ferritin, which are adsorbed on a functionalized layer on the surface. As a result the emitted wavelength and intensity of the emission changes, depending on the biomolecule.

HL 26: Focussed Session: Frontiers in Exploring and Applying Plasmonic Systems II (Joint Session of CPP, DS, HL, MM, and O, organized by DS)

With the increasing importance of plasmonics and the variety of its number of applications it becomes obvious that experimental characterization beyond the far-field optical standard methods and also theoretical tools that access the plasmonic behaviour on the atomic scale are indispensable for further development and improvement of the basic knowledge and thus, for new kinds of applications. The "Focused Session" gathers experts for unusual experimental methods (near-field studies with SNOM and EEL-TEM) and for the theoretical exploration of quantum effects in plasmonic excitations. Furthermore, new kinds of plasmonic applications (devices exploiting phase changes, alternative displays and holograms) will be introduced.

Organizers: Laura NaLiu (U Heidelberg) and Annemarie Pucci (U Heidelberg)

Time: Monday 16:30–17:15 Location: CHE 89

HL 26.1 Mon 16:30 CHE 89

Strong Coupling between Phonon-Polaritons and Plasmonic Nanorods — •Christian Huck[1], Jochen Vogt[1], Tomáš Neuman[2], Tadaaki Nagao[3], Rainer Hillenbrand[4,5], Javier Aizpurua[2], Annemarie Pucci[1], and Frank Neubrech[1,6] — [1]Kirchhoff Institute for Physics, Heidelberg, Germany — [2]Materials Physics Center (CSIC-UPV/EHU) and Donostia International Physics Center (DIPC), Donostia-San Sebastián, Spain — [3]WPI Center for Materials NanoArchitectonics, National Institute for Materials Science, Tsukuba, Japan — [4]CIC nanoGUNE and UPV/EHU, Donostia-San Sebastián, Spain — [5]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — [6]4th Physics Institute, Stuttgart, Germany

We perform far-field spectroscopy of metal nanoantennas, resonant in the infrared spectral region, placed on silicon oxide (SiO_2) layers of different thickness. Due to strong coupling between the plasmonic excitation of the metal antenna plasmons and the surface phonon-polaritons of thin SiO_2 layers a splitting of the plasmonic resonance is found in the respective spectra. Although the phonon-polaritons themselves are dark excitations under normal illumination, they strongly interact with plasmon-polaritons as we detailed for a planar SiO_2 layer beneath the nanostructures. The observed splitting can result in a transparency window, corresponding to suppression of antenna scattering, respectively "cloaking" of the antenna. The effect is a kind of induced transparency in which the strength of the phonon-polariton field plays the crucial role. It represents a further tuning possibility for the optical performance of infrared devices.

HL 26.2 Mon 16:45 CHE 89

Enhanced Infrared Spectroscopy of Single Small Fine Dust Particles with Resonant Plasmonic Nanoslits — •Jochen Vogt[1], Sören Zimmermann[2], Christian Huck[1], Michael Tzschoppe[1], Frank Neubrech[1,3], Sergej Fatikow[2], and Annemarie Pucci[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Heidelberg, Germany — [2]Division Microrobotics and Control Engineering, University of Oldenburg, Oldenburg, Germany — [3]4th Physics Institute, University of Stuttgart, Stuttgart, Germany

Guiding the way towards dust sensing devices based on surface-enhanced infrared (IR) absorption (SEIRA), our study demonstrates the potential of plasmonic nanostructures for chemically specific identification of single tiny fine dust particles. The model system under investigation consists of individual silica spheres with diameters below 240 nm placed at defined positions in resonant plasmonic nanoslits. With dimensions far below the wavelength, direct IR spectroscopic measurements of such particles are not possible in reasonable time scales. In our SEIRA setup, the characteristic phononic particle excitations of the silica spheres are enhanced by the strong near-field of the plasmonic nanoslits, which enables the IR spectroscopic identification of individual particles. The SEIRA signal enhancement of single particles at various positions along the nanoslit structure fully corresponds to the near-field enhancement profile of these structures with the optimal position for SEIRA sensing to be located at sites towards the slit middle.

HL 26.3 Mon 17:00 CHE 89

Transverse and Longitudinal Resonances in Plasmonic Gold Tapers — Surong Guo[1], Nahid Talebi[1], Wilfried Sigle[1], Ralf Vogelgesang[2], Gunther Richter[3], Martin Esmann[2], Simon F. Becker[2], Christoph Lienau[2], and •Peter A. van Aken[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Carl von Ossietzky University of Oldenburg, Oldenburg, Germany — [3]Max Planck Institute for Intelligent Systems, Stuttgart, Germany

Conically-shaped metallic tapers are one of the most common structures with concomitant capabilities of nanofocusing and field enhancement. We distinguish two different dynamic mechanisms, reflection and phase matching, of surface plasmons excited by relativistic electrons in three-dimensional gold tapers with various opening angles from 5° to 47° which are studied both experimentally and theoretically, by means of electron energy-loss spectroscopy and finite-difference time-domain numerical calculations, respectively. We observe distinct resonances along the taper shaft independent of opening angles. We show that the origin of these resonances is different at different opening angles and results from a competition between two coexisting mechanisms. For large opening angles ($> 20°$), phase matching between the electron field and that of higher-order angular momentum modes is the dominant contribution because of the increasing interaction length between electron and the taper near-field. In contrast, reflection from the taper apex dominates at small opening angles ($< 10°$). A gradual transition of these two mechanisms is observed for intermediate opening angles.

HL 27: Plasmonics and Nanooptics III: Light-Matter Interaction

Time: Monday 17:00–18:30 Location: TRE Ma

HL 27.1 Mon 17:00 TRE Ma

Momentum distribution of hot electrons in resonantly excited gold nanorods revealed by time of flight k-resolving photoemission spectromicroscopy — •Martin Lehr[1], Benjamin Foerster[2,3], Katja Krüger[2], Mathias Schmitt[2], Carsten Sönnichsen[2], Gerd Schönhense[1], and Hans Joachim Elmers[1] — [1]Institut für Physik, Johannes Gutenberg-Universität, Staudinger Weg 7, D-55128 Mainz, Germany — [2]Institut für physikalische Chemie, Johannes Gutenberg-Universität, Duesbergweg 10-14, D-55128 Mainz, Germany — [3]Graduate School for Excellence Materials Science in Mainz, Johannes Gutenberg University Mainz, Staudingerweg 9, D-55128 Mainz, Germany

We investigate plasmon assisted photoemission from individual Au nanorods using a time-of-flight momentum resolving photoemission electron microscope (ToF k-PEEM). The Au nanorods are taylored to obtain a localized plasmon polartion resonance wavelength of 800 nm with a linewidth of just 44 nm. The Au nanorods adhere to a transparent In-Sn oxide substrate enabling illumination from the rear side at normal incidence. The two momentum components parallel to the surface and the kinetic energy of the electrons are measured simultaneously. Both properties depend on laser power and polarization confirming a plasmon assisted emission process mediated by the optical field enhancement at the nanorod's ends. The exponential intensity decrease of emitted electrons with increasing kinetic energy reveals the distribution of hot electrons leading to an additional emission process with a characteristic homogeneous momentum distribution.

HL 27.2 Mon 17:15 TRE Ma

Plasmon polaritons in cubic lattices of interacting metallic nanoparticles — •Simon Lamowski[1], Felicitas Hellbach[1], Eros Mariani[2], Guillaume Weick[3], and Fabian Pauly[1] — [1]Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — [2]Centre for Graphene Science, Department of Physics and Astronomy, University of Exeter, Stocker Rd. EX4 4QL Exeter, UK — [3]Institut de Physique et Chimie des Matériaux de Strasbourg, Université de Strasbourg, CNRS UMR 7504, F-67034 Strasbourg, France

We investigate theoretically plasmon polaritons in cubic lattices of interacting spherical metallic nanoparticles [1]. Dipolar localized surface plasmons on each nanoparticle couple through the near field dipole-dipole interaction and form collective plasmons, which extend over the whole metamaterial. Coupling these collective plasmons in turn to photons leads to plasmon polaritons. We derive within a quantum model general semi-analytical expressions to evaluate both plasmon and plasmon-polariton dispersions that fully account for nonlocal effects in the dielectric function of the metamaterial. Within this model, we discuss the influence of different lattice symmetries and predict related polaritonic gaps within the near-infrared to the visible range of the spectrum that depend on wavevector direction and polarization.

[1] S. Lamowski, F. Hellbach, E. Mariani, G. Weick, and F. Pauly, arXiv:1606.04897.

HL 27.3 Mon 17:30 TRE Ma

Relaxation of single and collective electron excitations investigated with time- and energy-resolved PEEM — •Michael Hartelt[1], Anna-Katharina Mahro[1], Tobias Eul[1], Benjamin Frisch[1], Philip Thielen[1], Deirdre Kilbane[1,2], Mirko Cinchetti[1,3], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, Germany — [2]School of Physics, University College Dublin, Ireland — [3]Experimentelle Physik VI, Fakultät Physik, TU Dortmund, Germany

The generation of hot carriers through the internal decay of plasmons in metallic materials has received considerable attention lately, due to its wide range of potential applications [1]. Understanding the differences between photoinduced and plasmon-induced hot electrons is essential for the construction of devices for plasmonic energy conversion. To distinguish between the two processes, it is advantageous to make use of the time-resolved 2-photon-photoemission (TR-2PPE) method that is an established tool for the study of hot electron lifetimes [2] in combination with Photoemission Electron Microscopy (PEEM). This allows us to study hot electron dynamics on the femtosecond and nanometer scale by analyzing the energy distribution and relaxation dynamics of the photoemitted electrons. Here, we present first results of time and energy resolved PEEM (TR-ER-PEEM) measurements of localized and propagating plasmons (LSP and SPP) with focus on the relation between spectral features and local near-field distributions.

[1] Brongersma et al., Nature nanotechnology 10.1 (2015)
[2] M. Bauer et al., Progress in Surface Science 90, 319 (2015)

HL 27.4 Mon 17:45 TRE Ma

Parallel mapping of optical near-field interactions by molecular motor-driven quantum dots — Friedrich W. Schwarz[1], Hannah S. Heil[1], Heiko Gross[2], •Jens Ehrig[1], Bert Hecht[2], and Stefan Diez[1] — [1]B CUBE & cfaed, Technische Universität Dresden — [2]Nano-Optics and Biophotonics Group, Universität Würzburg

Absorption and emission rates of photons by quantum emitters strongly depend on the emitters' local environment. This enables the precise control of light–matter interactions, essential for the development of future opto-electronics devices. The design, characterization and optimization of such devices requires high-resolution, yet high-speed and non-invasive tools that allow the nm-precise mapping of the involved optical near-field interactions. Toward this end, we investigate the near-field interaction of optical dipole emitters with nanostructures by recording the fluorescence intensity of quantum dots attached to microtubules being transported across the nanostructure by molecular motors. The power of this parallel approach to near-field imaging is demonstrated by the nm-precise mapping of near-field interactions between individual quantum dots and nanoslits of 110 to 240 nm widths engraved in 25 nm gold layers. The results of these measurements are in excellent agreement with finite-difference time-domain simulations. Thus, by using a minimalistic biomolecular machinery, we are able to perform parallel superresolution mapping of near-field interactions in a virtually artifact-free fashion. We foresee broad applications, such as large-scale multi-probe imaging of meta-surfaces to further the understanding of light-matter interactions.

HL 27.5 Mon 18:00 TRE Ma

Adaptive spatial resolution in the 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

Optical devices based on nanostructures have many applications in different fields. For example, it has been shown that photonic crystal slabs can be used to control the polarization state emitted by quantum emitters [1]. One very efficient numerical method to model the optical properties of photonic crystal slabs and periodic arrays of nanoantennas is the Fourier modal method. However, due to the underlying Fourier basis, the Fourier modal method suffers from the Gibbs phenomenon, which results in spurious oscillations of the electromagnetic near fields around interfaces between different materials.

As an alternative to the Fourier basis, we have implemented a finite-difference basis for modal methods based on the approach in [2] and combined it with the coordinate transformation methods that are well-established in the standard Fourier modal method [3]. Thus, we have achieved significantly better convergence of the electromagnetic near fields as compared to the standard Fourier modal method as well as the finite difference modal method without coordinate transformations.

[1] S. V. Lobanov et al., Opt. Letters **40**, 1528 (2015).
[2] I. Semenikhin and M. Zanuccoli, JOSA A **30**, 2531 (2013).
[3] T. Weiss et al., Opt. Express **17**, 8051 (2009).

HL 27.6 Mon 18:15 TRE Ma

Strong Coupling of Single Excitons to Curved Optical Nanostructures — •Daniel Hernangómez-Pérez[1,2], Rui-Qi Li[2,3], Francisco José García-Vidal[2,4], and Antonio I. Fernández-Domínguez[2] — [1]Institute of Theoretical Physics, University of Regensburg, D-93050 Regensburg, Germany — [2]Departamento de Física Teórica de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [3]Key Laboratory of Modern Acoustics, MOE, Institute of Acoustics, Department of Physics, Nanjing University, Nanjing 210093, People's Republic of China — [4]Donostia International Physics Center (DIPC), E-20018 Donostia/San Sebastián, Spain

We systematically analyze plasmon-exciton coupling for a quantum

dot situated in-between two nanoparticles. To that purpose, we employ a systematic quasi-analytical approach inspired by transformation optics, which allows us to study the impact of geometry and material configurations in the quantum dynamics. We show that the coupling to multipolar dark modes close to the plasmon resonances allows to enter into a regime wheret the dynamics can be reversible and compare our findings to recent experiments. The findings presented here may serve as a guidance to additional future experiments and for the development of new quantum plasmonic devices. References: PRL 117, 107401 (2016), Nature 535, 127 (2016)

HL 28: Poster: Fundamentals of Perovskite Photovoltaics (joint session CPP, DS, HL)

Time: Monday 18:30–21:00 Location: P1A

HL 28.1 Mon 18:30 P1A

Hybrid photovoltaics based on diblock copolymer structured, mesoporous Ge thin films — •Andreas Hetzenecker[1], Nuri Hohn[1], Michael Giebel[2], Thomas F. Fässler[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]TU München, Chemie-Department, LS Anorganische Chemie mit Schwerpunkt Neue Materialien, Lichtenbergstr. 4, 85748 Garching

Hybrid photovoltaics opens new possibilities in solar cell design, combining the mechanical stability and high charge carrier mobility of semiconductors with the potentially cost-efficient, large scale production and flexibility of organic materials. The usage of poly(styrene-b-ethylene oxide) as a template and K_4Ge_9 Zintl clusters as an inorganic precursor [1] for sol-gel synthesis is a novel approach to produce mesoporous germanium structures. This method offers control over pore size and degree of porosity via the block lengths of the template and the reactant concentrations. Sponge-like germanium thin films were synthesized and characterized regarding their absorption behavior with UV/Vis spectroscopy. Structural analysis was performed via SEM and profilometry.

[1] M. M. Bentlohner et al., Angewandte Chemie International Edition, 55, 2441-2445 (2015).

HL 28.2 Mon 18:30 P1A

Ultrafast charge and exciton dynamics in $CH_3NH_3PbI_3$ — •Kestutis Budzinauskas[1], Yajun Gao[1], Elina Patsikatheodorou[1], Tobias Schneider[2], Selina Otlhof[2], Klaus Meerholz[2], and Paul H.M van Loosdrecht[1] — [1]University of Cologne, II physics institute — [2]University of Coglogne, Institute of chemical physics

Solar cells based on organic-inorganic perovskite semiconductors show a surprisingly high conversion effciency. Despite tremendous progress in the field of perovskite based devices, the fundamental photophysics responsible for the good performance are still not well understood. In order to obtain a better insight of the charge separation and recombination dynamics in these materials we have performed ultrafast time resolved absorption experiments in the VIS/NIR spectral range on pure MAPbI$_3$ (CH_3 NH_3PbI_3) films, as well as on multilayer systems which use PEDOT:PSS and $PC_{61}BM$ as charge selective extraction layers. Our experiments allow to selectively monitor diffusion and recombination processes as well as interfacial charge transfer and the formation of interfacial charge transfer states with a sub-100 fs time resolution

HL 28.3 Mon 18:30 P1A

Ultrafast charge and exciton dynamics in $CH_3NH_3PbI_3$ — •Kestutis Budzinauskas[1], Yajun Gao[1], Elina Patsikatheodorou[1], Tobias Schneider[2], Selina Otlhof[2], Klaus Meerholz[2], and Paul H.M. van Loosdrecht[1] — [1]University of Cologne, II physics institute — [2]University of Cologne, Institute of chemical physics

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HL 28.4 Mon 18:30 P1A

morphology evolution of titania films during in situ spray coating for perovskite solar cells — •Bo Su[1], Herbert A. Caller-Guzman[1], Volker Körstgens[1], Yichuan Rui[2], Yuan Yao[1], Stephan V. Roth[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]College of Chemistry and Chemical Engineering, Shanghai University of Engineering Science, Shanghai 201620, P. R. China — [3]DESY, Notkestr. 85, 22607 Hamburg, Germany

We combine a sol-gel route with spray coating to obtain porous titania films. Spray coating is used as deposition method since it is allowing for scaling-up to large scale production. A block copolymer template assisted sol-gel process is used to form nanostructured titania films. The structure evolution is probed with in situ GISAXS during the spray coating process, enabling the detection of characteristic length scales during fabrication. The morphology of the sprayed films is characterized ex-situ with SEM, TEM and optical microscopy as well. In addition, the crystalline structure of the titian films is probed with XRD. The perovskite solar cells based on sprayed titania films are characterized under AM 1.5G standard condition. We extract a structure-function relationship for different spray parameters.

HL 28.5 Mon 18:30 P1A

Influence of processing parameters on the morphology of perovskite solar cells — •Armin Schreiber, Johannes Schlipf, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Over the last decade, especially lead halide perovskites as an organic-inorganic hybrid compound received attention due to the exceptional rise in the power conversion efficiency (PCE) of research cells from 3.8 % in 2009 to more than 20 % in early 2016. The most common active layer material is methylammonium lead iodide (MAPbI$_3$). It can be fabricated using a solution conversion method consisting of firstly spin-coating lead iodide (PbI_2) and secondly immersing it in a solution of dissolved methylammonium iodide. This leads to strong preferential crystal orientations as evidenced by grazing-incidence small angle X-ray scattering (GIWAXS) measurements. The crystal orientation is tunable via temperature variation of precursors of the perovskite and the use of additives into the precursor or conversion solution [1]. We expand this study by the use of mixed solvent approaches with processing additives in order to further tune the time scales of the crystallization processes and gain more control of the film morphologies of perovskite thin films as well as improving the reproducibility and long-term stability.

[1] L. Oesinghaus et al., Adv. Mater. Interfaces 2016, 1600403

HL 28.6 Mon 18:30 P1A

Morphology of Perovskite-Based Hybrid Solar Cells — •Kiran Mathew John, Johannes Schlipf, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Organometal halide perovskites, have been shown to be great candidates for photovoltaics, owing to the strong solar absorption and the high mobility and low recombination rates of photo-generated charge carriers in these compounds. Subsequently, solar cells made from perovskites have reached efficiencies of more than 20%, making them comparable with commercially available silicon solar cells. The performance of the perovskite cells greatly depend on their crystal morphology. We fabricate and characterise different cells by varying processing parameters including film deposition methods, annealing temperature and solvent media. By means of X-ray scattering methods, we gain insight into the inner film morphology and thus are able to correlate morphology and photovoltaic performance, with the target to get better fundamental understanding.

HL 28.7 Mon 18:30 P1A

Polarisation resolved optical spectroscopy of single CsPbI3 nanocrystals — •Mirko Goldmann[1,2], Daniela Täuber[1,5], Juanzi Shi[1], Junsheng Chen[3], Maria E. Messing[4,5], Kaibo Zheng[3], and Ivan G. Scheblykin[1,5] — [1]Single molecule spectroscopy group, Lund University, Sweden — [2]TU Ilmenau, Germany — [3]2D spectroscopy group, Lund University, Sweden — [4]Solid State Physics, Lund University, Sweden — [5]NanoLund, Lund University, Sweden

Semiconducting metal halide nanocrystals are promising candidates for optoelectronic devices due to their high quantum yield and solution processability. Fully inorganic $CsPbI_3$ is more stable than $CH_3NH_3PbI_3$. Polarization resolved optical spectroscopy of single $CsPbI_3$ nanocrystals probes their cubic crystal structure and sperical shapes. Photoluminescence emission from freshly synthesized $CsPbI_3$ nanocrystals was found to be almost unpolarized. Several weeks old nanocrystals showed an increased appearance of polarized photoluminescence in agreement with the observation of elongated crystal shapes by TEM.

HL 28.8 Mon 18:30 P1A

Gold cluster growth kinetics at the metal-polymer interface of water-processed hybrid solar cells studied by in-situ GISAXS sputter deposition — •Adrian Haussmann[1], Volker Körstgens[1], Franziska Löhrer[1], Martin Wörle[2], Hristo Iglev[2], Reinhard Kienberger[2], Matthias Schwartzkopf[3], Alexander Hinz[4], Oleksandr Polonskyi[4], Thomas Strunskus[4], Franz Faupel[4], Stephan V. Roth[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]TU München, Physik-Department, LS Laser- und Röntgenphysik, James-Franck-Str. 1, 85748 Garching — [3]DESY, Notkestr. 85, 22607 Hamburg — [4]CAU Kiel, Institut für Materialwissenschaft, Kaiserstr. 2, 24143 Kiel

In this work the metal-polymer interface between gold contact and active layer of water-processed hybrid solar cells is investigated. The active layer consists of an aqueous soluble polythiophene and laser-ablated titania nanoparticles. Gold sputter deposition is applied to the active layer. To obtain full information of gold cluster growth kinetics during sputter process, in-situ time resolved grazing incidence small angle X-ray scattering (GISAXS) experiments and grazing incidence wide angle X-ray scattering (GIWAXS) are carried out. Different growth regimes of gold clusters are observed from the GISAXS and GIWAXS data analysis and discussed.

HL 28.9 Mon 18:30 P1A

Reduction of Hysteresis through PCBM in Planar Perovskite Solar Cells — •Yu Zhong[1], Carlos Andres Melo Luna[2], Richard Hildner[2], Cheng Li[1], and Sven Hüttner[1] — [1]Organic and Hybrid Electronics, Macromolecular Chemistry I, University of Bayreuth — [2]Experimental Physics IV, University of Bayreuth, Germany

Despite the development of organometal perovskite in solar cells, some problems still restrict its large-scale industrial application. Among these questions, it is urgent to address the hysteresis to realize highly efficient and reliable perovskite solar cells (PSC). The hysteresis is the discrepancy between two voltage-sweeping directions when performing a current-voltage (J-V) measurement. To suppress hysteresis, the introduction of [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) in the planar PSC has proved as an effective way. However, there is still no comprehensive understanding on it, which is the topic of this poster.

Evidences consistently show that the iodide ion migration is critical for the hysteresis behavior. Herein, we employ PL microscopy to in-situ investigate the ion migration process. By comparing the mobility of the ions in perovskite films with and without PCBM, it shows the decrease of ionic migration velocity when PCBM molecules are involved. Furthermore, temperature-dependent J-V measurements show that the activation energy of iodide ions increases in presence of PCBM molecules. Our experiment suggests that PCBM molecules passivate the iodide related defects and reduce the migration of iodide ions, thus suppressing the hysteretic behavior in PSC.

HL 28.10 Mon 18:30 P1A

Impact of additional PbI_2 and the grain size on optical properties in hybrid lead halide perovskites — •Tobias Meier[1], Fabian Panzer[1,2,3], Tanaji Gujar[4], Mukundan Thelakkat[4], and Anna Köhler[1,2] — [1]Experimental Physics II — [2]Bayreuth Institute of Macromolecular Research (BIMF) — [3]Department of Functional Materials — [4]Applied Functional Polymers, Macromolecular Chemistry, University of Bayreuth, 95440 Bayreuth, Germany

Hybrid lead halide perovskites are a promising candidate for the absorbing layer in solar cells due to their excellent optical properties i.e. a direct band gap, a high absorption coefficient throughout the entire visible spectrum and a low exciton binding energy. It is known that the precise stoichiometry of the additives during film preparation is important for the device performance. For example a small amount of typically 10% extra PbI_2 was found to be beneficial for the performance. However, the mechanism of how incorporations of additional PbI_2 influences the optical and electronic properties and the role of grain boundaries are not completely understood yet. We therefore performed temperature dependent steady-state absorption and photoluminescence spectroscopy to investigate the impact of additional PbI_2 and the grain size on the fundamental optical properties in thin films of $CH_3NH_3PbI_3$.

HL 28.11 Mon 18:30 P1A

Tuning the pore size of mesoporous titania films for hybrid solar cells — •Steffen Schlosser, Nuri Hohn, Lorenz Biessmann, Senlin Xia, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str 1, 85748 Garching

Hybrid solar cells combine the mechanical stability of inorganic and the versatility of organic semiconductors. Due to their potential for large-scale application, hybrid solar cells are especially interesting for low-cost industrial production. As an inorganic compound, mesoporous titania films are common for application in high-efficiency hybrid solar cells. The mesoporous character offers a high interfacial contact with the organic surfactant, usually a conjugated polymer. Challenges concerning these cells arise due to the difficulty of controlling their nanoscale structure, which affects conductivity and degree of backfilling. We focus on the tuning of the pore size of mesoporous titania nanostructures and its impact on the infiltration of the polymeric compound. Tuning of the pore sizes provides the possibility of enhancing the backfilling and thus has a positive impact on solar cell performance. In our experiments, a solution composed of an amphiphilic block copolymer and a precursor dissolved in an organic solvent is applied as a film. Immersion in an antisolvent leads to a structure formation process in the composite film, so that after calcination, a mesoporous titania film is obtained. Depending on the parameters used, the pore size can be controlled.

HL 28.12 Mon 18:30 P1A

Scanning force microscopy on perovskites — Ilka M. Hermes[1], Victor W. Bergmann[1], Dan Li[1], Alexander Klasen[1], Simon Bretschneider[1], Markus Mezger[1,2], Rüdiger Berger[1], Wolfgang Tremel[2], and •Stefan A.L. Weber[1,2] — [1]Max Planck Institute for Polymer Research, 55128 Mainz, Germany — [2]Johannes Gutenberg University, 55128 Mainz, Germany

In perovskite solar cells, nanoscale structures can have a huge impact on the device performance. For understanding this interplay, electrical scanning force microscopy (SFM) methods can correlate the nanoscale morphology with various surface properties: electrical conductivity (conductive SFM), surface potential in Kelvin probe force microscopy, (KPFM) or electromechanical coupling in piezoresponse force microscopy (PFM). This poster provides an overview on our activities in SFM on perovskite films and solar cells. We used KPFM to map the potential distribution on cross sections of perovskite solar cell devices in dark and under illumination, revealing distinct differences in the charging dynamics at different interfaces [1,2]. With PFM on micron-sized perovskite grains we observed a periodically alternating structure reminiscent of ferroelastic domain patterns [3]. Using a SFM under controlled humidity, the effects of reversible hydration in perovskite films on the morphology were studied [4]. Such experiments provide valuable information for the optimization of the light harvesting abilities in these materials and the fabrication processes. [1] Nat. Comm. 2014, 5. [2] ACS AM&I, 2016, 8 (30), 19402. [3] J. Phys. Chem. C (2016), 120, 5724. [4] J. Phys. Chem. C, 2016, 120 (12), 6363.

HL 28.13 Mon 18:30 P1A

Investigating the organometal halide perovskite crystallization in mesoscopic hole-conductor-free perovskite solar cells — •Oliver Filonik[1,2], Jia Haur Lew[2], Anish Priyadarshi[2], Nripan Mathews[2], and Eva M. Herzig[1] — [1]TU München, Munich School of Engineering, Herzig Group, 85748 Garching, Germany —

[2]School of Materials Science and Engineering, Nanyang Technological University, Nanyang Avenue, Singapore 639798, Singapore

Organometal halide perovskite based solar cells have emerged as the fastest-advancing photovoltaic technology to date, reaching certified solar cell efficiencies of up to 22.1%. Recently, the focus of research broadened beyond high efficiencies to key values like prolonged device lifetime and stability that are required for industrial implementation. A novel perovskite cell architecture utilizing a mesoporous scaffold with embedded perovskite addresses these challenges and is furthermore adaptable for industrial scale production. However, little is known about the perovskite crystal formation in mesoscopic scaffolds.

In this project, we fabricate a mesoscopic scaffold comprised of a mesoporous triple-layer of titania, zirconia and carbon by screenprinting and are investigating the influence of the processing additive 5-ammonium valeric acid iodide (5-AVAI) on the perovskite solution infiltration and perovskite crystallization. Hereby, our results grant us a better understanding of the perovskite crystallization processes in a mesoscopic scaffold and are of key importance for further developments.

HL 28.14 Mon 18:30 P1A

Fabrication and Characterization of Mesoscopic Perovskite Solar Cells — •Margret Eva Thordardottir[1,2], Oliver Filonik[1], Peter Müller-Buschbaum[2], and Eva M. Herzig[1] — [1]TU München, Munich School of Engineering, Herzig Group, 85748 Garching, Germany — [2]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

Photovoltaic solar cells have been regarded as a promising energy conversion method to keep up with the worlds increasing energy consumption. Organic solar cells yield promising prospects due to their low cost fabrication, light weight and mechanical flexibility. However, the efficiency of organic solar cells are inferior to commercial silicon solar cells. Organometal halide perovskite solar cells are a product of combining the advantages of organic and inorganic systems. The steep rise of the efficiency makes them the fastest-advancing solar cell technology to date. Properties of the perovskite material like large carrier diffusion lengths, high charge-carrier mobilities and low exciton binding energy all contribute to superior performance.
In this work, we fabricated mesoscopic perovskite solar cells by using a screenprinter. We analyze processing parameters and investigate the influence on the efficiency of the solar cell. To obtain fully printed solar cells, slot die coating is compared to drop casting of the perovskite materials onto the printed layers.

HL 28.15 Mon 18:30 P1A

Two-Photon Photoluminescence from Quantum-Dot-Like Perovskite Nanocubes — •Alexander Biewald[1,2], Veit Giegold[1,2], Richard Ciesielski[1,2], Fatma Meltem Aygüler[1,2], Nicolai Friedrich Hartmann[1,2], Pablo Docampo[3], and Achim Hartschuh[1,2] — [1]LMU Munich, Department Chemie and CeNS, 81377 Munich — [2]Nanosystems Initative Munich, 80799 Munich — [3]Newcastle University, Newcastle upon Tyne, UK

Perovskites are a promising material class for new solar cell and LED applications. Especially perovskite nanocubes, with sizes below 10 nm, are interesting because they exhibit quantum confinement which allows for tuning their optical transition energies similar to other inorganic semiconducting nanocrystals. We investigated the photoluminescence (PL) of individual $CsPbBr_3$ nanocubes deposited on glass upon pulsed two-photon excitation. Our setup combines a scanning confocal microscope and a pulse shaper in 4f geometry for amplitude and phase shaping of sub-20 fs laser pulses. We found that individual nanocubes show pronounced PL blinking, which we investigated in detail with respect to the characteristic on- and off-times. We also confirmed the non-linear intensity dependence of the PL that provides the basis for the coherent control of two-photon absorption in single nanocubes.

HL 28.16 Mon 18:30 P1A

Investigation of planar perovskite solar cells by means of electrical impedance spectroscopy — •Markus Jakob[1], David Kiermasch[1], Mathias Fischer[1], Phillip Rieder[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

Hybrid organic-inorganic perovskites have been recognized as a promising material for photovoltaic devices and became a hotspot in this research field over the last years. Toward the common goal of developing more efficient and stable devices better insight into the working principles is required. The interface between the crystalline perovskite and the charge selective layer has been found to be a crucial factor for the solar cell device performance. An accumulation of charged particles, either charge carriers or ions at the interface may lead to extraction barriers leading to a decrease in the overall efficiency. We investigate highly efficient solution processed perovskite solar cells in planar configuration by means of electrical impedance spectroscopy. The cells are fabricated with the well-known two step interdiffusion method using PbI_2 and CH_3NH_3I. We discuss our results for different device configurations and transport materials to identify their impact on the dielectric properties.

HL 28.17 Mon 18:30 P1A

Transient absorption spectroscopy of hole transport materials for perovskite solar cells — Jonas Hölzer, Johannes Klein, Mirko Scholz, Thomas Lenzer, and •Kawon Oum — Universität Siegen, Physikalische Chemie, Adolf-Reichwein-Str. 2, 57076 Siegen

Perovskite-based photovoltaic devices consist of multilayer arrangements containing mesoporous TiO2, an organic-inorganic perovskite and a hole transport material (HTM) as central elements. We present a steady-state and time-resolved UV-Vis-NIR absorption study of such devices featuring different triarylamine-based HTMs, enabling us to quantify the efficiency and time scale of the hole transfer process. In addition, direct photoexcitation of the HTMs on mesoporous TiO2 and Al2O3 thin films and in different organic solvents is investigated to understand their photophysics. They exhibit photoinduced electron injection into TiO2 and form radical cation-radical anion pairs on Al2O3 by exciton-splitting. Implications of these processes for the performance of HTMs in photovoltaic devices will be discussed.

HL 28.18 Mon 18:30 P1A

Investigation of the photophysical properties of methylammonium lead halide perovskite solar cells by electroluminescence spectroscopy — •Simon Berger[1], Philipp Rieder[1], David Kiermasch[1], Mathias Fischer[1], Kristofer Tvingstedt[1], Andreas Baumann[1,2], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research ZAE, 97074 Würzburg

Organo lead halide perovskite solar cells are in the focus of current research as one of the most promising materials in thin film photovoltaics. With many cell configurations being presented so far, we evaluated solution-processed planar as well as mesoporous perovskite solar cells in terms of their corresponding ability to emit light, using the technique of electroluminescence spectroscopy. In that manner, we probed the impact of different transport materials in regular as well as inverted layouts by evaluating the radiative efficiency of devices. Additionally, we studied the effect of incorporating bromine as well as chlorine to partly replace the iodine in the crystal structure of the perovskite layer on the processes relevant for the operation of a solar cell.

HL 28.19 Mon 18:30 P1A

Doping design for hole transport materials in perovskite solar cells — •Lorena Perdigón Toro, Christian M. Wolff, Malavika Arvind, and Dieter Neher — University of Potsdam, Soft Matter Physics

In planar perovskite solar cells, the active perovskite semiconductor is usually sandwiched between an organic hole transport material (HTM) and an electron transport material (ETM). The correct choice of these materials has been shown to be crucially important when aiming at high device efficiencies. A promising HTM is the polymeric hole conductor poly(triaryl amine) (PTAA), which given its energetic levels has been shown to be a suitable choice as hole transport and electron-blocking layer. Nonetheless, the relatively low hole mobility of PTAA can be limiting to the performance of the devices, particularly the fill factor and open-circuit voltage. In order to provide sufficient coverage and prevent shunt pathways, thicker hole transport layers (>20 nm) can be efficiently applied provided their mobility can be increased. Therefore, we employ the widely studied electron acceptor F4TCNQ and the strong Lewis acid tris(pentafluorohenyl)borane as dopants for PTAA. Optical spectroscopy of doped solutions and layers insights into the underlying doping mechanisms. The impact of doping on layer morphology is studied by AFM, while the electrical properties are studied with systematic conductivity measurements at different

operational conditions (e.g. elevated temperatures). Doped layers are optimized in working devices for highly efficient perovskite solar cells, reaching efficiencies above 18%.

HL 28.20 Mon 18:30 P1A

Temperature-dependent optical spectra of $(CH_3NH_3)PbBr_3$ single-crystals cleaved in ultrahigh vacuum — •Oskar Schuster[1], Max Wilhelm[1], Daniel Niesner[1], Ievgen Levchuk[2], Andres Osvet[2], Shreetu Shrestha[2], Miroslaw Batentschuk[2], Christoph Brabec[2,3], and Thomas Fauster[1] — [1]Lehrstuhl für Festkörperphysik, FAU Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany — [2]I-MEET, Department of Materials Science and Engineering, FAU Erlangen-Nürnberg, Martensstr. 7, D-91058 Erlangen, Germany — [3]ZAE Bayern, Haberstr. 2a, D-91058 Erlangen, Germany

Temperature-dependent optical spectroscopy determines basic properties like band gap, exciton binding energy, and direct or indirect character of the gap. Differences have been reported between freshly cleaved crystals compared to as-grown ones or thin films. We present an approach that determines the absorption of cleaved crystals from measured one-photon and two-photon induced photoluminescence spectra. The extracted low-temperature band gap and exciton binding energy of 22 meV are in excellent agreement with the ones determined from other techniques. The direct band gap increases with temperature at < 200 K, and decreases at higher temperature. The behavior is well described by the Bose-Einstein model. The associated exciton binding energy decreases for temperatures > 200 K. We find a second transition 60 meV (90 meV) below the direct gap in the orthorhombic (tetragonal) phase, consistent with a slightly indirect gap. Emission from this transition is significantly reduced after exposing the crystals to air.

HL 28.21 Mon 18:30 P1A

Photoinduced Charge Generation and Dynamics in Mixed Formamidinium Methylammonium Lead Halide Perovskite Thin Films as Observed by fs Transient Absorption Spectroscopy — •Jonas Horn[1,2,3], Iulia Minda[2], Heinrich Schwoerer[2], and Derck Schlettwein[1,3] — [1]Justus-Liebig-University Giessen, Institute of Applied Physics — [2]Stellenbosch University, Laser Research Institute, South Africa — [3]Justus-Liebig-University Giessen, Laboratory for Materials Science

Hybrid organic inorganic perovskite materials, in particular $FA_{1-x}MA_xPbI_{3-y}Br_y$ using formamidinium and methylammonium cations, are of great interest not only due to the rapid increase in power conversion efficiencies when applied in photovoltaic devices but also due to their astonishing optoelectronic properties. By means of transient absorption spectroscopy in the visible and near infrared spectral regions, temporal evolution of the population and depopulation of various electronic states and their associated spectral signatures was monitored. The detailed interpretation of the results leads to a consistent charge dynamic model of the initial photo-processes. Upon photoexcitation with 3.2 eV photon energy, hot electrons and holes are generated in the lowest conduction band and second highest valence band and relax to the band edges with a time constant of approximately 500 fs. Subsequently recombination, occurring on gradually faster time scales for hot versus cold electrons was shown and assigned to Auger- and bimolecular recombination.

HL 28.22 Mon 18:30 P1A

Dye-Sensitized Solar Cells based on Low-Temperature Electrodeposited ZnO and Co(II/III) Redox Electrolyte — •Raffael Ruess[1,2], Sebastian Haas[1,2], Andreas Ringleb[1,2], and Derck Schlettwein[1,2] — [1]Justus-Liebig-University Giessen, Institute of Applied Physics — [2]Justus-Liebig-University Giessen, Laboratory for Materials Science (LaMa)

Emerging photovoltaics, such as dye-sensitized solar cells (DSSCs), have received great interest in the recent years because of quite high record efficiencies (<14.3%) and low energy payback times. The present work is focused on DSSCs based on electrodeposited, porous zinc oxide which allows low preparation temperatures to further reduce energy consumption of cell production and allows the preparation on flexible polymer substrates. To reduce voltage loss in the cell and thus improve the power conversion efficiency, the commonly used I^-/I_3^- redox electrolyte in these DSSCs is replaced by a $Co(II/III)$ redox couple. Recombination, electrolyte diffusion and electron transport in the DSSC devices are studied by impedance spectroscopy, intensity modulated photocurrent and photovoltage spectroscopy and charge extraction techniques. It was found that the interaction of the cobalt redox mediator with zinc oxide at the interface lowers the conduction band position of ZnO and, thus, leads to a lower open-circuit photovoltage. However, efficient dye regeneration can be achieved due to sufficient mass transport through the nanoporous system resulting in high photon-to-electron conversion efficiencies.

HL 28.23 Mon 18:30 P1A

Temperature and illumination intensity dependent photoluminescence of methylammonium lead iodide perovskites — •Fabian Meier, Sebastian Reichert, Seth Niklas Schumann, Alexander Wagenpfahl, and Carsten Deibel — Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

Understanding recombination mechanisms of electrical charge carriers is of tremendous importance for understanding the extraordinary power conversion efficiencies, which increased from 4 % up to 21 %. We investigate thin films of methylammionium lead iodide perovskite on top of PEDOT:PSS layer and an ITO layer in terms of their stoichiometric ratio of methylammonium iodide and lead iodide. By confocal photoluminescence measurements we determine direct recombination of electric charges as function of time and spatial location. We discuss our results in terms of illumination intensity as well as temperature dependence and compare it to the energetically resolved emission spectra. We discuss recombination by tail states, also visible in EQE spectra, in view of the performance of solar cells based on the investigated perovskite layers.

HL 28.24 Mon 18:30 P1A

Stability and Performance of ZnO-based Dye-Sensitized Solar Cells in Contact to a Co(II/III) Redox Electrolyte — •Sebastian Haas[1,2], Raffael Ruess[1,2], and Derck Schlettwein[1,2] — [1]Justus-Liebig-University Giessen, Institute of Applied Physics — [2]Justus-Liebig-University Giessen, Laboratory for Materials Science (LaMa)

The use of $Co(II/III)$ electrolytes instead of the commonly used I^-/I_3^- redox electrolyte represents an attractive way to increase the efficiency of dye-sensitized solar cells (DSSCs). By this approach, attractive efficiencies of up to 14.3 % were reached for TiO_2-based cells. The present work is focused on DSSCs based on low temperature electrodeposited porous zinc oxide, to decrease further the already attractive energy payback time of DSSCs and allow preparation on temperature-sensitive substrates, e.g. polymer foils. Dye stability, electrolyte diffusion and recombination in the DSSC devices are studied by UV-Vis-spectroscopy, impedance spectroscopy and photocurrent-transients. It was found that the dyes $D149$ and $DN216$ are not stable at the ZnO surface in the presence of the $Co(II/III)$ redox couple. Furthermore, a small influence of a hindered diffusion in the DSSCs based on $Co(II/III)$ redox couple compared with DSSCs based on I^-/I_3^- redox electrolyte was observed.

HL 28.25 Mon 18:30 P1A

Temperature-dependent transient photocurrent measurements on organic-inorganic halide perovskite solar cells — •Ina Kelz[1], Nico Weber[1], Fabian Ruf[1], Tobias Abzieher[2], Nadja Giesbrecht[3], Meltem F. Aygüler[3], Pablo Docampo[3], Heinz Kalt[1], and Michael Hetterich[1,2] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Light Technology Institute (LTI), Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [3]Department of Chemistry, Ludwig-Maximilians-Universität München (LMU), 81377 Munich, Germany

Organic-inorganic halide perovskites as absorber material in solar cells show high power conversion efficiencies exceeding 20%. This is due to their promising properties such as a strong absorption coefficient and a low non-radiative carrier recombination. Additionally fabrication by low-cost production methods is possible. However, basic material properties of perovskite solar cells are not fully understood yet.

In order to gain a deeper insight into the electro-optic material properties temperature-dependent j-V-characteristics are measured. Organic-inorganic halide perovskites exhibit scan rate-dependent hysteresis effects which vary with various parameters such as illumination, bias voltage or temperature. Temperature dependent photocurrent transients show two regimes with different time constants, a fast component with a multi-exponential behaviour and a slow component which can be described by a single exponential function. The time constant of the slow component decreases for increasing temperature.

HL 28.26 Mon 18:30 P1A

High Energy Resolution Fluorescence Detected X-ray Ab-

sorption Spectroscopy on Lead Halide Perovskite Precursors — •Pascal Becker[1,2], Justus Just[1], Charles J. Hages[1], Oliver Müller[2], and Thomas Unold[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Germany — [2]Bergische Universität Wuppertal, Germany

Perovskites as photon absorbers in thin film solar cells have drawn immense attention resulting in a rapid rise in the achieved power conversion efficiencies exceeding 20 % within a few years. Despite the intensive research in this field little is known about the formation process of these perovskite thin films on an atomic level. X-Ray Absorption Spectroscopy (XAS) is a well suited method to investigate electronic and structural properties of thin film materials. Also, residual precursor phases can be identified by this method even when X-Ray Diffraction (XRD) fails to detect. By using high quality and high resolution reference spectra in a linear combination analysis the amount of these secondary phases can be quantified.

Therefore High Energy Resolution Fluorescence detected XAS (HERFD-XAS) measurements were performed on PbI_2, $PbBr_2$, $PbCl_2$ as well as $NH_3CH_3PbI_xCl_{3-x}$ at the Pb-L_2 edge. The data reveal a clear fine structure in near edge region as opposed to data from total yield fluorescence detected spectra.

HL 28.27 Mon 18:30 P1A

Capacitance spectroscopy on perovskite solar cells and MIS devices — •David Diering[1,2], Christian M. Wolff[2], Charles J. Hages[1], Thomas Unold[1], and Dieter Neher[2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [2]Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany

Hybrid organic-inorganic Perovskites are recently under strong focus for their tremendous rise in efficiency up to 21%. However, it is not fully understood why this class of material shows such a high performance. Capacitance spectroscopy is a powerful method to investigate defects which give rise to recombination processes and therefore influence the solar cell output.

By performing capacitance-voltage and admittance measurements on mixed perovskite {Cs/FA/MA}$PbI_{(3-x)}Br_x$ solar cells and metal-insulator-semiconductor(MIS) devices we are able to get information not only about defects but other important material properties such as the dielectric constant, charge carrier type and concentration. The data supports the previous theory of slight n-type to intrinsic behaviour. Further on, evidence for a deep defect level is found.

HL 28.28 Mon 18:30 P1A

Origin and Location of Trap States in Perovskite Films — •Tobias Seewald[1], Carola Ebenhoch[1], Philipp Ehrenreich[1], Rebecca Milot[2], Susanne Birkhold[1], Laura Herz[2], and Lukas Schmidt-Mende[1] — [1]Department of Physics, University of Konstanz, POB M 680, Konstanz 78457, Germany — [2]University of Oxford, Clarendon Laboratory, Parks Road, Oxford OX1 3PU, UK

Lead halide perovskites have experienced tremendous research interest within the last years. High power conversion efficiencies in combination with the ability of crystal formation during a solution casting process make this material class very attractive for photovoltaic application. For efficient charge carrier generation, it is essential to minimize non-radiative recombination that can be initiated by energetic trap states. For this purpose, we have studied polycrystalline methylammonium lead iodide perovskite films with varying crystal sizes. Morphology and crystallinity have been modified by means of methylamine gas induced defect healing. Time-resolved photoluminescence as well as pump-probe spectroscopy have been applied in order to relate trap state distribution with crystal sizes and grain boundaries. In this study we can demonstrate the importance of large crystal grains, which allow for high carrier mobilities and reduced non-radiative losses that are crucial for efficient solar cell devices.

HL 28.29 Mon 18:30 P1A

Vacuum chamber for in-operando grazing-incidence X-ray scattering experiments on novel thin-film solar cells — •Bernhard Kalis, Johannes Schlipf und Peter Müller-Buschbaum — TU München,Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

In the past few years hybrid perovskite solar cells have reached power conversion efficiencies of about 20%. Alternatively, organic and other types of hybrid solar cells offer potentially cheap energy supply. The photovoltaic performance of these novel solar cell materials seems to be directly linked to the morphology of the solar cell film. To understand these connections between structural changes of the absorber material due to the influences of temperature and humidity in addition to the aging of the solar cell we use the grazing-incidence small and wide angle X-ray scattering (GISAXS/GIWAXS) method during operation [1]. To fulfil and control all these environmental influences, a newly designed vacuum chamber comes to action that consists of several modules to provide multi-functionality. This Chamber has also the ability to be pre calibrated in order to minimize the expenditure of time during a beam time at a synchrotron such as the ELETTRA in Trieste, Italy or the DESY in Hamburg, Germany.

[1] C. J. Schaffer, C. M. Palumbiny, M. A. Niedermeier, C. Jendrzejewski, G. Santoro, S. V. Roth, P. Müller-Buschbaum, Advanced Functional Materials 2013, 25, 6760.

HL 28.30 Mon 18:30 P1A

Spectroscopic investigation of trap states related to loss mechanisms in hybrid perovskite solar cells — •Sebastian Reichert, Fabian Meier, Alexander Wagenpfahl, and Carsten Deibel — Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

Due to excellent electrical and optical properties of perovskite films for solar cell applications the pace of improvement related to power conversion efficiency and morphological optimisation has been unprecedented. The efficiency of methyl ammonium lead iodide (MAPI) solar cells is limited by the loss of charge carriers which is occurring within the active layer. Choosing a suitable model for those recombination mechanisms is still difficult, also due to the influence of the neighbouring transport or contact layers. We present photoluminescence transients of various MAPI thin films and compare these measurements to theoretical predictions by the charge carrier continuity equation for different recombination models. Depending on the processing conditions, the results indicate recombination assisted by tail states. The energetic trap distribution is quantified by thermally stimulated current measurements. We discuss the dominant recombination process in the examined MAPI films.

HL 29: Transport: Quantum Coherence and Quantum Information Systems - Theory (jointly with MA, HL)

Time: Tuesday 9:30–13:15 Location: HSZ 103

HL 29.1 Tue 9:30 HSZ 103

Adiabatic Quantum Simulations with Superconducting Qubits — •Nikolaj Moll, Panagiotis Barkoutsos, Daniel Egger, Stefan Filipp, Andreas Fuhrer, Marc Ganzhorn, Andreas Kuhlmann, Peter Müller, Marco Roth, Peter Staar, and Ivano Tavernelli — IBM Research – Zurich, Säumerstrasse 4, CH-8803 Rüschlikon, Switzerland

Quantum computing technology is improving fast and quantum computers with approximately 100 qubits appear feasible in the not so distant future. The quest for systems which profit of exponential speed-up and cannot be calculated on classical computers has recently triggered a lot of attention. Fermionic quantum systems, such as quantum chemistry or the Fermi-Hubbard model, are among the best candidates for exploiting the exponential speed-up. Such a quantum system can be implemented on a quantum computer based on superconducting qubits. However, the controlled realization of different types of interactions between qubits without compromising their coherence is essential. A coupling method between fixed-frequency transmon qubits can be achieved with the frequency modulation of an auxiliary capacitively coupled quantum bus. An adiabatic protocol for the Hydrogen molecule can be implemented on such a coupled qubit system.

HL 29.2 Tue 9:45 HSZ 103

Tunable, Flexible and Efficient Optimization of Control

Pulses for Superconducting Qubits, part I - Theory — •Shai Machnes[1,2], Elie Assémat[1], David Tannor[2], and Frank Wilhelm[1] — [1]Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany — [2]Weizmann Institute of Science, 76100 Rehovot

Quantum computation places very stringent demands on gate fidelities, and experimental implementations require both the controls and the resultant dynamics to conform to hardware-specific ansatzes and constraints. Superconducting qubits present the additional requirement that pulses have simple parametrizations, so they can be further calibrated in the experiment, to compensate for uncertainties in system characterization. We present a novel, conceptually simple and easy-to-implement gradient-based optimal control algorithm, GOAT [1], which satisfies all the above requirements.

In part II we shall demonstrate the algorithm's capabilities, by using GOAT to optimize fast high-accuracy pulses for two leading superconducting qubits architectures - Xmons and IBM's flux-tunable couplers.

[1] S. Machnes, D.J. Tannor, F.K. Wilhelm and E. Assémat, ArXiv 1507.04261 (2015)

HL 29.3 Tue 10:00 HSZ 103

Tunable, Flexible and Efficient Optimization of Control Pulses for Superconducting Qubits, part II: Applications — Shai Machnes[1,2], •Elie Assemat[1], David Tannor[2], and Frank Wilhelm[1] — [1]Saarland University, Saarbrücken, Germany — [2]Weizmann Institute of Science, Rehovot, Israel

In part I, we presented the theoretic foundations of the GOAT algorithm [1] for the optimal control of quantum systems. Here in part II, we focus on several applications of GOAT to superconducting qubits architecture. First, we consider a control-Z gate on Xmons [2] qubits with an Erf parametrization of the optimal pulse. We show that a fast and accurate gate can be obtained with only 16 parameters, as compared to hundreds of parameters required in other algorithms. We present numerical evidences that such parametrization should allow an efficient in-situ calibration of the pulse. Next, we consider the flux-tunable coupler by IBM [3]. We show optimization can be carried out in a more realistic model of the system than was employed in the original study, which is expected to further simplify the calibration process. Moreover, GOAT reduced the complexity of the optimal pulse to only 6 Fourier components, composed with analytic wrappers.

[1] S. Machnes et al., ArXiv 1507.04261v1 (2015)
[2] R. Barends et al., Phys. Rev. Lett. 100, 080502 (2013)
[3] D. C. McKay et al., ArXiv 1604.0307v2 (2016)

HL 29.4 Tue 10:15 HSZ 103

Symmetry Benchmarking of Quantum Algorithms — •Tobias Chasseur Chasseur[1], Felix Motzoi[1,2], Michael Kaicher[1], Pierre-Luc Dallaire-Demers[1], and Frank Wilhelm[1] — [1]Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany — [2]Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, Denmark

Scalable and robust benchmarking of quantum gates is essential on the path to a useful quantum computer, as current candidates such as superconducting qubit systems are set to leave the few qubit regime in the near future. Randomized Benchmarking and related approaches provide solutions for specific gates such as the Clifford group or a limited number of qubits; however a tool for benchmarking arbitrary gates without exponential scaling in the number of qubits seems prohibited by the inherent power of quantum computation. In this work we present a symmetry benchmarking protocol to estimate the implementation fidelity of specific algorithms with polynomial scaling. The proposed protocol relies on unitary 1-designs on the eigenspaces of algorithm-specific preserved quantities, as well as sequence structures similar to Randomized Benchmarking. It benchmarks the symmetry preservation of the implementation as an indicator for the overall fidelity. We demonstrate the protocol for the specific example of algorithms consisting of number preserving gates.

HL 29.5 Tue 10:30 HSZ 103

Implementation of Quantum Stochastic Walks — •Peter Schuhmacher[1], Luke Govia[2], Bruno Taketani[1], and Frank Wilhelm[1] — [1]Universität des Saarlandes, Saarbrücken, Germany — [2]Department of Physics, McGill University, Montreal, Quebec, Canada

Quantum walks are one of the most prominent frameworks in which to design and think about quantum algorithms. Both the continuous- and discrete-time versions have been shown to provide speed-up over classical information processing tasks, and can be regarded as universal quantum computers. Classical (probabilistic) and quantum unitary random walks yield different distributions due to interference effects. Combining the two, stochastic quantum walks (QSW) can be defined in an axiomatic manner to include unitary and non-unitary effects, and include both classical and quantum walks as limiting cases. While a general purpose quantum computer is still far over the horizon, intermediary technologies have been emerging with the promise to breach classical limitations. Within these, artificial intelligence is one exciting field where the use of quantum physics can lead to important improvements. Here, we focus on the physical realizability of both kinds of quantum stochastic walks (continuous-time and discrete-time).

HL 29.6 Tue 10:45 HSZ 103

Normal metal traps for superconducting qubits — •Roman-Pascal Riwar[1,2], Amin Hosseinkhani[1,3], Luke D. Burkart[2], Yvonne Y. Gao[2], Robert J. Schoelkopf[2], Leonid I. Glazman[2], and Gianluigi Catelani[1] — [1]Forschungszentrum Jülich, Germany — [2]Yale University, USA — [3]RWTH Aachen University, Germany

The coherence time of superconducting qubits is intrinsically limited by the presence of quasiparticles. While it is difficult to prevent the generation of quasiparticles, keeping them away from active elements of the qubit provides a viable way of improving the device performance. We develop theoretically and validate experimentally a model for the effect of a single small trap on the dynamics of the excess quasiparticles injected in a transmon-type qubit. By means of this model, we show that for small traps, increasing the size shortens the evacuation time of quasiparticles from the transmon. We further identify a characteristic trap size above which the evacuation time saturates to the diffusion time of the quasiparticles. In the diffusion limit, the geometry of the qubit and the trap become relevant. We compute the optimal trap number and placement for several realistic geometries. Finally, our estimates show that the dissipation introduced by the presence of normal metal traps is well below the losses observed in the transmon.

HL 29.7 Tue 11:00 HSZ 103

Proximity Effect in Normal-Metal Quasiparticle Traps — •Amin Hosseinkhani[1,2] and Gianluigi Catelani[1] — [1]Peter Grunberg Institut (PGI-2), Forschungszentrum Jülich, Jülich, Germany — [2]JARA-Institute for Quantum Information, RWTH Aachen University, Aachen, Germany

In many superconducting devices, including qubits, quasiparticle excitations are detrimental. A normal metal (N) in contact with a superconductor (S) can trap these excitations. However, the contact between N and S modifies the properties of both materials, a phenomenon known as proximity effect which has drawn attention since the '60s. Despite this long history, we find new analytical results for the density of states, which shows a square root threshold behavior at the minigap energy. In superconducting qubits, the trap must be placed far enough from a Josephson junction in order not to harm the qubit coherence. To estimate the minimum trap-junction separation, we study how the density of states in the superconductor depends on the distance from the trap. For high interface resistance between N and S, a separation of several (5-7) coherence lengths is sufficient.

15 min. break.

HL 29.8 Tue 11:30 HSZ 103

Generating Entangled Quantum Microwaves in a Josephson-Photonics Device — •Simon Dambach, Björn Kubala, and Joachim Ankerhold — Institute for Complex Quantum Systems, Ulm University, Ulm, Germany

The realization of efficient sources for entangled microwave photons is of paramount importance for many promising applications of quantum technology. In this talk, we demonstrate that Josephson-photonics devices are logical candidates for this task since they allow to create a broad range of different bi- and multipartite entangled states in a surprisingly simple way [1].

In a Josephson-photonics device, a Cooper pair tunneling across a dc voltage-biased Josephson junction simultaneously creates photons in several series-connected microwave cavities. The interplay of this multiphoton creation process and subsequent individual photon leakage from the cavities leads to a stationary state with complex entanglement properties. Sophisticated pulse-shaping schemes as required in conventional circuit-QED architectures are thus not necessary here. Varying experimental parameters in situ or by construction then allows to access the rich wealth of entangled states differing, e.g., in the

number of entangled parties or the dimension of state space. Such devices, besides their promising potential to act as a highly versatile source of entangled quantum microwaves, may be also an excellent playground for the abstract branch of quantum information theory to test entanglement criteria on naturally existing quantum states.
[1] S. Dambach, B. Kubala, and J. Ankerhold, arXiv:1609.08990

HL 29.9 Tue 11:45 HSZ 103

Theory of mode locking in pulsed semiconductor quantum dots — •Wouter Beugeling, Götz S. Uhrig, and Frithjof B. Anders — Lehrstuhl für Theoretische Physik 1/2, TU Dortmund, Dortmund, Germany

Electron spins in semiconductor quantum dots appear unsuitable for quantum computing at first sight, due to their fast decoherence caused by hyperfine interactions to the nuclear spins in the substrate. However, the coherence time is dramatically increased by periodic optical pulsing. The underlying mechanism is known as mode locking: Oscillation frequencies incommensurate with the pulse repetition rate are suppressed, and only resonant contributions remain. Because the resonant frequencies are set by the pulse repetition rate only, the system becomes effectively immune to perturbations induced by the hyperfine interactions and by variations between the individual quantum dots in an ensemble.

In this presentation, we explore the mechanism of mode locking with a combination of analytical and numerical methods. Exploiting the fact that the hyperfine interaction is small compared to the external magnetic field, we calculate the dynamics perturbatively. The resulting frequency distributions show clear signs of mode locking. We study the positions of the resonant frequencies and the rate at which mode locking sets in, and compare the results to other theoretical and experimental studies. We also discuss the influence of the hyperfine coupling strength, of the Zeeman effect of the nuclear spins, and of the pulse shape and detuning.

HL 29.10 Tue 12:00 HSZ 103

Higher Order Spin Correlation in Semi-Conductor Quantum Dots — •Nina Fröhling and Frithjof Anders — Technische Universität 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. Via quantum measurement theory we show that the experiment by Bechtold et al. (Phys. Rev. Lett. 117. 027402, 2016) can be described as a fourth order auto-correlation function. We compare our results obtained from a semiclassical approach, exact diagonalization and a Lanczos algorithm to the experimental results. In order to explain the observed long time dynamics in the forth order autocorrelation the nuclear Zeeman splitting and the strain induced anisotropic quadrupolar moment of the nuclei must be included.

HL 29.11 Tue 12:15 HSZ 103

Non-equilibrium nuclear spin distributions in a periodically pulsed quantum dot — •Natalie Jäschke and Frithjof Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44227 Dortmund

In pump-probe experiments single electron charged semiconductor quantum dots are subjected to periodic optical excitations. This mechanism generates electron and nuclear spin polarization. In the short time regime the decoherence of the electron spin polarization is governed by the hyperfine interaction with the nuclear spins. We aim for a theory that combines the effect of the periodic laser pump 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 Overhauser field bridges the time until the next laser pulse. On the one hand we analyze the time dependence of the electron spin dynamics and on the other hand present data for the non-equilibrium steady state spectral distributions of the Overhauser field for the long time limit. For the electron spin dynamics a revival effect right before the next pulse is observed. The Overhauser field shows mode locking effects in the component parallel to the external magnetic field.

HL 29.12 Tue 12:30 HSZ 103

Detection of coherent oscillations in proximitized quantum dot spin valves — Philipp Stegmann, Jürgen König, and •Stephan Weiss — Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany

Spin coherent oscillations in a proximitized quantum dot spin valve are resolved by means of full counting statistics of electrons [1]. Especially, generalized factorial cumulants [2,3] of the electronic distribution function are suitable for the detection of the transition between different spin states in the system. We furthermore study the influence of a tunnel coupled superconductor. Due to the presence of Andreev reflections, coherent oscillations between different spin states are modified, the Larmor frequency is renormalized. We explore that general factorial cumulants are able to distinguish different fundamental transport processes of the model [1].
[1] Ph. Stegmann, J. König, S. Weiss, submitted (2016)
[2] Ph. Stegmann, J. König, Phys. Rev. B **92**, 155413 (2015)
[3] Ph. Stegmann, J. König, Phys. Rev. B **94**, 125433 (2016)

HL 29.13 Tue 12:45 HSZ 103

Apparent pairing and subperiods in integer quantum Hall interferometers — •Giovanni Andrea Frigeri[1,3], Daniel Scherer[2], and Bernd Rosenow[3] — [1]Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany — [2]Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark — [3]Institut für Theoretische Physik, Universität Leipzig, Leipzig, Germany

We analyze the magnetic field and gate voltage dependence of the conductance in an integer quantum Hall Fabry-Pérot interferometer, taking into account the interactions between an interfering edge mode, a non-interfering edge mode and the bulk. For weak bulk-edge coupling and sufficiently strong inter-edge interaction, we observe that the interferometer operates in the Aharonov-Bohm regime with a flux periodicity halved respect to the usual expectation. Even in the regime of strong bulk-edge coupling, this behavior can be observed as a subperiodicity of the interference signal in the Coulomb dominated regime. We do not find evidence for a connection between a reduced flux period and electron pairing, though. Our results can reproduce recent experimental findings.

HL 29.14 Tue 13:00 HSZ 103

Interplay of Hamiltonian control and and decoherence: a caveat, some hope and a new simulation strategy — •Jürgen Stockburger — Institute for Complex Quantum Systems, Ulm University

Hamiltonian control and decoherence are intricately intertwined in low-temperature quantum systems. For controls which act on timescales shorter than the thermal time $\hbar\beta$, Markovianity can no longer be assumed (RWA breakdown) [1]. When open-system dynamics is mapped on a stochastic propagation, this case can be treated exactly, and standard optimal control techniques can be used to explore synergy effects between control and reservoir interaction. Quantum states can thus be purified [2] and systems entangled [3] by the combined effect of local control and dissipation.

This stochastic mapping can now be combined with non-perturbative projection techniques, requiring only moderate computational resources [4].
[1] Alicki, R., Lidar, D. A. and Zanardi, P., Phys. Rev. A **73**, 052311 (2006)
[2] Schmidt, R. *et al.*, Phys. Rev. Lett. **107**, 130404 (2011)
[3] Schmidt, R., Stockburger, J. T. and Ankerhold, J., Phys. Rev. A **88**, 052321 (2013)
[4] Stockburger, J. T., EPL (Europhysics Letters) **115**, 40010 (2016)

HL 30: Fundamentals of Perovskite Photovoltaics III (joint session CPP/DS/HL)

Time: Tuesday 9:30–12:30 Location: ZEU 222

Invited Talk HL 30.1 Tue 9:30 ZEU 222

Investigation of hybrid organic/inorganic perovskite systems and interfaces by photoelectron spectroscopy — •Selina Olthof — University of Cologne, Germany, Luxemburgerstrasse 116, 50939 Cologne

In recent years, the interest in hybrid organic - inorganic perovskites rose at a rapid pace due to their tremendous success in the field of photovoltaics. In addition to the thin film properties of the active layer, the performance of optoelectronic devices strongly depends on the appropriate energetic alignment between the active- and adjacent layers. In order to choose adequate transport materials for the increasingly complex hybrid perovskite compositions in a non-trial-and-error fashion, it is important to understand how the induced changes in band gap relate to shifts in the valence and/or conduction band.

In this talk, I will discuss recent findings regarding measurements of the electronic structure of various hybrid perovskites, covering lead as well as tin based systems and a variety of halogens using UV-, inverse, and x-ray photoelectron spectroscopy measurements (UPS/IPES/XPS). Furthermore, using these surface sensitive techniques the alignment at interfaces between different layers can be probed in-situ as well by performing a stepwise film preparation. Looking at various bottom contacts we find that chemical interactions, band bending, and interface dipole formation play an important role. Therefore, the nature of the substrate not only determines the energetic alignment but can lead to chemical reactions and influence film formation and crystallinity.

HL 30.2 Tue 10:00 ZEU 222

Influence of air and water on the electronic structure of CH3NH3PbI3-xClx mixed halide perovskite film surfaces — •Maryline Ralaiarisoa, Fengshuo Zu, and Norbert Koch — Humboldt-Universität zu Berlin, Institut für Physik & IRIS Adlershof, Brook-Taylor-Str. 6, 12489 Berlin, Deutschland

Water and oxygen under environmental conditions reveal to be both beneficial for device performance as well as detrimental to the stability of perovskite based solar cells and films. Within this controversy, an accurate and comprehensive description of the influence of these factors is still lacking, particularly on the electronic structure of perovskite films. We investigated the effect of water and air on the ionization energy (IE) and the electronic structure of perovskite films. To this end, we used photoelectron spectroscopy to monitor the electronic structure of perovskite films following a range of procedures, including thermal post-treatment, as well as air and oxygen exposure. After air exposure, we observe changes of work function (WF) and IE similar to those after pure oxygen exposure. Furthermore, our observations indicate that even without prior ambient air exposure residual water (from processing in a typical glove-box environment) can still be present on the surface of perovskite films, even under vacuum conditions. Such water adsorption seemingly increases the WF of the perovskite films. Our results underline how environmental conditions substantially affect the electronic structure of perovskite films, which will likely impact the energy level alignment in perovskite-based photovoltaic cells.

HL 30.3 Tue 10:15 ZEU 222

Modulated surface photovoltage spectroscopy of CH3NH3Pb(I,Br)3 thin films — •Celline Awino, Thomas Dittrich, Eva Unger, and Bernd Rech — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium-Photovoltaik, Kekuléstr. 5, 12489 Berlin, Deutschland

The investigation of electronic properties of CH3NH3Pb(I,Br)3 and their dependence on aging and light soaking is important for better understanding of the stability of solar cells based on related materials. Modulated surface photovoltage spectroscopy allows for the ex-situ and in-situ characterization of the band gap, tail states and deep defect states in the band gap, direction of modulated charge separation and diffusion length. It has been found, for example, that the Tauc gap and the energy of exponential tail states sensitively depend on the substrate and on soaking in nitrogen atmosphere and that light soaking has strong influence on the direction and amplitude of modulated charge separation.

HL 30.4 Tue 10:30 ZEU 222

Revealing the impact of the potential distribution within high performing Lead Methylammonium Tri-Iodide solar cells with organic contact materials — •Christian Müller[1,2,3], Bernd Epding[2,3], Ramos Bwalya[2,3], Michele Sessolo[4], Lidón Gil-Escrig[4], Henk Bolink[4], Robert Lovrincic[1,3], and Wolfgang Kowalsky[1,2,3] — [1]IHF, TU Braunschweig, Germany — [2]KIP, Universität Heidelberg, Germany — [3]InnovationLab, Heidelberg, Germany — [4]Instituto de Ciencia Molecular, Universidad de Valencia, Spain

Over the last few years the power conversion efficiency of organometal-halide perovskite (such as $CH_3NH_3PbI_3$, MAPI) based solar cells has skyrocketed at an unprecedented rate to values around 22%. However, the understanding of the physical process in the solar cells drags behind the progress of efficiency. For example, the influence of the potential distribution in such cells on their performance is so far not sufficiently studied.
We focus in this work on high performing fully vacuum processed MAPI solar cells with organic contact materials [1]. We will present SKPM measurements on p-i-n and n-i-p solar cell cross sections that map the potential distribution within the device with high spatial resolution. Performing measurements under different conditions enables us to determine the influence of potential barriers at the contact interfaces and of a poling on the cell efficiency.

[1] Energy Environ. Sci., 2016, 9, p. 3456-3463, C. Momblona et al.

HL 30.5 Tue 10:45 ZEU 222

Impact of Illumination on the Electronic and Chemical Structure of Mixed Halide Perovskites — •Fengshuo Zu[1], Patrick Amsalem[1], Ingo Salzmann[1], Rongbin Wang[1,2], Maryline Ralaiarisoa[1], Stefan Kowarik[1], Steffen Duhm[2], and Norbert Koch[1] — [1]Institut für Physik,Humboldt-Universität zu Berlin,12489 Berlin,Germany — [2]FUNSOM,Soochow-University,Suzhou,China

The seemingly n-type behavior of the perovskite films is largely intriguing since these films are calculated to be bipolar conductive. For exploring the fundamental physics of the n-type behavior, we investigate the effect of white-light illumination on the electronic structure of mixed halide perovskite thin films and of CH3NH3PbI3 single crystals using X-ray and ultraviolet PES, as well as UV-Vis absorption spectroscopy. The samples are found to be strongly n-type and, upon illumination, the valence band features shift by up to 0.7 eV to lower BE. We show this effect to be correlated with initial surface band bending due to the presence of donor levels likely consisting of reduced lead (Pb0) acting as surface traps. Upon short-time illumination, this phenomenon is found to be partially reversible, for prolonged illumination, however, a high concentration of metallic Pb0 is generated inducing strong Fermi-level pinning. This effect is accompanied by the formation of PbI2 defects within the film and a deficiency of iodine in the surface region. Experiments performed on CH3NH3PbI3 single crystal reveal the presence of a relatively high concentration of reduced Pb0 at the sample surface after cleaving, likewise, strongly pinning the Fermi-level even under high intensity illumination.

15 min break

HL 30.6 Tue 11:15 ZEU 222

Giant Rashba Splitting in $(CH_3NH_3)PbBr_3$ Organic-Inorganic Perovskite — Daniel Niesner[1], Max Wilhelm[1], Ievgen Levchuk[2], Andres Osvet[2], Shreetu Shrestha[2], Miroslaw Batentschuk[2], Christoph Brabec[2,3], and •Thomas Fauster[1] — [1]Lehrstuhl für Festkörperphysik, FAU Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany — [2]I-MEET, Department of Materials Science and Engineering, FAU Erlangen-Nürnberg, Martensstr. 7, D-91058 Erlangen, Germany — [3]ZAE Bayern, Haberstr. 2a, D-91058 Erlangen, Germany

A Rashba-type spin-split band structure has been predicted for organic-inorganic perovskite semiconductors. The effect has been proposed as one of the origins of the exceptionally long carrier lifetimes in the materials, forming the basis of their successful application in optoelectronics. Using angle-resolved photoelectron spectroscopy, we investigate the band structure of $(CH_3NH_3)PbBr_3$ single crystals cleaved in ultrahigh vacuum. The orthorhombic low-temperature phase and

the cubic room-temperature phase are studied. We apply a modified leading-edge method to identify the dispersion of the valence band edge. It reveals two valence band maxima, separated in k-space by 0.043 $Å^{-1}$. The dispersion is indicative of Rashba splitting. This interpretation is supported by the observation of circular dichroism in the orthorhombic phase. Extracted Rashba parameters of $\alpha_o = 7 \pm 1$ eV Å and $\alpha_c = 11 \pm 4$ eV Å in the orthorhombic and the cubic phase are amongst the largest reported to date.

HL 30.7 Tue 11:30 ZEU 222

Exploring the electronic band structure of (organo-)metal halide perovskite via photoluminescence anisotropy of individual nanocrystals — •Daniela Täuber[1], Mirko Goldmann[1,2], Juanzi Shi[1], Alexander Dobrovolsky[1], and Ivan Scheblykin[1] — [1]Chemical Physics, Lund University, Lund, Sweden — [2]TU Ilmenau, Germany

Understanding electronic processes in metal halide perovskites requires unraveling the origin of their electronic transitions. Light polarization studies can provide important information regarding transition dipole moment orientations. Investigating individual lead trihalide perovskite nanocrystals enabled us to detect the polarization of photoluminescence intensity and photoluminescence excitation, hidden in bulk samples by ensemble averaging. Polarization properties of $CH_3NH_3PbI_3$ crystals were correlated with their photoluminescence spectra and electron microscopy images [1]. We propose that distortion of PbI6 octahedra leads to peculiarities of the electronic band structure close to the band-edge. Namely, the lowest band transition possesses a transition dipole moment along the apical Pb-I-Pb bond resulting in polarized photoluminescence. Excitation of photoluminescence above the bandgap is unpolarized because it involves molecular orbitals delocalized both in the apical and equatorial directions of the perovskite octahedron. Trap-assisted emission at 77 K, rather surprisingly, was polarized similar to the bandgap emission.

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

[1] Täuber, D. et al., Nano Letters 16, 5087-5094, 2016.

HL 30.8 Tue 11:45 ZEU 222

Band Edge Engineering of Hybrid Halide Perovskites for Solar Cell Applications - Insights from Density Functional Theory — •Linn Leppert[1,2], Sebastian E. Reyes-Lillo[1,2], and Jeffrey B. Neaton[1,2,3] — [1]Molecular Foundry, Lawrence Berkeley National Laboratory — [2]Department of Physics, University of California Berkeley — [3]Kavli Energy NanoScience Institute at Berkeley

Efficiencies of solar cells based on hybrid halide perovskite absorbers have reached 22%, making them serious contenders to silicon solar cells. Nevertheless, the toxicity of lead, the material's instability, as well as pressing questions about the role of structural heterogeneities present challenges to its large scale fabrication and long term use. Recently it has been shown that photovoltaic properties vary significantly between different crystal facets of perovskite thin films, suggesting an appreciable effect of electric fields on the local electronic structure [1]. In this contribution, I will elucidate the coupling between electric polarization, which increases as a function of the macroscopic alignment of the organic moieties, and the band edge electronic structure. In particular the Rashba effect, an energy band splitting in k-space, increases with increasing polarization, indicating significant tunability with experimentally feasible applied fields. The effect can be tuned further by chemical substitution of the organic molecule as well as by anisotropic strain, allowing for considerable Rashba splitting even in the absence of electric fields [2]. [1] S. Leblebinci, L. Leppert, et al., Nature Energy 1, 16093 (2016). [2] L. Leppert et al., J. Phys. Chem. Lett. 7, 3683 (2016).

HL 30.9 Tue 12:00 ZEU 222

Computational serach for sulphide perovskites for solar energy conversion application — •Korina Kuhar, Mohnish Pandey, Kristian Sommer Thygesen, and Karsten Wedel Jacobsen — Center for Aromic-scale Materials Design (CAMD), Department of Physics, Technical University of Denmark, DK * 2800 Kgs. Lyngby, Denmark

Oxide perovskites are in general known to be wide band gap semiconductors which hampers their use for visible light absorption. However, recent experiments on the synthesis of inorganic sulphide perovskites, for example BaZrS3[1] and SrZrS3[2], with band gaps of 1.7 ev and 0.8-1 eV, respectively, show that sulphur is a possible supstitution to oxygen in inorganic perovskites to lower their band gaps. Several binary, ternary and quaternary sulphides are already known to have relevant band gaps. We perform a systematic investigation of the class of ABS3 compounds in eight phases using Density Functional Theory (DFT). The screening procedure applied is based on simple criteria such as stability, band gap in the visible part of the solar spectrum, high charge mobility and small tendency of the material to form defects. Finally we report a set of sulphide perovskites we found to be stable and have interesting properties for use as solar energy conversion materials.

1. DOI: 10.1021/acs.chemmater.5b04213 2. DOI: 10.1016/j.solidstatesciences.2005.02.010

HL 30.10 Tue 12:15 ZEU 222

Towards a multiscale statistical description of hybrid perovskite materials — •Jingrui Li[1], Jari Järvi[1,2], and Patrick Rinke[1] — [1]COMP Centre of Excellence, Aalto University, Finland — [2]Department of Physics, University of Helsinki, Finland

Hybrid perovskites (HPs), in particular methylammonium lead iodide ($MAPbI_3$), have received enormous interest in recent years as promising photoactive materials in emergent photovoltaic technologies. An important feature of HPs is their structural complexity introduced by the organic cations (e.g., MA^+). At room temperature or above, the MAs will be oriented (quasi-)randomly, forcing HPs into disordered structures. The disorder affects important materials properties such as the stability and electronic structure that are crucial for the application of HPs in novel photovoltaic devices. Our previous density-functional theory (DFT) study reveals that hydrogen bonding leads to an anisotropic interaction between the MA cations and the inorganic cage. The deformed cage and the MA orientation are interdependent, analogous to a chicken-and-egg paradox [1]. From the insight of this single unit cell model, we derive a multiscale scheme for disordered $MAPbI_3$ structures, in which the interaction between neighbouring MA ions is described by a pair model. We show that the total number of relevant pairs can be reduced to only 86 and then analyse DFT results for large, geometry optimized $MAPbI_3$ supercell models in terms of their "pair-mode" distribution. With our model we can then describe disordered HPs on length scales beyond a few nanometers.

[1] J. Li and P. Rinke, *Phys. Rev. B* **94** 045201 (2016).

HL 31: Organic Electronics and Photovoltaics III: Mobile and Trapped Charges

Time: Tuesday 9:30–12:45 Location: ZEU 260

HL 31.1 Tue 9:30 ZEU 260

A Kelvin-Probe study of the electrical transport in organic semiconductors — •Karl-Philipp Strunk[1], Valeria Milotti[1], Alexander Ullrich[2], and Christian Melzer[1] — [1]Centre for Advanced Materials, University of Heidelberg, Germany — [2]Chemiches Institut, Universität of Heidelberg, Germany

DC current-voltage measurements on organic field-effect transistors (organic FET or OFET) are commonly used to characterize the planar electrical transport in organic semiconductors. In this study we report an alternative AC dark-injection method giving likewise access to in-plane transport parameters of organic semiconductor thin films. Exposing a macroscopic FET-like structure to a periodic bias leads to a periodic change in surface potential which can be tracked via a Kelvin-Probe giving direct insight into the movement of lateral charge-carrier waves along the organic film. Tracking the temporal evolution of the surface potential distribution allows for the determination of the charge-carrier mobility at low currents, a regime which is conventionally hardly accessible. It will be shown that this regime allows for a mobility determination at P3HT based devices fairly independent on contact properties. In order to elucidate the influences of electrical properties like doping concentration, traps states and injection barriers on the device response, time-dependent finite-element simulations have been carried out.

HL 31.2 Tue 9:45 ZEU 260

Spin dynamics and spin current in a high-mobility polymer — •Thorsten Arnold[1], Andreas Lücke[2], Uwe Gerstmann[2], Wolf Gero Schmidt[2], and Frank Ortmann[1] — [1]Institute for Materials Science, Center for Advancing Electronics Dresden and Dresden Center for Computational Materials Science, Technische Universität Dresden, 01069 Dresden, Germany — [2]Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn, Germany

Organic semiconductors are characterized by small spin-orbit coupling, which leads to a relatively long spin relaxation time. This makes them particularly interesting materials for spintronics. We describe spin transport in the thiophene-based polymer PBTTT using a recently developed generalization of the Kubo formalism to spin and an appropriate definition of the spin current operator in tight-binding form to investigate the spin conductivity tensor in PBTTT. The transfer integrals of the Hamiltonian and spin current operator are extracted from the DFT band structure with and without spin-orbit coupling. The spin propagation and spin conductivity for different spin-orbit transfer integral models are compared and the energy dependence and relaxation are analyzed.

HL 31.3 Tue 10:00 ZEU 260

Virtual screening for high carrier mobility in organic semiconductors — •Christoph Schober, Karsten Reuter, and Harald Oberhofer — Technische Universität München

Low carrier mobilities still hamper the use of organic semiconductors in many applications. Using a staged virtual screening approach we compute the electronic couplings and intramolecular reorganization energies as two main descriptors for charge mobility for a set of 95445 molecular crystals extracted from the Cambridge Structural Database (CSD). Descriptor calculations are performed using efficient density functional theory methods developed in our group, together with a fully automated workflow system for data preparation and verification. As a final step, based on the calculated coupling values we identify materials with long-range charge percolation pathways. We readily find many acclaimed compounds, as well as a number of most promising materials that have not yet been considered for an application in organic electronics. Together with the unique meta-data provided in the CSD the large descriptor database allows to extract important trends and correlations that will further accelerate the theoretical design and discovery of high mobility organic semiconductors.

C. Schober, K. Reuter, H. Oberhofer, *J. Chem. Phys.* **2016**, *144*, 054103.
C. Schober, K. Reuter, H. Oberhofer, *J. Phys. Chem. Lett.* **2016**, *7*, 3973-3977.

HL 31.4 Tue 10:15 ZEU 260

Utilizing Schottky barriers to suppress short channel effects in organic transistors — •Antón F. Fernández and Karin Zojer — Institute of Solid State Physics and NAWI Graz, Graz University of Technology, Graz, Austria

High switching speeds constitute one of the optimization targets for organic thin film transistors (OTFT). Reducing the channel length is a major handle to boost the switching speed of OTFTs. However, upon reducing the channel length one has to cope with undesired short-channel effects, i.e., a loss of saturation, a reduced ON-OFF ratio, and a disproportionally larger impact of the contact resistance. We demonstrate by virtue of device simulations that the ON-OFF-ratio of a short channel transistor is enhanced by orders of magnitude when a Schottky barrier at the injecting contact is intentionally introduced. The key effect is the efficient suppression of the OFF-current while trading in only a small loss in the ON current. We show that, in fact, it is possible to establish a minimal Schottky barrier such that the short channel transistors can be operated without premature turn-on while retaining an ON current as large as expected from Gradual Channel approximation. This strategy is suited for staggered and coplanar transistor architectures.

HL 31.5 Tue 10:30 ZEU 260

Direct Au-C contacts based on biphenylene for single molecule transport — •Narendra P. Arasu and Héctor Vázquez — Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnická 10/112, Prague, Czech Republic

Metal-molecule contacts strongly influence the mechanical, electronic and conducting properties of molecular junctions [1]. Here we use Density-Functional Theory (DFT) and Non-Equilibrium Green's Function (NEGF) methods to study biphenylene-based molecular circuits. We expect that at the Au surface the biphenylene molecule will break a weak intramolecular C-C bond and form covalent bonds to the substrate. Direct Au-C metal-molecule links were shown to be highly-conducting [2,3]. With these Au-C links to the substrate, we then consider several linker groups at the other end of the molecule, which is contacted by a Au tip. We calculate the mechanical properties of the junctions from tip approach trajectories and find that Au-C bonds are stable under the stress induced by the approaching tip. We then discuss the conductance of the junction focusing on the dependence of transport behaviour on linker chemistry.

[1] F. Schwarz et al., J. Phys.: Condens. Matter 26, 474201 (2014).
[2] Z. L. Cheng et al., Nat. Nanotechnol 6, 353-357 (2011).
[3] W. Chen et al., J. Am. Chem. Soc 133, 17160 (2011).

HL 31.6 Tue 10:45 ZEU 260

Controlling the transport in organic electronics via self-assembled Monolayers — •Anja Förster[1], Sibylle Gemming[2,3], and Gotthard Seifert[1] — [1]TU Dresden, Center for Advancing Electronics Dresden (cfaed), 01062 Dresden, Germany — [2]Institute of Ion Beam Physics and Material Research, Helmholtz-Zentrum Dresden Rossendorf, Center for Advancing Electronics Dresden (cfaed), Bautzner Landstr. 400, 01328 Dresden, Germany — [3]Insitute of Physics, TU Chemnitz, 09107 Chemnitz, Germany

Self-assembled monolayers (SAM) can be used to control the transport in organic field-effect transistors. The SAM creates a dipole moment induced electric field that is able to change the major transport type in organic materials.

In the case of fluoroalkyl SAMs, their strong dipole moment induces electric fields up to 10^9 V/m. These fields are strong enough to affect the underlying organic material up to a distance of 10-20 Å from the SAM. Due to the orientation of the dipole moments this leads to a hole dominated transport.

Amine-based SAMs, on the other hand, enhance the electron transport as their dipole moment is counter-directional to the one from fluoroalkyl SAMs. Due to their lower absolute dipole moment, their effect is not as strong as for fluoroalkyl SAMs.

Finally, we exemplarily show for pentacene how the SAM molecules connect to the organic material. The resulting distance of the SAM layer to the organic material determines the maximum strength of the dipole moment induced electric field.

15 min break

HL 31.7 Tue 11:15 ZEU 260

Electronic components embedded in a single graphene nanoribbon — •Peter Jacobse[1,2], Fabian Schulz[3], Adri van den Hoogenband[2], Marc-Etienne Moret[2], Robertus Klein-Gebbink[2], Peter Liljeroth[3], and Ingmar Swart[1] — [1]Debye Institute for Nanomaterials Science, Utrecht University, PO Box 80000, 3508 TA Utrecht, The Netherlands — [2]Princetonplein 1 — [3]2Department of Applied Physics, Aalto University School of Science, PO Box 15100, 00076 Aalto, Finland

On-surface synthesis offers a convenient route to atomically well-defined graphene nanoribbons (GNRs) with a precisely controlled width and edge structure. In addition to monocomponent ribbons, GNR heterojunctions joining two semiconducting segments with different band gaps (through ribbon width) or different band-alignment (through nitrogen substitution) have been demonstrated. The driving force in this direction is to build more functionality into a single ribbon for applications in GNR-based electronics or photovoltaics. However, the GNR equivalents of a metal-semiconductor junction or a tunnel barrier have not yet been realized. We embed these junctions in a single GNR by joining armchair GNRs belonging to the metallic (5-atom wide) and semiconducting (7-atom wide) families through on-surface synthesis. We characterize the atomic scale geometry and electronic structure by combined atomic force microscopy (AFM), scanning tunneling microscopy (STM) and conductance measurements. The GNR equivalent of a tunnel barrier constitutes a first step towards complete electronic devices built into a single GNR.

HL 31.8 Tue 11:30 ZEU 260

Thermoelectric thin films based on a polymer/nanoparticle nanocomposite — •Nitin Saxena[1,2], Mihael Coric[3], Anton Greppmair[4], Jan Wernecke[5], Mika Pflüger[5], Michael Krumrey[5], Martin S. Brandt[4], Eva M. Herzig[3], and Peter Müller-Buschbaum[1,2] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]Center for Nanoscience, LMU München, 80539 München, Germany — [3]TU München, Munich School of Engineering, 85748 Garching, Germany — [4]TU München, Walter-Schottky-Institut and Physik-Department, 85748 Garching, Germany — [5]PTB, BESSY II Helmholtz-Zentrum Berlin, 12489 Berlin, Germany

Thermoelectric materials pose a compelling technology for power generation from renewable energies, since temperature gradients are transformed into voltages and thus electrical power. So far, highly efficient thermoelectrics comprise rare and/or toxic inorganic materials, and require cost- and energy-intensive fabrication. These points hinder their large-scale application. In order to overcome these limitations, we pursue a hybrid approach combining the semiconducting polymer blend PEDOT:PSS for its high electrical conductivity and inorganic nanoparticles in order to reduce thermal conductivity within the thin film. Beside the thermoelectric properties, we investigate the thermal conductivity of pristine PEDOT:PSS and of the hybrid film, in order to ultimately calculate the figure-of-merit ZT. Tender resonant x-ray scattering (T-ReXS) is used to derive a morphological model, and describe the influence of the nanoparticles on the thermoelectric properties.

HL 31.9 Tue 11:45 ZEU 260

Modelling long-term isothermal charge decay in modified PTFE electrets — •Dmitry Rychkov — University of Potsdam, Potsdam, Germany

Electret stability is usually best characterised by means of charge decay as a function of time. In highly stable electret materials, charge-decay measurements require very lengthy experiments even at elevated temperatures. Isothermal charge-decay curves, however, can be modelled if thermally-stimulated discharge data are known. Here, we attempt to deal with this problem for electrets made from chemically modified polytetrafluoroethylene (PTFE) films. PTFE films were treated with TiCl4 vapor in a flow-type reactor and electrically charged in a positive corona discharge. Using the charge-transport theory by Simmons, frequency factors and energy spectra for the relevant surface traps have been extracted from thermally stimulated surface-potential decay curves. The data were then used to calculate isothermal charge-decay curves at different temperatures. A detailed comparison between the modelled and the experimental curves reveals good agreement at elevated temperatures. At lower temperatures, however, the modelled isothermal charge-decay curves deviate from the experimental ones and show a slower decay, which indicates that additional mechanisms that are not covered in the theory may contribute to the electret-charge decay in this temperature range. We propose a simple phenomenological model to illustrate the effects of such mechanisms and to determine the applicability limits of our charge-decay modelling method.

HL 31.10 Tue 12:00 ZEU 260

Large area three-dimensional polarization control in P(VDF-TrFE) polymer films on graphite — •Robert Roth[1], Martin Koch[1], Jakob Schaab[2], Martin Lilienblum[2], Thomas Thurn-Albrecht[1], and Kathrin Dörr[1] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, 06099 Halle, Germany — [2]Department of Materials, ETH Zürich, Vladimir-Prelog-Weg 1-5/10, 8093 Zürich, Switzerland

Ferroelectric polymers are attractive candidates for functional layers in electronic devices like non-volatile memories, piezo- and magnetoelectric sensors, and capacitor-based high speed energy storage devices. Unfortunately, such thin films often reveal low di- and piezoelectric responses due to reduced crystalline and electrical dipole order, leading to compensation effects and low effective electric performance. One of the best characterized and often applied ferroelectric polymers is poly(vinylidene fluoride-co-trifluoroethylene) (P(VDF-TrFE)). We will present results on micron-sized domains with three dimensional ferroelectric polarization alignment in P(VDF-TrFE) films on graphite. The ferroelectric domains have been achieved by a combined procedure of electrical poling and mechanical annealing with an atomic force microscopy tip. They show strongly increased lateral and vertical piezoresponse compared to the as-prepared film and can be deliberately written and switched.

HL 31.11 Tue 12:15 ZEU 260

Significanlty enhanced charging efficiency for higher piezoelectricity in polymer ferroelectrets — •Xunlin Qiu — Department of Physics and Astronomy, University of Potsdam, 14469 Potsdam, Germany

Ferroelectrets are internally charged polymer foams or cavity-containing polymer-film systems. They are charged through a series of dielectric barrier discharges (DBDs) inside the cavities which interact with the internal polymer surfaces [1]. The breakdown strength of the gas strongly influences the charging process. A gas with a lower breakdown strength has a lower charging voltage, but leads to a lower remanent polarization. Charging in gases with higher breakdown strength requires higher voltage but allows higher remanent polarization. Here, a charging scheme involving gas exchange during charging is proposed [2]. The cavities of a tubular-channel fluoroethylenepropylene (FEP) ferroelectret are first filled with helium (lower breakdown strength), so that DBDs can be easily triggered by applying a relatively low voltage. The charging voltage should not be turned off until the gas inside the cavities has been replaced with nitrogen or air (having higher breakdown strength), in order to achieve higher remanent polarization. With the proposed charging scheme, the charging efficiency and hence the resultant piezoelectricity of ferroelectrets can be significantly enhanced.

[1] X. Qiu, W. Wirges and R. Gerhard, J. Appl. Phys. 110, 024108 (2008).

[2] X. Qiu, Appl. Phys. Lett. 109, 222903 (2016).

HL 31.12 Tue 12:30 ZEU 260

Tuning the Electronic Properties of 3D Covalent Organic Networks by Collective Electrostatic Design — •Veronika Obersteiner, Andreas Jeindl, Johannes Götz, Aurelie Perveaux, and Egbert Zojer — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria

Covalent organic frameworks have recently attracted substantial interest as materials for photovoltaics applications, as they can be synthesized mimicking donor-acceptor bulk heterojunctions.

On the basis of first-principle results we propose a novel design strategy for analogous 3D organic networks, where a band offset between different semiconducting segments can be achieved by introducing periodic arrangements of dipolar elements into the material. Exploiting the resulting collective electrostatic effects, we are able to manipulate the electronic landscape of the 3D networks in a controlled way,thereby, achieving spatially confined pathways for electrons and holes. The distinct advantage of this approach over conventional strategies for achieving the band offset by using chemically distinct donor and acceptor units is that the magnitude of the band offset can be tuned continuously. The suggested electrostatic design strategy also enables the realization of more complex structures like quantum-cascades and 'quantum-checkerboards'.

HL 32: Focussed Session: Frontiers in Exploring and Applying Plasmonic Systems I (Joint Session of CPP, DS, HL, MM, and O, organized by DS)

With the increasing importance of plasmonics and the variety of its number of applications it becomes obvious that experimental characterization beyond the far-field optical standard methods and also theoretical tools that access the plasmonic behaviour on the atomic scale are indispensable for further development and improvement of the basic knowledge and thus, for new kinds of applications. The "Focused Session" gathers experts for unusual experimental methods (near-field studies with SNOM and EEL-TEM) and for the theoretical exploration of quantum effects in plasmonic excitations. Furthermore, new kinds of plasmonic applications (devices exploiting phase changes, alternative displays and holograms) will be introduced.

Organizers: Laura NaLiu (U Heidelberg) and Annemarie Pucci (U Heidelberg)

Time: Tuesday 9:30–12:45 Location: CHE 89

Topical Talk HL 32.1 Tue 9:30 CHE 89

Driving nanophotonics to the atomic scale — •Javier Aizpurua — Center for Materials Physics (CSIC-UPV/EHU) and DIPC, San Sebastian, Spain

Plasmonic nanogaps are formed at the junction of two metallic interfaces and provide a great opportunity to explore atomic-scale morphologies and complex photochemical processes by optically monitoring the excitation of their intense surface plasmonic modes. In recent years, optical spectroscopy of these cavities has proven to be extremely sensitive to atomic-scale features that determine the chemistry and the optoelectronics in the gaps. In this regime, classical theories often fail to address the fine details of the optical response, and more sophisticated quantum models based on condensed matter theory techniques are needed. Additionally, theoretical approaches based on quantum electrodynamics (QED) can be properly developed to address the complex coupling of subnanometric optical cavities with electronic and vibrational states of molecules nearby. A few experimental situations in optoelectronics, molecular spectroscopy and optomechanics, where optics is proven to address the atomic scale and thus quantum effects are shown to be of paramount importance, will be described.

Topical Talk HL 32.2 Tue 10:00 CHE 89

Transverse and Longitudinal Resonances in Plasmonic Gold Tapers — Surong Guo[1], Nahid Talebi[1], Wilfried Sigle[1], Ralf Vogelgesang[2], Gunther Richter[3], Martin Esmann[2], Simon F. Becker[2], Christoph Lienau[2], and •Peter A. van Aken[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Carl von Ossietzky University of Oldenburg, Oldenburg, Germany — [3]Max Planck Institute for Intelligent Systems, Stuttgart, Germany

Conically-shaped metallic tapers are one of the most common structures with concomitant capabilities of nanofocusing and field enhancement. We distinguish two different dynamic mechanisms, reflection and phase matching, of surface plasmons excited by relativistic electrons in three-dimensional gold tapers with various opening angles from 5° to 47° which are studied both experimentally and theoretically, by means of electron energy-loss spectroscopy and finite-difference time-domain numerical calculations, respectively. We observe distinct resonances along the taper shaft independent of opening angles. We show that the origin of these resonances is different at different opening angles and results from a competition between two coexisting mechanisms. For large opening angles ($> 20°$), phase matching between the electron field and that of higher-order angular momentum modes is the dominant contribution because of the increasing interaction length between electron and the taper near-field. In contrast, reflection from the taper apex dominates at small opening angles ($< 10°$). A gradual transition of these two mechanisms is observed for intermediate opening angles.

Topical Talk HL 32.3 Tue 10:30 CHE 89

Nanoimaging and control of polaritons in 2D materials — •Rainer Hillenbrand — CIC nanoGUNE, San Sebastian, Spain

A promising solution for active control of light on the nanometer scale are plasmons in graphene, which offer ultra-short wavelengths, long lifetimes, strong field confinement, and tuning possibilities by electrical gating. Here, we discuss scattering-type scanning near-field optical microscopy (s-SNOM) for real-space imaging of graphene plasmons [1-3] in nanoresonators [4] and hBN-graphene heterostructures [5]. We also introduce THz near-field photocurrent nanoscopy and discuss its application for imaging acoustic graphene plasmons in a graphene-based THz detector [6]. Further, we discuss ultraslow hyperbolic volume and surface phonon polaritons in boron nitride flakes [7,8].

[1] J. Chen et al., Nature, 487, 77 (2012) [2] Z. Fei et al., Nature 487, 82 (2012) [3] P. Alonso-González et al., Science 344, 1369 (2014) [4] A. Y. Nikitin et al., Nat. Photon. 10, 239 (2016) [4] A. Woessner et al., Nat. Mater. 14, 421 (2015) [6] P. Alonso-González et al., Nat. Nanotechnol. DOI: 10.1038/nnano.2016.185 [7] E. Yoxall et al., Nat. Photon. 9, 674 (2015) [8] P. Li et al, Nano Lett. DOI: 10.1021/acs.nanolett.6b03920

15 min. break.

Topical Talk HL 32.4 Tue 11:15 CHE 89

Switchable infrared nanophotonic elements enabled by phase-change materials — •Thomas Taubner — Institute of Physics (IA), RWTH Aachen University

The strong confinement and enhancement of light when coupled to surface waves or nanoparticles is key for various applications in nanophotonics such as sensing, imaging or the manipulation of light fields. In the mid-infrared spectral range, metallic nanoantennas and materials supporting surface phonon polaritons (SPhPs) can be used as building blocks of such devices. Often, their optical functionality is only obtained at a fixed wavelength, determined by the geometric design and the material properties.

By using phase-change materials (PCMs) as tunable environment for nanophotonic resonators, their resonance frequency can be altered in a non-volatile, reversible way. PCMs offer a huge change in refractive index due to a phase transition from their amorphous to crystalline state, which can be thermally, optically or electrically triggered. We present results on thermal and optical switching, as well as addressing of individual IR resonances of both systems, metallic nanoantennas and resonators for SPhPs. SPhPs on polar dielectrics exhibit lower losses and larger Q-values compared to metallic nanoantennas, and their confinement can be even increased by adding ultrathin, switchable PCM layers. We show the all-optical, non-volatile, and reversible switching of the SPhPs by controlling the structural phase of the PCM [1], opening the door for re-configurable metasurfaces.

[1] P. Li et al., Nat. Mat. 15, 870 (2016).

Topical Talk HL 32.5 Tue 11:45 CHE 89

Nonlocal response in plasmonic nanoparticles: How much quantum? — •N. Asger Mortensen — Technical University of Denmark

Plasmonics is commonly explored and interpreted within the framework of classical electrodynamics. On the other hand, with the increasing ability to explore plasmonics in nanostructures with yet smaller characteristic dimensions, intrinsic length scales of the electron gas are anticipated to manifest in a nonlocal plasmonic response and other quantum corrections to the light-matter interactions. In nanoparticles, nonlocal response promotes frequency blueshifts and nonlocal damping of high-order modes, as has been observed in single-particle EELS. As to the quantum mechanical origin of these effects, one can quantify the degree of nonclassical effects from an energy perspective. This provides a direct link between the experimentally observed resonance blueshift and the fraction of electromagnetic energy attributed to quantum degrees of freedom.

Topical Talk HL 32.6 Tue 12:15 CHE 89

Short-range plasmonics — •Harald Giessen — University of Stuttgart, Stuttgart, Germany

Short-range plasmons with extreme light compression down to 60 nm with light wavelength of 800 nm are demonstrated. Also, the formation of orbital angular momentum of plasmons with subfemtosecond resolution is studied.

HL 33: Quantum Dots: Optical Properties I

Time: Tuesday 9:30–13:00 Location: POT 81

Invited Talk HL 33.1 Tue 9:30 POT 81

Deterministic Single Quantum Dot Devices: Building Blocks for Photonic Quantum Networks — •Stephan Reitzenstein — Institute of Solid State Physics, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

The emerging field of photonic quantum technologies relies crucially on the availability of practical quantum light sources. Prime candidates to realize such sources are self-assembled semiconductor quantum dots (QDs). This is explained by their superb optical properties in terms of the quantum efficiency, the single photon purity and the high photon indistinguishability. Moreover, QDs allow for the generation of entangled photon pairs and more complex photon states. Still, it is a great challenge to further develop these key building blocks beyond proof-of-principle demonstrations towards scalable quantum devices enabling advanced systems such as multi-partite quantum networks.

In this talk, I will review exciting progress in the field of QD based devices with a focus on the development of practical and efficient quantum light sources for future photonic quantum networks. This includes important aspects such efficient light extraction strategies, deterministic nanoprocessing technologies and the quantum optical evaluation of the photon sources. In particular, I will introduce in-situ electron beam lithography, which allows for the realization of QD based quantum devices with high process yield. The talk will conclude with an outlook on upcoming challenges such as entanglement swapping using QD based quantum light sources.

HL 33.2 Tue 10:00 POT 81

Non-linear two-photon resonance fluorescence of a single artificial atom — •Jonathan Müller, Lukas Hanschke, Per-Lennart Ardelt, Manuel Koller, Tobias Simmet, Alexander Bechtold, Kai Müller, and Jonathan Finley — Walter Schottky Institut, TU-München, 85748 Garching, Germany

Resonance fluorescence that arises from the interaction of a coherent light field with a two level system, has led to the development of numerous physical breakthroughs in atomic quantum optics. Increasing the complexity of the physical systems, first predictions for a non-linear counterpart of resonance fluorescence were made theoretically already 30 years ago.

We present non-linear resonance fluorescence studies for the two-photon excitation of individual semiconductor quantum dots. Monitoring the population evolution for increasing Rabi frequencies we observe an s-shaped behavior as a clear signature of the non-linear excitation process. Quantum optical simulations based on a 4-level system provide excellent agreement with the measurements and reveal the crucial role of the environmental coupling to LA-phonons which leads to a redistribution of the population between the levels. Finally, we directly measure the formation of dressed states in the non-linearly driven system that emerge from the resonant two-photon interaction between the coherent light field and the 4-level artificial atom. Our results open the route for investigating a range of optical phenomena from entangled photon pairs to photon bundles resulting from the coherent non-linear interaction in two-photon resonance fluorescence.

HL 33.3 Tue 10:15 POT 81

Solid-state ensemble of highly entangled photon sources at rubidium atomic transitions — •Michael Zopf[1], Robert Keil[1], Yan Chen[1], Bianca Höfer[1], Jiaxiang Zhang[1], Fei Ding[1,2], and Oliver G. Schmidt[1,3] — [1]Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [2]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstraße 2, 30167 Hannover, Germany — [3]Merge Technologies for Multifunctional Lightweight Structures, Technische Universität Chemnitz, Germany

Semiconductor InAs/GaAs quantum dots grown by the Stranski-Krastanov method are among the leading candidates for the deterministic generation of polarization entangled photon pairs. Despite remarkable progress in the last twenty years, many challenges remain for this material, such as extremely low yield (<1% quantum dots can emit entangled photons), low degree of entanglement, and large wavelength distribution. Here we show that, with an emerging family of GaAs/AlGaAs quantum dots grown by droplet etching and nanohole infilling, it is possible to obtain a large ensemble (close to 100%) of polarization-entangled photon emitters on a wafer without any post-growth tuning. Under pulsed resonant two-photon excitation, all measured quantum dots emit single pairs of entangled photons with ultra-high purity, high degree of entanglement (fidelity up to F = 0.91, with a record high concurrence C = 0.90), and ultra-narrow wavelength distribution at rubidium transitions. Therefore, a solid-state quantum repeater can be practically implemented with this new material.

HL 33.4 Tue 10:30 POT 81

Resonantly excited quantum dots: from quantum beats in temporal domain to two-photon interference of remote sources — •J. H. Weber[1], H. Vural[1], M. Müller[1], C. Schneider[2], S. L. Portalupi[1], S. Höfling[2,3], and P. Michler[1] — [1]IHFG, IQST Center and SCoPE, Universität Stuttgart — [2]Physikalisches Institut, Universität Würzburg — [3]School of Physics and Astronomy, University of St. Andrews, UK

Two-photon interference is a crucial building block for photonic quantum information technology such as linear optical quantum computation and quantum-enhanced phase determination. For such applications, highly indistinguishable single photons are essential. Single semiconductor quantum dots are promising emitters because of their high brightness, indistinguishability and on-demand single photon emission. Resonant excitation is proven to strongly reduce dephasing mechanisms. In the present study, we carry out coherent and on-demand initialization of the two-level system: in contrast to the commonly observed Rabi oscillations, here we prove this coherent initialization by the observation of strongly pronounced quantum beats in the temporal dynamics of the spontaneous emission. Furthermore, high indistinguishability of the subsequently emitted photons could be shown by exploiting the Hong-Ou-Mandel effect. To scale photonic quantum information processing with quantum dots, two-photon interference of distinct sources is crucial. Therefore, two remote quantum dots were tuned into resonance, accomplishing two-photon interference of the on-demand generated resonance fluorescence.

HL 33.5 Tue 10:45 POT 81

Photoelectron generation and capture in the resonance fluorescence of a 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, Germany. — [2]Chair of Applied Solid State Physics, Ruhr-University Bochum, Germany.

The ultimate goal for self-assembled quantum dots (QDs) as single photon sources is a transform-limited photon stream. This goal has not yet been reached, as spectral wandering of the center frequency of the QD transition is still observed. The major sources of this spectral jitter are charge and nuclear spin noise. Charge noise can arise from charging/discharging of trap states that are filled by photoexcited free charge carriers. Furthermore, these photoexcited electrons can relax into the QD, quenching the transitions in a resonant measurement.

Time-resolved resonance fluorescence on a single self-assembled quantum dot (QD) is used to analyze the generation and capture of photoinduced free charge carriers [1]. We directly observe the capture of electrons into the QD as an intensity reduction of the exciton transition and in the appearence of a non-equilibrium trion resonance. The exciton transition is quenched until the captured electron tunnels out of the dot again in the order of milliseconds. Our results demonstrate that even under resonant excitation, excited free electrons are generated and can negatively influence the optical properties of a QD.

[1] A. Kurzmann et al., Appl. Phys. Lett. **108**, 263108 (2016).

Coffee Break

HL 33.6 Tue 11:30 POT 81

Ultrafast electric control of a quantum dot exciton — •Amlan Mukherjee[1,2,3], Alex Widhalm[1,3], Nandlal Sharma[1,3], Andreas Thiede[2,3], Dirk Reuter[1,3], and Artur Zrenner[1,3] — [1]Department Physik, Universität Paderborn, Paderborn, Germany — [2]Höchstfrequenzelektronik, Universität Paderborn, Paderborn, Germany — [3]Center for Optoelectronics and Photonics Paderborn (CeOPP), Universität Paderborn, Paderborn, Germany

The excellent optical properties of single InGaAs QDs combined with ultrafast electric control allow for the realisation of new coherent optoelectronic functionalities. Universal coherent control can be achieved by combining the control of occupancy using optical pulses with phase control using electric pulses within the dephasing time of the ground state QD exciton. To implement fast electric phase control, we have designed a SiGe:C hetero-bipolar electronic circuit for the generation of ultrafast electric signals, which act as phase gates for a single QD. Our current circuit design generates rise times below 15 ps and it is fully operational at liquid Helium temperatures. In Ramsey experiments we demonstrate a coherent electric phase manipulation over up to 20π and the realisation of a π phase change within 35 ps. Also, such ultrafast electrical pulses can be used in combination with cw excitaion to perform an adiabatic rapid passage for robust exciton generation. We report results from our attempts to perform the electrically chirped excitation of an exciton.

HL 33.7 Tue 11:45 POT 81

Highly indistinguishable and strongly entangled photons from symmetric GaAs quantum dots — •Daniel Huber[1], Marcus Reindl[1], Yongheng Huo[2,1], Huiying Huang[1], Johannes S. Wildmann[1], Oliver G. Schmidt[2], Armando Rastelli[1], and Rinaldo Trotta[1] — [1]Institute of Semiconductor and Solid State Physics, Johannes Kepler University, Linz, Altenbergerstr. 69, 4040, Austria — [2]Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstr. 20, 01069 Germany

The development of scalable sources of non-classical light is fundamental to unlock the technological potential of quantum photonics. Among the systems under investigation, semiconductor quantum dots (QDs) are currently emerging as near-optimal sources of indistinguishable single photons. However, experiments on conventional Stranski-Krastanow InGaAs QDs have reported non-optimal levels of entanglement and indistinguishability of the emitted photons. For applications such as entanglement teleportation and quantum repeaters, these criteria have to be met simultaneously. In this talk, I will present a material system that has received limited attention so far: GaAs QDs grown via droplet etching. I will demonstrate that under resonant excitation these highly symmetric QDs deliver photon pairs with high degree of indistinguishability and with an unprecedented degree of entanglement fidelity. The results suggest that if QD entanglement resources will be used for future quantum technologies, GaAs might be the material system of choice
[arXiv:1610.06889] .

HL 33.8 Tue 12:00 POT 81

Deterministically fabricated bright single-photon sources with a backside gold mirror — •Sarah Fischbach[1], Alexander Thoma[1], Esra Burcu Yarar Tauscher[1], Ronny Schmidt[1], Arsenty Kaganskiy[1], Fabian Gericke[1], André Strittmatter[1,2], Tobias Heindel[1], Sven Rodt[1], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Germany — [2]Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg, Germany

Combinations of quantum dots (QDs) and deterministically fabricated microlenses can act as efficient single-photon sources with low $g^{(2)}(0)$-values and a high photon indistinguishability. Applications in the field of advanced quantum communications, however, require in addition high extraction efficiencies as well as a flexible technology platform, which can be extended for strain tuning or electrical contacts.
Here, we realize a deterministic single-photon source based on a QD microlens with a backside gold mirror, providing high reflectivity even at large angles of incidence. The utilized flip-chip process with thermocompression gold bonding was realized with a distance of 60 nm between mirror and QD to achieve a maximum enhancement of the emission. The geometry of the structures is optimized using finite-element simulations. Suitable target QDs are selected by cathodoluminscence lithography at cryogenic temperatures and are integrated into devices by 3D in-situ electron-beam lithography. Photoluminescence measurements demonstrate high extraction efficiencies as well as a second order autocorrelation value $g^{(2)}(0) < 0.02$.

HL 33.9 Tue 12:15 POT 81

Theoretical modelling of absorption spectra from differently charged quantum dots — •Matthias Holtkemper, Doris E. Reiter, and Tilmann Kuhn — Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Semiconductor quantum dots (QDs) are promising structures for realisations in quantum information technology and spintronics. Apart from the ground state exciton also excited exciton states become relevant for dynamical processes like optical spin control, relaxation or charged biexciton cascades. Here we present a systematic analysis of absorption spectra for negatively, neutrally and positively charged QDs with a focus on excited excitonic states. To be specific, we model the QD using kp-theory within a configuration interaction approach. The QD confinement is approximated by a harmonic potential. We include the direct and short range exchange Coulomb interaction. The role of the different interactions is investigated in detail to give a fundamental understanding of the relevant effects. We discuss trends in the spectra while tuning the interaction strengths and study the differences and commonalities between differently charged QDs.

HL 33.10 Tue 12:30 POT 81

Bulk AlInAs on InP(111) as a novel material system for pure single photon emission — •Michael Deppisch[1], Sebastian Unsleber[1], Christian M. Krammel[2], Minh Vo[1], Christopher D. Yerino[3], Paul J. Simmonds[4], Minjoo Larry Lee[3,5], Paul M. Koenraad[2], Christian Schneider[1], and Sven Hoefling[1,6] — [1]Technische Physik and Wilhelm Conrad Roentgen Research Center for Complex Material Systems, Physikalisches Institut, Universitaet Wuerzburg, Am Hubland, D-97074 Wuerzburg, Germany — [2]Department of Applied Physics, Eindhoven University of Technology, Eindhoven 5612 AZ, The Netherlands — [3]Department of Electrical Engineering, Yale University, PO Box 208284, New Haven, CT 06520, USA — [4]Boise State University, Departments of Physics and Materials Science and Engineering, Boise, ID 83725, USA — [5]Department of Electrical and Computer Engineering, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA — [6]SUPA, School of Physics and Astronomy, University of St. Andrews, St. Andrews, KY16 9SS, UK

We report on quantum light emission from bulk AlInAs grown on InP(111) substrates. Indium rich clusters in the bulk $Al_{0.48}In_{0.52}As$ (AlInAs) were observed, resulting in quantum dot (QD)-like energetic traps for charge carriers. QD-like emission signals appear as sharp lines in our photoluminescence spectra at near infrared wavelengths around 860 nm, and with linewidths as narrow as 50 μeV. Moreover, single photon emission is demonstrated as we extract $g^{(2)}$-values as low as $g^{(2)}_{\mathrm{cw}}(0) = 0.05$ for continuous wave excitation and $g^{2}_{\mathrm{pulsed,\ corr}}(0) = 0.24$ for pulsed excitation.

HL 33.11 Tue 12:45 POT 81

Deterministic generation of bright single resonance fluorescence photons from a Purcell-enhanced quantum dot-micropillar system — •Stefan Gerhardt[1], Sebastian Unsleber[1], Yu-Ming He[1,3], Sebastian Maier[1,3], Niels Gregersen[4], Martin Kamp[1], Christian Schneider[1], and Sven Hoefling[1,2,3] — [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 — [4]Department of Photonics Engineering, Technical University of Denmark, Ørsteds Plads, 2800 Kgs. Lyngby, Denmark

We report on the observation of bright emission of single photons generated via pulsed, resonance fluorescence conditions from a quantum dot deterministically centered in a micropillar cavity device via cryogenic optical lithography. The brightness of the QD fluorescence is greatly enhanced on resonance with the fundamental mode of the pillar, leading to an overall device efficiency of $\nu = (74 \pm 4)\,\%$ for a single photon emission as pure as $g^{(2)}(0) = 0.0092 \pm 0.0004$ with a two-photon wave packet overlap up to $\nu = (88 \pm 3)\,\%$.

HL 34: Two-dimensional materials III (joined session with TT)

Time: Tuesday 9:30–13:15 Location: POT 51

HL 34.1 Tue 9:30 POT 51

Optical properties of organic/inorganic and all-inorganic lead halide perovskite nanoplatelets — •Jasmina A. Sichert[1,2], Yu Tong[1,2], Verena A. Hintermayr[1,2], Alexander F. Richter[1,2], Bernhard Bohn[1,2], Lakshminarayana Polavarapu[1,2], Carlos Cardenas-Daw[1,2], Alexander S. Urban[1,2], and Jochen Feldmann[1,2] — [1]Chair for Photonics and Optoelectronics, Department of Physics and Center for Nanoscience (CeNS), Ludwig-Maximilians-Universität (LMU), Amalienstaße 54, 80799 Munich, Germany — [2]Nanosystems Initiative Munich (NIM), Schellingstraße 4, 80799 Munich Germany

In recent years, organic/inorganic and all-inorganic lead halide perovskite have shown great potential for photovoltaics as well as for light-emitting applications. We have successfully synthesized two-dimensional methylammonium and cesium lead halide perovskite nanoplatelets of varying thickness down to one monolayer.[1,2] With decrease in crystal thickness we observed quantum-size effects and an increase in the exciton binding energy. In the extreme case of a perovskite sheet only a single unit cell thick, the screening of the exciton decreases significantly, resulting in a huge exciton binding energy of several hundred meV in the thin nanoplatelets. We conducted time-resolved photoluminescence spectroscopy to further investigate the effect of the crystal thickness on the optical properties of the nanoplatelets.

[1] Sichert et al., Nano Lett. 15, 6521-6527 (2015)
[2] Tong et al., Angew. Chem. 55, 13887-13892 (2016)

HL 34.2 Tue 9:45 POT 51

Band-gap and exciton binding-energy renormalizations due to excited carriers in monolayer TMDs — •Daniel Erben[1], Christopher Gies[1], Malte Rösner[1,2], Alexander Steinhoff[1], Matthias Florian[1], Michael Lorke[1], Tim Wehling[1,2], and Frank Jahnke[1] — [1]Insitute for Theoretical Physics, University of Bremen, Germany — [2]Bremen Center for Computational Materials Science, University of Bremen, Germany

Coulomb interaction between charge carriers in atomically thin layers of transition-metal dichalcogenides (TMDs) has been shown to be exceptionally large due to the weak screening in the thin layer itself. It causes strong renormalization effects which change the electronic properties and the optical response of the material.

We investigate excited-state optical properties of the typical monolayer TMDs MoS_2, $MoSe_2$, WS_2 and WSe_2 by solving the semiconductor Bloch equations on the full Brillouin zone using the SXCH-approximation for the Coulomb interaction. Excitonic resonances shift in absolute value and relative to each other with increasing carrier density. This effect is a result of a band-gap reduction due to many-particle renormalizations and a reduction of the binding energy due to screening of the Coulomb interaction and Pauli blocking, which we analyse and compare in detail for MoS_2, $MoSe_2$, WS_2 and WSe_2. Our calculations predict a transition from a direct to an indirect band-gap in molybdenum and tungsten disulfides in the presence of highly excited carriers. The selenides stay indirect for different excitations.

HL 34.3 Tue 10:00 POT 51

Phase separation and composition fluctuation effects on electronic and optical properties of $(BN)_{1-x}(C_2)_x$ 2D alloy — •Ivan Guilhon[1], Lara K Teles[1], Marcelo Marques[1], and Friedhelm Bechstedt[2] — [1]Grupo de Materiais Semicondutores e Nanotecnologia, Instituto Tecnológico de Aeronáutica, DCTA, 12228-900 São José dos Campos, Brazil — [2]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, D-07743 Jena, Germany

$(BN)_{1-x}(C_2)_x$ alloys are promising materials for band gap engineering in two-dimensional electronics. Despite the importance of microstructural features, such as phase separation and composition fluctuation. The current theoretical studies of such monolayer alloys are often restricted to investigate "guessed" nonrandom structures.

Using DFT calculations combined with a statistical approach to account for disorder effects, we study the properties of these 2D alloys as a function of their average composition. A complete scenario of how thermodynamic conditions affect the distribution of atoms is provided. The solubility limits and critical temperature are studied by constructing a T-x phase diagram.

In this context, we calculate the energy gap as a function of the composition and optical absorbance spectra are predicted for different compositions. Our predictions are compared with the experimental findings. We reproduce the experimentally found absorption spectra with a two-peak pattern for intermediate carbon concentrations and identify them with phase-segregated instead of homogeneous alloys.

HL 34.4 Tue 10:15 POT 51

Electron-phonon interaction in transition metal dichalcogenides — •Nicki F. Hinsche[1], Arlette Sohanfo Ngankeu[2], Sanjoy Mahatha[2], Marco Bianchi[2], Charlotte Sanders[2], Philip Hofmann[2], and Kristian S. Thygesen[1] — [1]Center for Atomic-scale Materials Design, Technical University of Denmark, 2830 Kgs. Lyngby, Denmark — [2]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNANO), Aarhus University, 8000 Aarhus C, Denmark

Atomically thin layers of Transition Metal Dichalcogenides (TMD) attract remarkable interest due to their extraordinary electronic and optical properties and are often quoted as semiconductor analogues of graphene. Possessing direct band gaps in the visible frequency range and exhibiting high electronic mobilities at room temperature, TMD's are emerging candidates for next generation electronic and optoelectronic applications [1]. By means of DFT electronic-structure and Boltzmann transport calculations [2], we discuss the impact of microscopic electron-phonon interaction onto the renormalization of the electronic structure and the phonon-limited electronic transport properties for two prototypical TMD's: TaS_2 and WS_2. Our analysis and conclusions will be drawn closely to recent experimental findings [3].

[1] F. A. Rasmussen and K. S. Thygesen. Journ. of Phys. Chem. C **13** 169 (2015) [2] N. F. Hinsche *et al.*, ACS Nano **9** 4406 (2015) [3] C. E. Sanders *et al.*, Physical Rev. B. **94** 081404 (2016)

HL 34.5 Tue 10:30 POT 51

Spin Degenerate Regimes for Single Two-Dimensional Quantum Dots on Transition Metal Dichalcogenide Monolayers — •Matthew Brooks and Guido Burkard — Department of Physics, University of Konstanz, D-78464, Germany

Strong spin orbit coupling in transition metal dichalcogenides (TMDCs) monolayers results in spin resolvable band structures about the K (K') valleys such that the eigenbasis of a 2D quantum dot (QD) on a TMDC monolayer in zero field is described by the Kramers pairs $|+\rangle = |K'\uparrow\rangle, |K\downarrow\rangle$ and $|-\rangle = |K\uparrow\rangle, |K'\downarrow\rangle$. This coupling limits the usefulness of single TMDC QDs as qubits due to the inherent difficulty of generating superposition states of the valley degree of freedom. Possible regimes of spin degenerate states overcoming the spin orbit coupling in monolayer TMDC QDs are investigated in both zero field, where the spin and valley degrees of freedom become fourfold degenerate, and in some magnetic field, localised to the K' valley. Such regimes are shown to be achieved in MoS_2, where the spin orbit coupling is sufficiently low that the spin resolved conduction bands intersect at points about the K (K') valleys and as such may be exploited by selecting suitable critical dot radii.

HL 34.6 Tue 10:45 POT 51

Electron Spin Relaxation in a Transition-Metal Dichalcogenide Quantum Dot — •Alexander Pearce and Guido Burkard — University of Konstanz, Konstanz, Germany

We study the relaxation of a single electron spin in a circular quantum dot in a transition-metal dichalcogenide monolayer defined by electrostatic gating. Transition-metal dichalcogenides provide an interesting and promising arena for quantum dot nano-structures due to combination of spin-valley physics and strong spin-orbit coupling. First we will discuss which bound state solutions in different B-field regimes can be used as the basis for qubits, at low B-fields combined spin-valley Kramers qubits and at large B-fields spin qubits. Then we will discuss the relaxation of a single electron spin mediated by electron-phonon interaction via various different relaxation channels. Rashba spin-orbit admixture mechanisms allow for relaxation by in-plane phonons arising either from the deformation potential or by piezoelectric coupling, additionally direct spin-phonon mechanisms involving out-of-plane phonons allow for relaxation. We find that the relaxation rates

scale as $\propto B^4$ and $\propto B^2$ for in-plane phonons coupling via deformation potential and piezoelectric coupling respectively, while relaxation due to the direct spin-phonon coupling scales as $\propto B^2$. In the low B-field regime we also discuss the role of impurity mediated spin relaxation which will arise in disordered quantum dots.

Coffee Break

Invited Talk HL 34.7 Tue 11:30 POT 51

Influence of dark states on excitonic spectra of transition metal dichalcogenides — •Malte Selig[1,2], Dominik Christiansen[1], Gunnar Berghäuser[1,2], Ermin Malic[2], and Andreas Knorr[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Berlin, Germany — [2]Chalmers University of Technology, Department of Physics, SE-412 96 Gothenburg, Sweden

In monolayers of transition metal dichalcogenides, excitonic effects play a significant role: Besides bright excitons, dark exciton states are formed by electrons and holes with opposite spin or constitute excitons with non-vanishing center of mass momentum well above the lightcone. Evaluating the excitonic states it turns out, that in tungsten based materials some of these dark states are energetically located below the optical accessible ones. Here, we develope excitonic Bloch equations for excitonic polarizations and densities under the influence exciton phonon interaction, adressing the strong impact of low lying dark states. We investigate the dephasing of the excitonic polarization through exciton phonon scattering [1] and the phonon mediated formation and thermalization of exciton densities. It turns out that coupling to low lying dark states is crucial for luminescence yield and lifetime. The presented results can explain several recent experimental results.

[1] M. Selig et al.,Nature Commun. 7,13279 (2016)

HL 34.8 Tue 12:00 POT 51

Transport measurements in graphene-WSe_2 heterostructures — •Tobias Völkl[1], Tobias Rockinger[1], Martin Drienovsky[1], Kenji Watanabe[2], Takashi Taniguchi[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Universität Regensburg, Germany — [2]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

Bringing graphene into proximity to WSe_2 was proposed as a way to induce a high spin orbit coupling strength in graphene, while maintaining the high intrinsic mobility of graphene. We therefore investigated the transport properties of graphene-WSe_2 heterostructures.

Placing graphene onto a WSe_2-flake resulted in mobilities around 10000 cm^2/Vs of graphene. Further a weak antilocalization behavior was observed, which indicates a high spin orbit coupling strength induced by the WSe_2.

Higher mobilities around 100000 cm^2/Vs were achieved by encapsulation of graphene between WSe_2 and hBN. In these samples no weak antilocalization behavior could be observed. We attribute this to a transition from diffusive to the quasiballistic regime. Also a feature dependent on the sample width arises in the low magnetic field range. We attribute this to a magneto size effect which further indicates quasiballistic behavior.

HL 34.9 Tue 12:15 POT 51

Electrical behavior of the oxidation of atomically thin $HfSe_2$ under ambient conditions — •Christopher Belke, Hennrik Schmidt, Benedikt Brechtken, Johannes C. Rode, Dmitri Smirnov, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover

12 years after the discovery of graphene [1], two-dimensional materials are of rising importance in the research and development section. An example for those layered materials are TransitionMetalDichalcogenide (TMD) with the chemical formula MX_2 , where M is a transition metal and X a chalcogenide [2]. Some materials are very fragile in ambient conditions. One of them is the n-type semiconductor hafnium diselenide ($HfSe_2$) [3]. During the fabrication the samples were prepared under nitrogen atmosphere or were covered with PMMA. An increasing resistance was measured while the sample was oxidized under ambient conditions, as well as a change of the electric field effect was observed.

[1] A. K. Geim et al., Nature Materials, **6**, 183 (2007)
[2] A. K. Geim, and I. V. Grigorieva, Nature **499**, 419 (2013)
[3] M. Kang et al. APL **106**, 143108 (2015)

HL 34.10 Tue 12:30 POT 51

ab initio **study of the transport properties in bulk and monolayer MX_3 (M = Ti, Zr, Hf and X = S, Se) compounds.** — •Yasir Saeed — Qatar Environment and Energy Research Institute (QEERI), Hamad Bin Khalifa University (HBKU), Qatar Foundation, P.O. Box 5825, Doha, Qatar

Two dimensional (2D) materials are best candidates for thermoelectric application due to their low thermal conductivity which is key property to achieve high efficiency for their usage in the filed of energy harvesting. Owing to that, here we present a study on electronic as well as thermal transport of bulk and monolayer MX_3 compounds (M = Ti, Zr, and Hf and X = S and Se) are investigated by by density functional theory and semi-classical Boltzmann theory. The bandgap amounts to rather similar value for bulk and monolayer, only the shape of band near Fermi level changes slightly, which results in a modified effective mass. We found that monolayer MX_3 compounds are good TE materials than bulk. Also *p*-type monolayer TiS_3 has twice large PF at 600 K than its room temperature value. However, monolayer $Zr/HfSe_3$ compounds showing promising behavior as a *n*-type TE materials at elevated high temperature of 600 K. In-plane tensile strain is also possible to tune the bandgap to increase S and disorder the monolayer lattice to minimize κ, therefore turns out to be a highly efficient approach for creating high performance TE materials.

HL 34.11 Tue 12:45 POT 51

Nonlinear Hall voltage from magnetic hot-spots — •Karina A. Guerrero Becerra, Andrea Tomadin, Andrea Toma, Remo Proietti Zaccaria, Francesco De Angelis, and Marco Polini — Istituto Italiano di Tecnologia, via Morego 30, I-16163 Genova, Italy

Electromagnetic simulations have recently shown that specifically designed plasmonic nanostructures are able to enhance and localize an oscillating magnetic field within a micro-meter area. These magnetic hot-spots, generated by forcing the plasmonic resonances of planar nanostructures to generate displacement currents of coil-type shape, have been shown to operate in the NIR [A. Nazir, *et. al.* Nano. Lett., 14, 3166-3171 (2014)] and in the MIR [S. Panaro, *et. al.* Nano. Lett., 15, 6128-6134 (2015)] frequency regions. Operating frequencies can be extended towards the THz regime. Here we propose that magnetic hot-spots might be probed through transport measurements by exploiting the response of the 2D electron gas (2DEG) hosted in a graphene bar, placed within the hot-spot area. We study the response of the 2DEG, being subject to the oscillating in-plane electric field of the radiation driving the coil-type resonance, and to the localized magnetic field induced by it. We found that the response of the graphene 2DEG drives a rectification effect giving rise to a measurable Hall-like dc voltage, being sensitive to the operational frequency of the hot-spot. We discuss the conditions under which the predicted dc voltage is experimentally accessible, within the range of frequencies from THz to MIR. We show that the electric and magnetic fields within the hot-spot launch graphene plasma waves.

HL 34.12 Tue 13:00 POT 51

Exchange Interaction for Quantum Dots in TMDCs — •Alessandro David, Andor Kormanyos, and Guido Burkard — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

We study the properties of double quantum dots in Transition Metal Dichalcogenides (TMDCs) where trapped electrons comprise not only the usual spin and valley degrees of freedom, but also a spin-orbit splitting in the spectrum. The spin-orbit coupling splits the four-fold spin and valley degeneracy into two Kramers pairs with correlated spin and valley states. We consider two different situations where the spin-orbit splitting is either much larger or comparable to the tunneling. Our aim is to use such systems filled with only two electrons for quantum information processing. In the case of large spin-orbit splitting, it turns out that there is a fourfold degenerate ground state (well separated from higher states) where, with a simple redefinition of Pauli matrices, we can obtain a CNOT gate in the same way it was obtained in the quantum computer proposed by Loss and DiVincenzo. In the case of small spin-orbit splitting, we have to consider a 16 dimensional subspace, but it is still possible to obtain a unitary evolution operator, that also depends on the value of spin-orbit splitting.

HL 35: Focus Session: Topological Insulators on Coupled Quantum Wells (joined session with TT)

Time: Tuesday 9:30–12:45 Location: POT 151

Invited Talk HL 35.1 Tue 9:30 POT 151

Edge conduction in the 2D topological insulator candidate InAs/GaSb — •Susanne Mueller, Matija Karalic, Christopher Mittag, Lars Tiemann, Thomas Tschirky, Quansheng Wu, Alexey A. Soluyanov, Atin Nath Pal, Christophe Charpentier, Matthias Troyer, Werner Wegscheider, Klaus Ensslin, and Thomas Ihn — Physics Department ETH Zurich, 8093 Zurich, Switzerland

We have studied transport measurements in mesoscopic Hall bars in the electrically tunable double quantum well structure InAs/GaSb. Helical edge states are predicted to dominate transport in the hybridization gap at zero magnetic field. We measure the non-local resistances and find a scaling according to Landauer-Büttikers expectations for helical edge modes [1]. No dependence on edge length could be observed in these devices, despite recent findings of trivial edges in this material system [2, 3]. To deepen the discussion, we are currently investigating the edge length dependence over a broader range of sample sizes and complete the discussion with clear experimental signature for the inverted phase [4] and the effect of strain on the bulk band structure [5], having in mind that an optimized bulk insulator is a necessary starting point for an edge study.

[1] S. Mueller et al., Phys. Rev. B 92, 081303 (2015)
[2] F. Nichele et al., New J. Phys. 18, 083005 (2016)
[3] B.-M. Nguyen et al., Phys. Rev. Lett. 117, 077701 (2016)
[4] M. Karalic, S. Mueller et al., Phys. Rev. B 94, 241402 (2016)
[5] L. Tiemann, S. Mueller et al., arXiv: 1610.06776

HL 35.2 Tue 10:00 POT 151

Topological Dirac Semimetals in GeSbTe vdW Heterostructures — •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 spectral and topological properties of hexagonal TeSb[Te(GeTe)$_n$]SbTe van-der-Waals (vdW) heterostructures (GST-KH) as a function of strain, GeTe content and spin-orbit coupling (SOC) using density functional theory. We show that C_{3v} rotation symmetry stabilizes a massive 3D topological Dirac semimetal (TDSM) phase [1] in the entire family, thus going beyond previous topological insulator (TI) + normal insulator (NI) superlattice (SL) models [2]. The TDSM bulk Dirac cones move along k_z, proportional to the SOC profile and hybridization balance of corresponding interface states that gives rise to emergent magnetic gauge fields. The avoided crossings naturally allow perturbative hopping to build a tunable TDSM-heterostructure model and to include the c_S protected massive TDSM phase into the SL TI-to-NI transition as an expanded onset of the critical point where TDSM and 3D TI features merge. We attribute the TDSM dispersion of GST-KH to the internal $X(\mathrm{AX})_n$ film between polarizing SbTe caps and thereby create a link to generalized AX_2. To our knowledge, this is the first example of a (massive) TDSM in a vdW superlattice [*].

[*] doi.org/10.13140/RG.2.2.15113.85606

[1] B. Yang and N. Nagaosa, Nature Commun. 5, 4898 (2014)
[2] J. Tominaga et al, Adv. Mat. Inter. 1, 1300027 (2014)

HL 35.3 Tue 10:15 POT 151

Fractional quantum Hall effect in the $N = 2$ Landau level in bilayer graphene — Georgi Diankov[1], •Chi-Te Liang[1,2], François Amet[3,4], Patrick Gallagher[1], Menyoung Lee[1], Andrew Bestwick[1], Kevin Tharratt[1], William Coniglio[5], Jan Jaroszynski[5], Kenji Watanabe[6], Takashi Taniguchi[6], and David Goldhaber-Gordon[1] — [1]Department of Physics, Stanford University, Stanford, California 94305, USA — [2]Department of Physics, National Taiwan University, Taipei 106, Taiwan — [3]Department of Physics, Duke University, Durham, North Carolina 27708, USA — [4]Department of Physics and Astronomy, Appalachian State University, Boone, NC 28608, USA — [5]National High Magnetic Field Laboratory, Tallahassee, Florida 32310, USA — [6]Advanced Materials Laboratory, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305, Japan

To date, most fractional quantum Hall (FQH) studies have focused on the $N = 0$ lowest Landau level (LL). Here we report transport measurements of FQH states in the $N = 2$ LL (filling factors $4 < |\nu| < 8$) in bilayer graphene, a system with spin and valley degrees of freedom in all LLs, and an additional orbital degeneracy in the 8-fold degenerate $N = 0/N = 1$ LLs. In contrast with recent observations of particle-hole asymmetry in the $N = 0/N = 1$ LLs of bilayer graphene. The particle-hole symmetric FQH states in the $N = 2$ LL display energy gaps of a few Kelvin, comparable to and in some cases larger than those of fractional states in the $N = 0/N = 1$ LLs.

Invited Talk HL 35.4 Tue 10:30 POT 151

Progress in Edge Channel Transport of Two-Dimensional Topological Insulators — •Hartmut Buhmann — Physikalisches Institut, EP3, Universität Würzburg, Würzburg, Germany

The discovery of the quantum spin Hall (QSH) effect is already ten years old. However, an undisturbed edge channel transport has rarely been reported especially for samples which exceed a few micrometers in size, even though the QSH-states are protected against backscattering by time reversal symmetry. The reasons are manifold but mainly due to the fact that two-dimensional topological insulators are based on narrow gap semiconductors. Small disturbances and inhomogeneity may already result in potential fluctuations which introduce locally metallic electron or hole puddles. Edge channels traversing such puddles are no longer protected and backscattering destroys the expected perfect quantized conductance.

In this presentation I will review the experimental observations on two-dimensional topological insulators and give examples of how one can achieve almost perfect quantization in narrow gap samples. Taking special care during the fabrication process and taking advantage of charge accumulation at certain interfaces of the sample layer stack it becomes possible to observe quantized edge channel conductance even in sample exceeding the elastic mean free path. With these samples it is now possible to address various still open questions on the specific properties of the transport in helical edge channel as for example aspects of the magnetic field and temperature dependence.

Coffee Break

Invited Talk HL 35.5 Tue 11:30 POT 151

Transport and capacitance in HgTe-based topological insulators — •Dieter Weiss — Universität Regensburg, D-93040 Regensburg, Germany

The discovery of 2D and 3D topological insulators (TI) has opened an exciting area of condensed matter physics. It has been theoretically predicted and recently shown experimentally [1-3] that strained HgTe films constitute a 3D TI with a high-mobility 2D-electron gas enclosing the insulating bulk of HgTe. Here, I will show both transport and capacitance data obtained from different metal-oxide HgTe devices. Using top gates we can tune the gate voltage and thus explore quantum transport and quantum capacitance at different positions of the Fermi level E_F. Experiments on mesoscopic structures like nanowires and antidot superlattices made from strained 3D-HgTe films provide further evidence of the peculiar nature of topological surface states.

Work done in collaboration with D. A. Kozlov, D. Bauer, J. Ziegler, H. Maier, R. Fischer, S. Weishäupl, Z. D. Kvon, N. N. Mikhailov, and S. A. Dvoretsky

[1] C. Brüne et al., Phys. Rev. Lett. **106**, 126803 (2011)
[2] D. A. Kozlov et al., Phys. Rev. Lett. **112**, 196801 (2014)
[3] D. A. Kozlov et al., Phys. Rev. Lett. **116**, 166802 (2016)

HL 35.6 Tue 12:00 POT 151

Gate-tunable spin-charge conversion in single-layer graphene — •Masashi Shiraishi[1], Sergey Dushenko[1], Yuichiro Ando[1], Hiroki Ago[2], Taishi Takenobu[3], Susumu Kuwabata[4], and Teruya Shinjo[1] — [1]Kyoto University, Japan — [2]Kyushu University, Japan — [3]Nagoya University, Japan — [4]Osaka University, Japan

The small spin-orbit interaction of carbon atoms in graphene promises a long spin diffusion length and the potential to create a spin field-effect transistor. However, for this reason, graphene was largely overlooked

as a possible spin-charge conversion material. In this presentation, an electric gate tuning of the spin-charge conversion voltage signal in single-layer graphene is reported [1]. Using spin pumping from an yttrium iron garnet ferrimagnetic insulator and ionic liquid top gate, we determined that the inverse spin Hall effect is the dominant spin-charge conversion mechanism in single-layer graphene. From the gate dependence of the electromotive force we showed the dominance of the intrinsic over Rashba spin-orbit interaction, a long- standing question in graphene research. Our study shows a simple spatial inversion symmetry breaking is not sufficient for generating the inverse Rashba-Edelstein effect, which is contrary to a conclusion in the other study [2].

References: [1] S. Dushenko, M. Shiraishi et al., Phys. Rev. Lett. 116, 166102 (2016). [2] J.B.S. Mendes et al., Phys. Rev. Lett. 115, 226601 (2015).

Invited Talk HL 35.7 Tue 12:15 POT 151

Giant Spin-Orbit Splitting in Inverted InAs/GaSb Double Quantum Wells — •Fabrizio Nichele[1], Morten Kjaergaard[1], Henri J. Suominen[1], Rafal Skolasinski[2], Michael Wimmer[2], Binh-Minh Nguyen[3], Andrey A. Kiselev[3], Wei Yi[3], Marko Sokolich[3], Michael J. Manfra[4], Fanming Qu[2], Arjan J. A. Beukman[2], Leo P. Kouwenhoven[2], and Charles M. Marcus[1] — [1]Center for Quantum Devices and Station Q Copenhagen, Niels Bohr Institute, University of Copenhagen, Universitetsparken 5, 2100 Copenhagen, Denmark — [2]QuTech, Delft University of Technology, 2600 GA Delft, The Netherlands — [3]HRL Laboratories, 3011 Malibu Canyon Road, Malibu, California 90265, USA — [4]Department of Physics and Astronomy and Station Q Purdue, Purdue University, West Lafayette, Indiana 47907 USA

We present transport measurements and numerical simulations that reveal a giant spin-orbit splitting of the bands in inverted InAs/GaSb quantum wells close to the hybridization gap. The splitting results from the interplay of electron-hole mixing and spin-orbit coupling, and can be larger than the hybridization gap. We experimentally investigate the band splitting as a function of top gate voltage for both electronlike and holelike states. Unlike conventional, noninverted two-dimensional electron gases, the Fermi energy in InAs/GaSb can cross a single spin-resolved band, resulting in full spin-orbit polarization. In the fully polarized regime we observe exotic transport phenomena such as quantum Hall plateaus evolving in e^2/h steps and a nontrivial Berry phase.

HL 36: Organic Semiconductors (joined session with CPP, DS)

Time: Tuesday 9:30–13:15 Location: POT 251

HL 36.1 Tue 9:30 POT 251

Femtosecond time-resolved spectroscopy of an acceptor-donor-acceptor oligomer film — •Ephraim Sommer[1], Antonietta De Sio[1], Elena Mena-Osteritz[2], Peter Bäuerle[2], and Christoph Lienau[1] — [1]Institut für Physik, Carl-von-Ossietzky Universität Oldenburg — [2]Institut für Organische Chemie II und Neue Materialien, Universität Ulm

Conjugated oligomers are gaining increasing popularity for application in organic solar cells as photoactive materials thanks to their high production reproducibility and device efficiencies [1]. However, a detailed understanding of the initial charge transfer in such systems is missing. Recently, in polymer based active materials it was found that coherent vibronic coupling plays an important role in this process [2]. This raises the question whether this also holds for oligomers. To answer this, we investigate a novel A-D-A-type oligomer by pump-probe and 2D electronic spectroscopy with femtosecond time resolution. Upon selective excitation of the donor unit, we observe strong peak-shifts of the exciton signals as a most dominant feature at early times. Moreover, the signal shows long lived vibrational oscillations. Such a peak shift cannot be explained within a vibronically coupled dimer model including only one dominant vibrational mode like in [2]. Our preliminary results suggest that the photoinduced charge transfer may occur via a conical intersection between the donor and acceptor potential energy surfaces. We will discuss theoretical modelling aimed at validating this idea.

[1] R. Fitzner et al., Adv. Funct. Mater., 12, (2015)
[2] A. De Sio et al., Nat. Commun., 7, (2016)

HL 36.2 Tue 9:45 POT 251

Polariton bottleneck dynamics in organic microcavities — •Felix Lemke, Hartmut Fröb, and Karl Leo — IAPP, TU Dresden, Germany

Organic molecules are known to be promising candidates for strong coupling experiments due to their large exciton binding energy. Simultaneously, organic materials reveal large inhomogeneously broadened absorption spectra, complicating the investigation. Even so, small organic molecules have advantages in processing, stability (to ambient conditions and high optical excitation) and lifetime.

In this work we will present a method to investigate the microcavity polariton properties utilizing the oligomer Bu4-Ph4-DIP. We perform angle-resolved streak camera measurements and compare the data with a rate-equation model. Simulation and measurement agree very well. From this, we can see directly the influence of the polariton bottleneck, which proofs, that our system is in the strong coupling regime. Moreover, we can extract the characteristic time constants and gain an insight into the polariton dynamics.

HL 36.3 Tue 10:00 POT 251

Charge-exciton quenching in organic transistors — •Wouter Koopman[1,2], Stefano Toffanin[2], and Michele Muccini[2] — [1]Universität Potsdam, Potsdam, Deutschland — [2]CNR-ISMN, Bologna, Italien

Organic Light-Emitting Transistors (OLETs) possess a huge potential for the design of highly integrated multifunctional optoelectronic systems and intense nanoscale light sources, such as the long-searched-for electrically pumped organic laser. In order to fulfill these promises, the efficiency and brightness of the current state-of-the-art devices have to be increased. The dominating quenching process limiting the external quantum efficiency in OLETs is charge-exciton interaction. A comprehensive understanding of this quenching process is therefore of paramount importance. The present talk reports a systematic investigation of charge-exciton interaction in organic transistors employing time-resolved photoluminescence electro-modulation (PLEM) spectroscopy on the picosecond timescale. The results show that the injected charges reduce the exciton radiative recombination in two ways: (i) charges may prevent the generation of excitons and (ii) charges activate a further non-radiative channel for the exciton decay. Moreover, the transient PLEM measurements clearly reveal that not only trapped charges, as it is was already reported in literature, but rather the entire injected charge density contributes to the quenching of the exciton population. Finally, lessons for the design of high-efficiency OLET are disused.

HL 36.4 Tue 10:15 POT 251

Investigating the doping efficiency of organic semiconductors by thermoelectric measurements — •Bernhard Nell[1], Markus Krammer[2], Karin Zojer[2], and Koen Vandewal[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials, Technische Universität Dresden, Dresden, Germany — [2]Institute of Solid State Physics, Technische Universität Graz, Graz, Austria

We use thermovoltage (Seebeck effect) and temperature-dependent conductivity measurements on doped organic semiconductors to determine the dominating type of charge carriers introduced by the dopant and to gain insight into the position of the transport level with respect to the Fermi level. The investigation of fullerene dopants with a high degree of fluorination in various amorphous host materials allows us to tune the energy level offset between host and dopant and to study their influence on Fermi level position and overall doping efficiency systematically. Combining thermoelectric measurements with Kinetic Monte Carlo simulations gives further insight into the influence of Coulomb interactions on the trapping of mobile charge carriers in doped organic semiconductors. We find that at low doping concentrations a high amount of charge carriers is immobilized in trap states, leading to a reduced doping efficiency. Upon increasing the doping concentration, the trap states are subsequently passivated and an increased doping efficiency can be observed. Furthermore the doping efficiency

is increased upon fluorination of the dopant molecules and we find a correlation between the energy level offset and the doping efficiency, at the same molar concentration.

HL 36.5 Tue 10:30 POT 251

Vibronic coherence in a reference organic photovoltaic blend — •Antonietta De Sio[1], Ephraim Sommer[1], James Lim[2], Susana F. Huelga[2], Martin B. Plenio[2], Giulio Cerullo[3], and Christoph Lienau[1] — [1]Institut für Physik, Universität Oldenburg, Germany — [2]Institut für Theoretische Physik, Universität Ulm, Germany — [3]Department of Physics, Politecnico di Milano, Italy

The microscopic mechanisms underlying charge separation in organic solar cells are still highly debated. Although recent theoretical work [1] suggests that vibronic couplings may lie at the origin of efficient charge generation in such systems, clear experimental evidence on the role of vibronic coherence for charge separation is still lacking. Here we use ultrafast two-dimensional electronic spectroscopy with 10-fs time resolution to investigate the initial dynamics of excitons and polaronic species in P3HT and P3HT:PCBM thin films with different acceptor concentration. Our experimental results, supported by theoretical simulations, show that strong vibronic coupling favors exciton delocalization and accelerates charge separation even in presence of disorder, resulting in long-lived coherent oscillatory dynamics of strongly correlated excitons and polaron pair states, mutually coupled to a dominant vibrational mode. These results allow us to gain fundamental new insights into the initial dynamics of charge separation and may open up new perspectives for optimizing devices [2,3].

[1] Tamura et al, JCP 137, 22A540, 2012. [2] Falke et al, Science 344, 1001, 2014. [3] De Sio et al, Nat.Commun. 2016 in press.

HL 36.6 Tue 10:45 POT 251

Crystalline Packing Motifs in Pentacene-like Organic Semiconductors — •Michael Klues and Gregor Witte — Fachbereich Physik, Universität Marburg, Germany

While the impact of chemical modifications on the molecular electronic system can be well computed, the influence on solid state properties is hardly predictable. In fact already slight chemical modifications, like the introduction of heteroatoms or small side groups, often lead to dramatically changed crystal structures and thereby rather different charge carrier mobilities or exciton binding energies. Within a comparative study of various pentacene-like organic semiconductors, based on a Hirshfeld analysis [1] we reveal correlations between molecular properties and packing motives. By choosing molecules with nearly identical geometrical dimensions the complexity of intermolecular interactions is considerably reduced and effects of electrostatic potentials, hydrogen bonds and atom sizes can be carved out. Thereby, we attain a simple rule for predicting the occurrence of herringbone packing motifs and point out the relevance of hydrogen bonds for parallel molecular arrangements as found previously for partially fluorinated HBC. [2] Furthermore we suggest a route to increase intermolecular orbital overlap by integration of large heteroatoms in the periphery of aromatic systems which yields an improved charge carrier mobility in the case of DNTT.

[1] M.A Spackman; D. Jayatilaka, CrystEngComm, 11, 19, (2009)

[2] T. Breuer et al., Phys. Chem. Chem. Phys., (2016), DOI: 10.1039/C6CP06126E

Coffee Break

HL 36.7 Tue 11:30 POT 251

Strongly reduced inhomogeneous broadening of molecular aggregates in hybrid nanostructure system — •Xuan Trung Nguyen[1], Antonietta De Sio[1], James Lim[2], Alexandra Markovic[3], Julia Witt[3], Gunther Wittstock[3], Susana Huelga[2], Martin Plenio[2], and Christoph Lienau[1] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg, Germany — [2]Institut für Theoretische Physik and IQST, Universität Ulm, Germany — [3]Institut für Chemie, Carl von Ossietzky Universität Oldenburg, Germany

The applications of nanostructures based on organic molecular aggregates range from solar cells to all-optical switching. These aggregates are often modeled as disordered systems that exhibit inhomogeneously broadened absorptive line shapes. In such a system, disorder localizes the exciton wavefunction and leads to limited exciton transport efficiency, which is important in devices like solar cells. By using linear and non-linear spectroscopy, we show that the inhomogeneous broadening of a model J-aggregate cyanine dye is strongly reduced in the presence of an ultrathin gold layer and the resulting optical spectra display almost perfect Lorentzian line shapes. Supported by theoretical simulations, we explain the experimental results in terms of increased delocalization of the exciton wavefunction due to electronic coupling to surface plasmon polaritons supported by the aggregate-gold. This coupling can average out the disorder effect and thus increase the exciton transport efficiency.

HL 36.8 Tue 11:45 POT 251

The Influence of Molecular Packing on Charge-Transfer States at the Pentacene/Perfluoropentacene Interface — •Andre Rinn[1], Tobias Breuer[1], Julia Wiegand[2], Michael Beck[2], Jens Hübner[2], Michael Oestreich[2], Gregor Witte[1], and Sangam Chatterjee[3] — [1]Faculty of Physics and Materials Science Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, D-30167 Hannover, Germany — [3]Institute of Experimental Physics I, Justus-Liebig University Giessen, Heinrich-Buff-Ring 16, D-35392 Gießen, Germany

We study different model systems of intermixed and layered heterostructures of pentacene and perfluoropentacene by means of time resolved photoluminescence spectroscopy to investigate the impact of molecular packing at the interface on the optical properties. We assign the different PL signals visible in the heterostructures to their respective origin and find an increase in the PL intensity of the charge-transfer signal for pi-stacking at the interface. Significantly slower carrier dynamics are measured for the charge-transfer states when compared to bulk exciton emission which are quenched by singlet exciton fission.

HL 36.9 Tue 12:00 POT 251

Three-dimensional confinement and exciton-polaritons in open organic microcavities — •Simon Betzold[1], Marco Dusel[1], Jürgen Ohmer[2], Utz Fischer[2], Christof P. Dietrich[1], and Sven Höfling[1,3] — [1]Technische Physik, Universität Würzburg — [2]Institut für Biochemie, Universität Würzburg — [3]SUPA, School of Physics and Astronomy, University of St Andrews

Frenkel excitons, characteristic of organic semiconductors, possess large binding energies making them stable at room temperature, rendering polariton experiments at ambient air conditions possible. Organic materials further exhibit very large oscillator strengths and thus strongly interact with a cavity field. Since organic materials are very sensitive to the deposition of semiconductor layers on top of them, we use an open cavity system, which makes non-invasive investigation 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 exemplary investigate the strong exciton-photon coupling between a fluorescent protein and the dielectric cavity. We emphasize that the open cavity approach can easily be extended to more complex systems like photonic lattices and active regions including 2D monolayer materials or hybrid organic-inorganic bilayers.

HL 36.10 Tue 12:15 POT 251

Improving lasing properties of a hybrid OLED/microcavity structure — •Stefan Meister, Robert Brückner, Markas Sudzius, Hartmut Fröb, and Karl Leo — IAPP, TU Dresden, Germany

Organic materials have many advantages which can be utilized in different kinds of devices such as light-emitting diodes, solar cells, or even lasers. Some examples are the spectrally separated broad absorption and emission spectra, the possibility to build very thin and flexible devices, and the fact of having an intrinsic four-energy-level-system.

The goal of realizing an electrically driven organic solid state laser is so far well beyond reach. As a first step, we incorporate an OLED into a microcavity (MC) consisting of two Distributed Bragg Reflectors (DBR). These devices are investigated electrically and with a microphotoluminescence setup to determine the optical functionality. The optical measurements further allow to compare it to standard organic MCs. These insights are analyzed and addressed with the help of photolitography to improve the quality of the metal layers. Further, different very thin (60nm - 0.15mm) encapsulation methods are tested

to allow measurements under ambient conditions.

HL 36.11 Tue 12:30 POT 251

High temperature stable single carrier hole only devices — •Shahidul Alam[1,2], Peter Fischer[3], Ulrich S. Schubert[1,2], and Harald Hoppe[1,2] — [1]Center for Energy and Environmental Chemistry Jena (CEEC Jena) Friedrich-Schiller-Universität Jena Philosophenweg 7a 07743 Jena, Germany — [2]Institute of Organic and Macromolecular Chemistry Friedrich-Schiller-Universität Jena Humboldtstr. 10 07743 Jena, Germany — [3]Institut für Werkstofftechnik, TU Ilmenau, Gustav-Kirchhoff-Str. 6, 98693 Ilmenau, Germany

Thin hole transport layers (HTL) are crucial elements in organic semiconductor based devices. Metal oxides are an encouraging material class for this purpose. Metal oxides can be used to modify either of the two contacts in a device for improved wettability as well as chemical and electronic compatibility of the contacts with the organic layer. Several materials like NiO, V2O5, WO3 and MoO3 have demonstrated encouraging prospective for performing as efficient charge transport layers. Among them molybdenum oxide (MoO3) attracted extensive interest due to its superior performance. In order to evaluate charge transport properties of annealed semiconductor films, devices are required to be stable at high annealing temperature. Whereas PEDOT:PSS has generally proper charge injection and extraction properties, these may drastically change upon heating above certain temperature. In this work, we show that a MoO3 interlayer can efficiently substitute PEDOT:PSS as hole transport layer within single carrier hole only devices (SCHD), because of its better stability at high annealing temperature.

HL 36.12 Tue 12:45 POT 251

Tuning the conductivity in organic-based charge-transfer materials: A combined NEXAFS and electrical transport study — •Antonia Morherr[1], Sebastian Witt[1], Alisa Chernenkaya[2], Katja Medjanik[2], Gerd Schönhense[2], Harald O. Jeschke[3], Roser Valentí[3], and Cornelius Krellner[1] — [1]Physikalisches Institut, Goethe Universität, 60438 Frankfurt am Main — [2]Institut für Physik, Johannes Gutenberg-Universität, 55099 Mainz — [3]Institut für theoretische Physik, Goethe Universität, 60438 Frankfurt am Main

Single crystals of the novel charge transfer complexes phenanthrene- and picene/TCNQ-F_x (x=0,2,4) were grown by physical vapor transport [1] and investigated by electrical transport measurements, near-edge X-ray absorption spectroscopy (NEXAFS) and density functional theory calculations. The electrical conductivity and the mobility of the samples increase with increasing acceptor strength. The activation energy of the complexes was studied by temperature dependent measurements and compared to the electrical band structure investigated by NEXAFS [2]. The results were compared to the DFT calculations for the electrical band structure and simulated NEXAFS spectra.

[1] A. Morherr et al., Physica B 496, 98-105 (2016)
[2] A. Chernenkaya et al., J. Chem. Phys. 145, 034702 (2016)

HL 36.13 Tue 13:00 POT 251

Three-dimensional photonic confinement of imprinted pillars in an organic Tamm-plasmon structure — •Marco Dusel[1], Simon Betzold[1], Christof P. Dietrich[1] und Sven Höfling[1,2] — [1]Technische Physik, Julius-Maximilians-Unversität Würzburg, Am Hubland, 97074 Würzburg — [2]SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, UK

The fluorescence of organic solids at room temperature is governed by the radiative decay of Frenkel excitons that are characterized by large exciton binding energies and short Bohr radii compared to inorganic semiconductors. Due to their very large oscillator strength, organic materials further strongly interact with light, in particular in microcavities.

So far, photonic confinement within the cavity plane has mainly been achieved by tailoring the dielectric part of the cavity. Here, we present a novel technology that enables 3D photonic confinement within the active organic layer of a Tamm-plasmon structure (metal-clad cavity) by laterally imprinting pillars. The fabricated pillars have diameters ranging from 7 to 20 μm and heights between 2 and 4 μm. The developed technology enables far more complicated photonic potentials including coupled pillars, chains and lattices.

HL 37: III-V Semiconductors

Time: Tuesday 9:30–12:30 Location: POT 112

HL 37.1 Tue 9:30 POT 112

GaAs Based Nanowire Lasers and their integration onto Silicon Waveguides — •Tobias Kostenbader, Thomas Stettner, Jochen Bissinger, Daniel Ruhstorfer, Philipp Zimmermann, Gerhard Abstreiter, Gregor Koblmüller, and Jonathan Finley — Walter Schottky Institut and Physik Department, Technische Universität München

III-V semiconductor nanowires (NW) have been demonstrated to be a highly promising candidate for nanoscale coherent light sources suitable for on-chip data communication [1].

In this work we present a study of coaxial GaAs-AlGaAs NW lasers with either bulk GaAs or single and multiple coaxial GaAs quantum wells (QW) as active gain media. We observe single mode lasing of both bulk and core-multishell NW lasers, as confirmed by characteristic s-shaped input-output behavior when subject to optical pumping, as well as a blueshift of the emission due to quantum confinement in the QWs. We show that the emission energy and gain of the NW laser can be controlled epitaxially during growth.

Furthermore, we present a monolithic integration scheme that enables the site-selective growth of GaAs-AlGaAs core-shell NW lasers on silicon-on-insulator and silicon ridge waveguides (WGs). Here, an 80nm thick dielectric interlayer at the NW-WG interface ensures high modal reflectivities and allows lasing operation on the ridge WG. Our results represent a step towards III-V NW lasers that can be site-selectively integrated on silicon.

[1] B. Mayer, et al. Nano Lett. 16 (1), pp 152-156(2016).

HL 37.2 Tue 9:45 POT 112

Ferromagnetic (Ga,Mn)P: magneto-transport properties and co-doping effect — •Chi Xu[1,2], Ye Yuan[1,2], Mao Wang[1,2], Hendrik Hentschel[1,2], Roman Böttger[1], Manfred Helm[1,2], 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]Technische Universität Dresden, D-01062 Dresden, Germany

The III-Mn-V based diluted magnetic semiconductor offers an opportunity to explore various aspects of carrier transport in the presence of cooperative phenomena. In this work, GaP is chosen as a host semiconductor for magnetic dopants due to its large bandgap (2.2 eV) and short bond length (0.545 nm) with the possibility of obtaining strong p-d hybridization . We have prepared Mn-doped GaP by combining ion implantation and pulsed laser melting and make a systematic investigation on the magnetic and transport properties of (Ga,Mn)P by varying Mn concentration as well as by Zn co-doping. All samples show insulating behavior and different negative magnetic resistance are observed, which indicate that the local moment from Mn 3d electrons have interaction with the holes introduced by Zn co-doping.

HL 37.3 Tue 10:00 POT 112

GaSb-based Double Barrier Resonant Tunneling Diodes with Ternary Emitter Prewells — •Andreas Pfenning[1], Georg Knebl[1], Fabian Hartmann[1], Robert Weih[1], Andreas Bader[1], Monika Emmerling[1], Martin Kamp[1], Sven Höfling[1,2], and Lukas Worschech[1] — [1]Technische Physik, Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), 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

We demonstrate room temperature operation of GaSb/AlAsSb double barrier resonant tunneling diodes with pseudomorphically grown emitter prewell structures consisting of the ternary compound semiconductors GaInSb and GaAsSb. At room temperature, no resonant tunneling is observed for structures without emitter prewells. For resonant tunneling structures comprising emitter prewells, room temperature resonant tunneling is evident with pronounced current resonances and regions of negative differential resis-

tance. The respective peak-to-valley current ratios are 1.45 and 1.36 for $Ga_{0.84}In_{0.16}Sb$ and $GaAs_{0.05}Sb_{0.95}$ emitter prewells, respectively. The incorporation of a ternary emitter prewell leads to an enhanced Γ-L valley energy separation with respect to bulk GaSb. A repopulation of the Γ-valley states and a depopulation of the L-valley states is achieved and undesired transport channels via L-valley states are reduced.

HL 37.4 Tue 10:15 POT 112

In-Plane Gate transistors for use of sensing gaseous and liquid dielectric environments. — •Benjamin Feldern, Sascha R. Valentin, Arne Ludwig, and Andreas D. Wieck — Angewandte Festkörperphysik, Ruhr-Univesität Bochum, 44801 Bochum, Germany

For the purpose of sensing dielectrics, In-Plane-Gate (IPG) transistors are written in Gallium-Arsenide based high-electron-mobility-transistor (HEMT) structures using focused ion beam implantation. These FIB-implanted IPGs are to be used to sense dielectrics in different compositions. Using the Petrosyan-Stikh formula for the depletion length of the implanted region in addition to the representation of the IPG by a parallel-plate geometry by de Vries and Wieck, the dielectric constant of the environment can be calculated and analysed. We demonstrate an influence of the dielectric on the properties, while a quantitative analysis still shows some deviations. Beyond this, also surface treatments were performed and tested on their influence of the sensing capability. It was found that surface depletion was increased by both exposure of the IPGs to an N_2-Plasma as well as dipping in N_2H_8S.

HL 37.5 Tue 10:30 POT 112

Bond strength inversion in (In,Ga)As — •Stefanie Eckner[1], Konrad Ritter[1], Philipp Schöppe[1], Erik Haubold[1], Sven Bauer[1], Erich Eckner[2], Mark C. Ridgway[3], and Claudia S. Schnohr[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Institut für Optik und Quantenelektronik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [3]Department of Electronic Materials Engineering, Research School of Physics and Engineering, The Australian National University, Canberra ACT 0200, Australia

Mixed semiconductors feature different first nearest neighbour pairs whose bond stretching force constants determine fundamental material properties, including their vibrational behaviour and the local atomic arrangements. The latter are particularly crucial for strained thin films and nanostructures and influence other key material properties like the band gap energy. In this study, (In,Ga)As grown by metal organic chemical vapour deposition was studied using extended x-ray absorption fine structure spectroscopy. Measurements were performed at the Ga-K- and In-K-edge at nine different temperatures. The resulting temperature evolution of the bond length variation yields the Ga-As and In-As effective bond stretching force constants. The values obtained for the ternary alloys show a remarkable size inversion with regard to the values in the binary materials, meaning that bond stretching force constants determined for binary III-V-semiconductors are not readily transferable to ternary systems.

Coffee Break

HL 37.6 Tue 11:15 POT 112

Optical confinement and conversion of exciton polaritons in a structured (Al,Ga)As microcavity — •Alexander S. Kuznetsov, Paul Helgers, Klaus Biermann, and Paulo V. Santos — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

Optical microcavity (MC) exciton polaritons (EPs) are strongly coupled light-matter entities useful for studying quantum phenomena. Due to the macroscopic de Broglie wavelength and small effective mass of EPs, effects of confinement and quantum phases manifest themselves in micrometer sized potentials and Kelvin-temperature range. In particular, confinement of EPs by dynamic acoustic potentials [1] and optical beams [2] benefits realization and manipulation of Bose-Einstein-like quantum phases of EPs. Here we show that much stronger EPs confinement occurs in laterally structured (Al,Ga)As MC fabricated by etching-MBE-overgrowth technique. Lateral confinement is due to the cavity geometry and thus purely optical. This allows for investigation of localization and motion of unperturbed EP gas. Spatially resolved photoluminescence studies reveal quantization of EPs dispersion and wave functions amplitudes due to the confinement, typical of such structures [3]. Closer optical examination reveals conversion of EP to bare excitons and vice-versa across the strong coupling boundaries, a new possibility for manipulation of quantum information.

[1] E. A. Cerda-Méndez et al., PRL 111, 146401 (2013)
[2] J. Schmutzler et al., Phys. Rev. B 91, 195308 (2015)
[3] R. I. Kaitouni et al., Phys. Rev. B 74, 155311 (2006)

HL 37.7 Tue 11:30 POT 112

Evaluation of growth parameters of InAs nanowires toward vertical field effect transistor devices — •Stampfer Lukas, Jonathan Becker, Stefanie Morkötter, Julian Treu, Gerhard Abstreiter, Jonathan J. Finley, and Gregor Koblmüller — Walter Schottky Institut and Physik Department, Technische Universität München, 85748 Garching

InAs nanowires (NWs) show great promise for future electronic applications due to their high charge-carrier-mobility, their integrability on common silicon semiconductor technology and the feasibility of high precision epitaxial on-chip-growth. The unique geometrical shape and high aspect ratio of NWs allow for effective wrap gating on standing NWs and therefore hold great potential for field effect transistors with low subthreshold-swing and minimized short-channel effects.

In this work the effects of growth conditions of nominally undoped InAs were evaluated with respect to the structural and electrical transport properties. The catalyst-free MBE grown NWs were characterized via HRTEM and back-gated planar 4-terminal measurements. The electrical measurements revealed room-temperature mobilities ranging from 500 to 2200 $\frac{cm^2}{Vs}$ depending on growth conditions, on-off ratios above 103 at 4.2 K and an electron density of of $10^{17}\,cm^3$ limited by surface state mediated electron accumulation. From temperature-dependent FET measurements different carrier activation behavior was found and directly correlated with the different microstructure. First endeavors in the fabrication of vertical single-NW InAs FET devices via advanced selective area epitaxy growth are presented.

HL 37.8 Tue 11:45 POT 112

Strain distribution in highly mismatched GaAs/(In,Ga)As core/shell nanowires — •Leila Balaghi[1,2], René Hübner[1], Genziana Bussone[3], Raphael Grifone[3], Mahdi Ghorbani[1], Arkady Krasheninnikov[1], Gregor Hlawacek[1], Jörg Grenzer[1], Harald Schneider[1], Manfred Helm[1,2], and Emmanouil Dimakis[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]cfaed, TU Dresden, 01062 Dresden, Germany — [3]PETRA III , Deutsches Elektronen-Synchrotron (DESY), 22607 Hamburg, Germany

The core/shell nanowire (NW) geometry is suitable for the pseudomorphic growth of highly mismatched semiconductor heterostructures, where the shell thickness can exceed significantly the critical thickness in equivalent planar heterostructures. We have investigated the accommodation of misfit strain in self-catalyzed GaAs/(In,Ga)As core/shell NWs grown on Si(111) substrates by molecular beam epitaxy. The NWs have their axis along the [111] crystallographic direction, six $\{1\bar{1}0\}$ sidewalls, and their crystal structure is predominantly zinc blende. For strain analysis, we used Raman scattering spectroscopy, transmission electron microscopy, X-ray diffraction and photoluminescence spectroscopy. Within a certain range of core/shell dimensions and shell composition, our findings reveal that the elastic energy in NWs without misfit dislocations can be confined exclusively inside the core, allowing for the shell to be strain-free. The experimental results are also compared with theoretical simulations of the strain (continuum elasticity theory) and phonon energy (density functional theory).

HL 37.9 Tue 12:00 POT 112

Formation of self-organized nanostructures by droplet epitaxy on AlGaAs(111)B — •Alexander Karlisch and Dirk Reuter — Optoelektronische Materialien und Bauelemente, Universität Paderborn, 33098 Paderborn, Germany

Quantum dots (QDs) on the (111)-surface of (Al)GaAs are potential emitters of entangled photons due to the reduced fine structure splitting. QDs on this surface can be grown by the droplet epitaxy (DE) method, where group III metal droplets are formed in a first step and crystallized under As-flux in a second step. In this contribution we present a study on the formation of group III metal droplets on $Al_{0.33}Ga_{0.66}As$(111)B and their crystalization due to an As flux. The samples are grown by solid-source molecular beam epitaxy on a GaAs(111)B substrate with 1° miscut towards (211). Atomic-force microscopy measurements show density and shape of nanostructures

formed by DE at different substrate temperatures and deposition rates after droplet formation and after crystallization, respectively.

HL 37.10 Tue 12:15 POT 112

Optical Characterization of Quaternary GaInAsBi Semiconductor Alloys — •Julian Veletas[1], Lukas Nattermann[1], Thilo Hepp[1], Kerstin Volz[1], and Sangam Chatterjee[2] — [1]Faculty of Physics and Materials Science Center, Philipps-Universität Marburg, D-35032 Marburg, Germany — [2]I. Physikalisches Institut, Justus-Liebig-Universität Gießen, D-35392 Gießen, Germany

Dilute bismuth-containing semiconductor alloys such as GaAsBi are attracting significant attention due to their promising characteristics in near- and mid-infrared laser applications. The incorporation of Bismuth leads to a strong reduction of the bandgap commonly described by an anti crossing process in the valence bands of the host material. Consequently, the split-off band separation ΔSO also increases. This leads to a suppression of non-radiative Auger recombination and, thus an enhanced performance of future devices. For example, ΔSO even surpasses the bandgap energy Egap for more than 4% bismuth incorporation in GaInAsBi alloys. Here, we study a series of GaInAsBi/GaInAs/InP epilayers grown by metal-organic vapor-phase epitaxy. Modulation spectroscopy is applied to identify the optical transitions in the quaternary alloy. Comparing the results with temperature-dependent photoluminescence data measurements reveals only a small Stokes Shift and very little disorder signatures.

HL 38: Zinc Oxide

Time: Tuesday 9:30–11:15 Location: POT 06

HL 38.1 Tue 9:30 POT 06

Al-doped ZnO nanowires grown by PLD — •Alexander Shkurmanov, Chris Sturm, Holger Hochmuth, and Marius Grundmann — Universität Leipzig, Inst. for Exp. Phys. II, Linnéstr. 5, 04103 Leipzig, Germany

ZnO nanowires (NWs) attract a lot of interest and can be used as building blocks for different devices e.g. light emitters, resonators and sensors. At the same time, doping of the ZnO NWs by Al leads to increase of their conductivity [1], luminescence intensity [2], and optical transmission [3] in comparison with undoped ZnO. This makes doped ZnO NWs promising for a wide range of applications.

Here we present the growth of Al doped ZnO NWs on ZnO seed layers by pulsed laser deposition (PLD). We demonstrate that the choice of the seed layer as well as a growth temperature determine the shape of the NWs and allow to vary diameter of the NWs diameter from 550 nm to less than 7 nm. Furthermore, by comparing the NW growth of undoped ZnO wires on the same kind of the seed layers allows deeper insight into the growth mechanism of the ZnO wires.

[1] G. Zimmermann et al., Phys. Status Solidi RRL 4, 3-4 2010
[2] C.-L. Hsu et al., RSC Adv., 4, 2980, 2014
[3] C. M. Garcia et al., Advances in Materials Physics and Chemistry, 2, 56, 2012

HL 38.2 Tue 9:45 POT 06

Unambiguous identification of Sn_3O_4 using Raman spectroscopy and ab initio calculations — •Christian T. Reindl[1], Martin Becker[1], Bianca K. Eifert[2], Marcel Giar[2], Lilan Zheng[3], Angelika Polity[1], Yunbin He[3], Christian Heiliger[2], and Peter J. Klar[1] — [1]I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen — [2]Institut für Theoretische Physik, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen — [3]Faculty of Materials Science and Engineering, Hubei University, Wuhan 430062, China

A lot is known about the two stable tin oxides SnO and SnO_2. Both physes have been intensively investigated and are widely used in applications such as transparent conducting oxides, gas sensors, and lithium ion batteries. Over the last century many attempts have failed to identify the metastable oxide occuring at an intermediate Sn:O stochiometry. Using Raman spectroscopy as the experimental backbone and ab initio density functional theory (DFT) calculations we are able to distinguish different candidates and finaly identify the intermediate phase as Sn_3O_4. The samples evaluated are of different origin. One kind was grown utilizing ion beam sputter deposition (IBDS) directly, whereas the second kind was first ion beam sputtered as SnO and annealed to form the intermediate phase. The third kind was a SnO layer produced by pulsed laser deposition which was oxidized to the intermediate phase afterwards. All three variants show none or only slight traces of SnO or SnO_2, respectively and are in excellent agreement with the calculated Sn_3O_4 spectra.

HL 38.3 Tue 10:00 POT 06

Polymer passivated zinc oxide thin film transistors — •Torsten Balster, Jonas Köhling, Marlis Ortel, and Veit Wagner — Department of Physics and Earth Sciences, Jacobs University Bremen gGmbH, Campus Ring 1, 28759 Bremen, Germany

Thin film transistors with ZnO as active layer were prepared by pulsed spray pyrolysis method, in order to investigate the passivation of surface trap states. These states are known to have significant influence on mobility, hysteresis and stability of transistors. Promising candidates for the passivation are polymer classes containing an oxygen with free electron pairs, which can coordinate with Zn-atoms at the surface.
After the pulsed spray pyrolysis deposition of the ZnO films, poly methyl methacrylate, which has a carbonyl group in the monomer, was spin-coated from solution onto the TFT and annealed afterwards. After this treatment, no hysteresis and only a minor onset voltage variation during bias stress could be observed. However, the onset was shifted to lower values in comparison to the untreated surface. Furthermore, the influence of the molecular chain length and the solvent on the electronic properties will be discussed.

Coffee Break

HL 38.4 Tue 10:30 POT 06

Defects and defect complexes in zinc oxide revisited: Self-consistent hybrid functional calculations — •Daniel Fritsch[1], Benjamin Morgan[1], and Aron Walsh[1,2] — [1]Department of Chemistry, University of Bath, BA2 7AY Bath, UK — [2]Department of Materials, Imperial College London, SW7 2AZ London, UK

Zinc oxide exhibits *n*-type conductivity, arising from intrinsic defects and hydrogen impurities, and this can be enhanced by aliovalent doping with group-III elements. Al-doping of ZnO is a particular example of this doping strategy with great potential for use in future technologies and devices. The effect of Al-doping depends on the delicate interplay between intrinsic point defects (V_{Zn}, V_O, Zn_i, O_i) and substituted Al (Al_{Zn}). In particular, our understanding of possible complex formation, such as the aluminum–zinc-vacancy complex (Al_{Zn}-V_{Zn}), is far from complete and requires further detailed investigations.

Most recent density functional theory calculations of ZnO doping have used hybrid functionals, which introduce a fraction of Hartree-Fock exchange into available exchange-correlation potentials based on intuition or experimental calibration. A recent self-consistent hybrid functional [1] offers a new approach for parameter-free hybrid functional investigations and removes this level of empiricism. Having used this new self-consistent hybrid method, we will present calculated results for bulk ZnO, its intrinsic defects, and the important Al_{Zn}–V_{Zn} defect complex, and compare them to available experimental and theoretical data.

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

HL 38.5 Tue 10:45 POT 06

Second-Harmonic Generation in ZnO/(Zn,Mg)O Multiple Quantum Wells — •Johannes Mund[1], Dmitri R. Yakovlev[1], Sergey Sadofev[2], Cedrik Meier[3], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, Germany — [2]Institut für Physik, AG Photonik, Humboldt-Universität zu Berlin, Germany — [3]Department Physik, Nanophotonik & Nanomaterialien, Universität Paderborn, Germany

Non-linear optical properties of $ZnO/Zn_{0.9}Mg_{0.1}O$ multiple quantum wells with well width varied from 1.8 to 10 nm are studied by second-harmonic generation (SHG).

We succeed to detect the 1S quantum well exciton and show qualitatively the quantum confinement of this state in narrow QW as well

as the quantum confined stark effect in broader QW. A comparison to spectra of ZnO bulk material and a pure ZnMgO layer confirms that the observed resonance has its origin in the MQW structure. SHG spectra are compared with photoluminescence and reflectivity spectra to identify exciton transitions. Also SHG rotational diagrams are measured and relative values of components of the non-linear susceptibility tensor are evaluated.

HL 38.6 Tue 11:00 POT 06

Microdisks coupled with Waveguides of II/VI quantum well heterostructures — •Gesa Schmidt, Torsten Rieger, Detlev Grützmacher, and Alexander Pawlis — PGI-9 and JARA-FIT, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

Waveguides and microdisks were fabricated from II/VI quantum wells (QWs) grown by molecular beam epitaxy on GaAs substrates. They provide suitable components for integrated-optical devices in the blue/green spectrum. Additionally, doping of the QWs with fluorine allows modern devices such as low-threshold lasers and single photon sources and their integration. To this end, the introduction of an Al_2O_3 interlayer, fabricated by selective post-growth oxidation of an AlAs buffer between the GaAs and the II/VI heterostructure, provides improved waveguiding and reduced photon leakage. Al_2O_3 is optically transparent for the emission from the QWs and has considerably smaller refractive index compared to the II/VI material.

We present optical properties and photon-guiding characteristics of microdisk cavities with adjacent waveguide membranes. The analysis of spatial-resolved μ-photoluminescence measurements along the waveguide demonstrates the photon transfer between microdisk and waveguide. Moreover, we observed lasing at specific whispering gallery modes of our microdisks, which denote efficient photon guiding along the waveguide. Our findings demonstrate functional operation of microdisk-waveguide couplers based on ZnSe/(Zn,Mg)Se QW structures and their potential for larger scale integrated-optical systems in the blue/green spectral range.

HL 39: Plasmonics and Nanooptics IV: Light-Matter Interaction

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

HL 39.1 Tue 10:30 TRE Ma

Rolled-up active microtubes containing tuneable grating couplers for the excitation of surface plasmon polaritons — •Jan Siebels[1], Hoan Vu[1], Alf Mews[1], Stefan Mendach[2], and Tobias Kipp[1] — [1]Institut für Physikalische Chemie, Universität Hamburg — [2]Institut für Angewandte Physik, Universität Hamburg

Grating structures can be utilized in order to overcome the momentum mismatch between an incident photon and a surface plasmon polaritons (SPPs) at a metal/dielectric interface. We implemented grating structures with gradually varying effective refractive indices into active microtubes containing GaAs quantum wells. The grating consists of triangularly shaped silver bars–varying the filling-factor in the direction perpendicular to the periodicity. This allows for a position-dependent coupling of the quantum well emission to the SPP. To characterize these systems we implemented a photoluminescence mapping technique by means of a streak camera which allows simultaneous recording of spectral distribution and related decay characteristics. The spatially resolved data reveals spectral shifts and changes of the decay lifetime that can be attributed to localized excitation of SPPs due to the embedded gratings. We gratefully acknowledge financial support by the Deutsche Forschungsgemeinschaft (DFG) via ME3600/1.

HL 39.2 Tue 10:45 TRE Ma

Tip-Enhanced Raman Spectroscopy of a MoS2 / Au Nanoparticle (2D crystal/Plasmonic) Heterostructure — •Mahfujur Rahaman[1], Raul D Rodriguez[1], Gerd Plechinger[2], Stefan Moras[1], Christian Schüller[2], Tobias Korn[2], and Dietrich RT Zahn[1] — [1]Semiconductor Physics, Technische Universität Chemnitz, Germany — [2]Fakultät für Physik, Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany

Tip-enhanced Raman spectroscopy (TERS) has been rapidly improved over the last decade and opened up opportunities to study phonon properties of materials on a nanometre scale. We report on TERS of a 4-layer MoS2 flake deposited onto a Au nanostructured surface, thus forming a 2D crystal/plasmonic heterostructure. Au nanotriangles are prepared by nanosphere lithography and then MoS2 is mechanically exfoliated on top of it. The TERS spectra are acquired under resonance conditions at 638 nm excitation using a Xplora/AIST-NT TERS system. We obtain a spatial resolution of 10 nm in TERS imaging. We observe the highest enhancement of the Raman intensity of MoS2 on top of Au nanotriangles due to the strong electromagnetic confinement between the tip and single triangle. Our results enable us to determine the local strain in MoS2 induced after the heterostructure formation. The maximum frequency shift of E2g mode is determined to be 3.2 cm-1 which is equivalent to 1% of biaxial strain induced in the film. Our results will help the understanding of the structural and mechanical degrees of freedom to the nanoscale optoelectronic properties of future MoS2/plasmonic based devices.

HL 39.3 Tue 11:00 TRE Ma

Strong Exciton-Plasmon Coupling on Core-Shell Nanoparticles — •Wouter Koopman, Felix Stete, and Matias Bargheer — Universität Potsdam, Potsdam, Deutschland

Strong-coupling of molecular excitons to localized plasmons in metal nanoparticles offers a new approach for the investigation and utilization of quantum-effects at room temperature. On the other hand, the fabrication of core-shell molecule-metal nanoparticles is possible by well-established, economic wet-chemical methods. Plasmon-exciton coupling could therefore offer an attractive route for the facile implementation of robust, scalable nanoscale quantum systems. This talk will address the presence of strong exciton-plasmon coupling in two simple nanoparticle geometries: core-shell spheres and rods. We will elaborate on the different possible coupling regimes and discuss the pitfalls when one wants to distinguish these experimentally. In particular we show that relying solely on extinction spectrum to classify the coupling regime, as often encountered in literature, can lead to a wrong identification of the regime. In addition, we will address the pronounced dependence of coupling-strength on the particle size and on the dielectric environment and discuss how to use these factors to tailor the coupling.

HL 39.4 Tue 11:15 TRE Ma

SPP-Light Interaction in the Space-Time Domain — •David Janoschka, Pierre Kirschbaum, Pascal Dreher, Michael Horn-von Hoegen, and Frank J. Meyer zu Heringdorf — Faculty of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg, Germany

Focusing of Surface Plasmon Polaritons (SPPs) with nanooptical elements extends the comprehension of nonlinear phenomena on Au surfaces. We use femtosecond-laser-pulses (<15 fs) to excite SPPs, which can be observed in a direct conceptual visualization in our Photoemission Electron Microscope (PEEM). Focused Ion Beam (FIB) milled structures on Au provide a great control over the shape of the SPP phase fronts. As such, we are able to achieve the formation of a strong SPP-field induced nanofocus with circular shaped excitation structures. This causes highly localized electron emission, exclusively by the SPP-SPP interaction, which was introduced as plasmoemission in previous work.

Here, we investigate the differences between photoemission and plasmoemission. We are in particular interested in the SPP-SPP-interaction in the presence of other nanooptical elements like nanoholes and nanoparticles, especially in the strong field enhancement caused by these nanooptical elements.

HL 39.5 Tue 11:30 TRE Ma

Resonant excitation of isolated helical nanostructures in the visible range — Katja Höflich[2], Enno Hansjürgen[1], Heiko Kollmann[1], Silke Christiansen[2], Christoph Lienau[1], and •Martin Silies[1] — [1]AG Ultrafast Nano-Optics, Carl von Ossietzky Universität Oldenburg, Germany — [2]Nanoscale Structures and Microscopic Analysis, Helmholtz-Zentrum Berlin, Germany

Circular dichroism is a phenomenon that describes the extinction difference in chiral objects when excited by left and right-handed circular

polarized light. While the circular dichroism of single biomolecules is rather low, the signal can be enhanced by several orders of magnitude using artificial, i.e. plasmonic chiral nanostructures. Thus, the study of these plasmonic structures is a vivid field of research. Here, confocal white-light spectro-microscopy is employed to measure extinction spectra of single silver helices with sub-micrometer dimensions fabricated using electron beam induced deposition for left- and right-handed circular excitation. Circular dichroism spectra of isolated right-handed helices show - besides a near-IR resonance for light at the same handedness - a distinct resonance for left-handed circular polarized light in the visible range around 600 nm. While the resonant behavior for the right-handed circular polarized light is expected [1], the emergence of a pronounced left-handed resonance is surprising. Finite element modeling reliably reproduces the observed spectral features and suggests that a pseudo current at the outer surface of the helices locally switches the polarization state of the incident polarization. [1] Gansel et al. Science 325, 1513 (2009)

HL 39.6 Tue 11:45 TRE Ma

The detection of attenuated waveguide modes in SiO_2 on silicon covered with gold-nanoparticles using photo emission electron microscopy — •Alwin Klick[1], René Wagner[1], Malte Grossmann[1], Laith F. Kadem[2], Jost Adam[3], Till Leissner[3], Horst-Günter Rubahn[3], Christine Selhuber-Unkel[2], and Michael Bauer[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel — [2]Institut für Materialwissenschaft, Christian-Albrechts-Universität zu Kiel — [3]Mads Clausen Instituttet, Syddansk Universitet

We present a time-resolved photoemission electron microcopy study of propagating electromagnetic modes in the UV spectral regime in SiO_2 covered with self-assembled gold nanospheres on a silicon substrate. Comparison with simulations using the finite element method confirms that guided light modes in the SiO_2 slab are detected. Furthermore, we show that the gold nanospheres play a key role in the observation of guided modes using PEEM due to their high electron density substantially enhancing the detected photoemission yield. Analytic calculations which take into account the size of the nanospheres and their distribution on the surface show that plasmonic interactions have negligible impact on the light mode properties.

HL 39.7 Tue 12:00 TRE Ma

Near-field investigation of geometric and material resonances in semiconductor nanowires with doped segments — •Lena Jung[1], Dmitriy S. Boyuk[2], Amar T. Mohabir[2], Michael A. Filler[2], and Thomas Taubner[1] — [1]I. Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, Georgia 30332, United States

Doped semiconductors (SCs) allow for tunability of plasmon resonances via gating or doping. We investigate Si nanowires (NWs) with doped segments with infrared near-field microscopy (s-SNOM). In s-SNOM, optical near-fields that are excited via laser-illumination of a metalized AFM tip interact with the sample. This enables to determine the samples dielectric properties with a high resolution only limited by the tip radius (∼25 nm). By combining the Drude model for doped SCs with models for the tip-sample interaction, carrier properties of the doped SC can be obtained by spectroscopic imaging in the range of a near-field resonance close to the plasma edge. Additionally, the doped segments in the NWs act as resonators for mid-IR light due to their geometry. Localized surface plasmon (LSP) resonances have been observed in the far-field. Different growth conditions revealed differences in the shape of the spectra, explained by variations in the sharpness of the segment boundaries [1]. Goal of our investigations is to distinguish these different effects and to determine carrier properties, boundary sharpness and map the LSP resonance given by the segment geometry.

[1] Chou et al., ACS Nano **9**, 1250 (2015)

HL 39.8 Tue 12:15 TRE Ma

Single-particle spectroscopy of bare and porphyrin-covered silver clusters with multi-photon photoemission electron microscopy — •Klaus Stallberg and Winfried Daum — Institute of Energy Research and Physical Technologies, TU Clausthal, Leibnizstraße 4, 38678 Clausthal-Zellerfeld, Germany

Coupling of optical excitations in dye molecules with plasmonic excitations in metallic nanostructures holds the potential to provide control over light-matter interaction at a nanoscale level. Plasmonic-excitonic coupling has been reported for dye-coated metallic nanoparticles by application of particle-averaging methods. We apply multi-photon photoemission electron microscopy (nP-PEEM) with tunable-laser excitation to study localized surface plasmon resonances (LSPR) of individual silver clusters, which are grown under UHV conditions on silicon substrates. Simulations elucidate the influence of the supporting substrate on the LSPR, most notably an amplification of LSP modes with a polarization normal to the substrate. For particles covered with porphyrin (ZnTPP) the simulations predict the appearance of a second LSPR near the optical absorption (Soret-) band of the ZnTPP molecules, a consequence of coupling between the plasmonic near-field and and the excitonic polarization inside the ZnTPP layer. Depending on their spectral positions, both LSP modes are predicted to spectrally repel each other as a result of additional coupling between the LSP modes. In our laser spectroscopic nP-PEEM experiments we observe such spectral shifts for silver particles covered with a ZnTPP layer of only four monolayers.

HL 39.9 Tue 12:30 TRE Ma

Linear ultra-broadband spectral interferometry for probing coherent surface plasmon polariton propagation in the time domain — Jue-Min Yi[1], •Vladimir Smirnov[1], Dongchao Hou[1], Heiko Kollmann[1], Zsuzsanna Pápa[2], Péter Dombi[2], Sven Stephan[1], Daniel Espeloer[1], Christoph Lienau[1], and Martin Silies[1] — [1]AG Ultrafast Nano-Optics, Carl von Ossietzky Universität Oldenburg, Germany — [2]Wigner Research Centre for Physics, 1121 Budapest, Hungary

Surface Plasmon Polaritons (SPPs) are evanescent coherent wave packets that can both confine the energy of light to metallic nanostructures and transport energy over mesoscopic distances [1]. They can then be used to generate and process information coded as optical signal to realize nanometer-scale all-optical circuitry. The propagation properties of these SPPs are defined by the geometry and composition of nanostructures. Here, we introduce a new ultra-broadband far-field spectral interferometry method to completely characterize coherent SPP propagation in metallic nanostructures, which allows the reconstruction of the plasmonic field in time domain [2]. Group velocity and dispersion of SPPs are determined with high precision in a broad frequency range in the visible and near-infrared regions, and the propagating SPP field at large distance is thus displayed with high time resolution. Our results shed new light on characterizing the interplay between nanostructure geometry and coherent SPP propagation.

[1] M.L.M. Balistreri, et al., Science 294, p.1080 (2001)
[2] J.Yi, et al., submitted to ACS Photonics (2016)

HL 39.10 Tue 12:45 TRE Ma

(The Road to) Understanding Localization of Light in Nanosponges — •Felix Schwarz[1], Jan Vogelsang[3], Germann Hergert[3], Dong Wang[2], Heiko Kollmann[3], Petra Gross[3], Erich Runge[1], Christoph Lienau[3], and Peter Schaaf[2] — [1]TU Ilmenau, Institut für Physik und IMN MacroNano, 98693 Ilmenau — [2]TU Ilmenau, Institut für Werkstofftechnik und IMN MacroNano, 98693 Ilmenau — [3]Carl von Ossietzky Universität, Institut für Physik and Center of Interface Science, 26129 Oldenburg

Disorder on the nanometer scale can lead to localization of light and huge electromagnetic field enhancement, which in turn can be used for non-linear optics and for the study and exploitation of quantum optical processes. Most recently, long-lived, highly localized plasmons on the surface of nanoporous gold-nanoparticles (nanosponges) with an unmatched excitation efficiency were reported based on photoemission. Surprisingly, first calculations show that on these sponges localization takes place on the same length scale as the typical pore size. To optimally tailor the disorder for potential applications and increase the understanding of this unusual localization process, we systematically examine the influence of the specific type of disorder. Far-field scattering and near-field properties are calculated for different correlation functions and filling fraction of the sponges. Furthermore, a multiscale approach is presented, where parts of the surface can be simulated with increased resolution while the antenna resonances are evaluated in an effective-medium picture. Very good agreement with experimental data regarding the field enhancement and lifetime is reported.

HL 40: Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - III

Time: Tuesday 10:30–13:00 Location: GER 38

Invited Talk HL 40.1 Tue 10:30 GER 38

Including spin effects in the strong-coupling limit of DFT — •Paola Gori-Giorgi[1], Juri Grossi[1], Derk Pieter Kooi[1], Klaas Giesbertz[1], Michael Seidl[1], Aron Cohen[2], and Paula Mori-Sanchez[3] — [1]Vrije Universiteit Amsterdam, The Netherlands — [2]University of Cambridge, UK — [3]Universidad Autonoma de Madrid, Spain

The exact strong-coupling limit of density functional theory (DFT) reveals a different mathematical structure with respect to the one of traditional approximations for the exchange-correlation (xc) functional: instead of the local density, local density gradients, or quantities related to the Kohn-Sham orbitals, some integrals of the density appear in this limit. In the recent years, xc functionals directly inspired to this mathematical structure have been constructed and implemented in an efficient way. However, the leading terms (exact or approximate) in the strong-coupling limit of DFT are intrinsically semiclassical and, as such, do not incorporated the spin dependence. In this talk, I will present the first study on the incorporation of the spin-dependence in the exact strong-coupling limit in simple one-dimensional cases. I will then discuss approximations for our findings and routes to the construction of spin-dependent xc functionals for strong coupling. Comparison with exact calculations for the Hohenberg-Kohn functional in the strong-coupling regime confirms the accuracy of our expressions for the leading terms.

HL 40.2 Tue 11:00 GER 38

Strong correlation from the Random Phase Approximation and beyond — •Thomas Olsen and Kristian Thygesen — Department of Physics, Technical University of Denmark

We assess the performance of the Random Phase Approximation (RPA) for strongly correlated systems and discuss different routes to venture beyond RPA. It is well-known that RPA reproduces the dissociation curve of molecular H2 correctly and thus accurately captures the strong static correlation inherent in the dissociation limit. It is thus natural to ask whether RPA is able to describe the strongly correlated Mott insulators as well. In particular, the accurate description of antiferromagnetic systems is complicated by the fact that the magnetic order often emerges from a detailed interplay between direct exchange and super-exchange couplings, which are respectively exchange and correlation effects. Whereas DFT+U, semi-local and hybrid functionals are often capable of describing either exchange or super-exchange accurately, RPA is shown to give an accurate account of both. We will finally show that RPA can be improved by either including non-local kernel in the framework of TDDFT or including electron-hole interactions in the irreducible response function. Only the latter approach improves the description of strong correlation, whereas the former approach improves atomization energies significantly compared to RPA.

HL 40.3 Tue 11:15 GER 38

Surface and adsorption energy calculations within the random phase approximation — •Per Schmidt and Kristian Thygesen — Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

The application of density functional theory (DFT) to the calculation of adsorption and surface energies is ever increasing and as a theory, it has the potential to e.g. guide experiments in the search of better catalysts. However, a previous study[1] shows that with standardly used semi-local functionals, DFT is not able to accurately predict surface and adsorption energies simultaneously. By tuning the functional, either the predicted surface or adsorption energies can be improved at the expense of the other. For a few cases however, it has been shown[1] that the many-body approach, the random phase approximation (RPA), yields both excellent surface and adsorption energies.

In this work we expand the use of the RPA method to eight adsorption reactions over 20 transition metal surfaces using the electronic structure code GPAW. We report the difference in surface and adsorption energies compared with the standard DFT functionals: PBE, RPBE and BEEF-vdW. We find that RPA does in general predict less stable surfaces, in better agreement with experiments and the average change in adsorption energies varies between ± 0.5 eV. The RPA values could be used to guide construction of new density-functionals aimed at improving surface science calculations.

[1] L. Schimka, J. Harl, A. Stroppa, A. Grüneis, M. Marsman, F. Mittendorfer, and G. Kresse, Nature Materials 9, 741 (2010).

HL 40.4 Tue 11:30 GER 38

Large-scale cubic-scaling RPA correlation energy calculations using a Gaussian basis — •Jan Wilhelm and Jürg Hutter — University of Zurich, Winterthurerstrasse 190, 8057 Zurich, Switzerland

The random phase approximation (RPA) for computing the electron correlation energy has emerged as an accurate tool for predicting the properties of molecules and condensed phase systems. RPA combines a number of attractive features, most importantly that long-range van der Waals interaction is included, in contrast to semilocal density functionals. The drawback connected with RPA is the computational cost: For canonical implementations of RPA, the numerical effort grows as quickly as $O(N^4)$ with the system size N. We present an algorithm for computing the RPA correlation energy in a Gaussian basis requiring $O(N^3)$ operations and $O(N^2)$ memory. The cubic-scaling RPA method is based on the resolution of the identity (RI) with the overlap metric, a reformulation of RI-RPA in the Gaussian basis and imaginary time as well as the use of sparse linear algebra. We report a massively parallel implementation which is the key for the application to large systems. As first benchmark of the method, we show the RPA correlation energy of thousands of water molecules in a high-quality cc-TZVP basis. For a comparison, the canonical RPA method is restricted to 500 water molecules using the whole Piz Daint supercomputer for two hours. Our RPA algorithm enables the application of RPA to large systems where van der Waals interactions play an important role, e.g. for predicting the adsorption energy of large molecules on surfaces.

HL 40.5 Tue 11:45 GER 38

Semi-local exchange functionals showing ultranonlocal response: the hope to replace exact exchange — •Thilo Aschebrock and Stephan Kümmel — Theoretical Physics IV, University of Bayreuth, D-95440 Bayreuth, Germany

The widespread success of Density Functional Theory (DFT) is based on a favorable ratio of accuracy to computional cost, especially with semi-local approximations to the exchange-correlation energy. However, functionals such as the local density approximation (LDA), generalized-gradient approximations (GGA) or meta-generalized-gradient approximations (meta-GGA), typically miss important exact exchange features related to the derivative discontinuity. These are essential for accurately describing long-range charge transfer processes. The electrical response of molecular chains, which is dramatically overestimated by local and semi-local density functionals, is a prime example. The key to its correct description is a term in the Kohn-Sham exchange potential that counteracts the external field and has been named "ultranonlocal". We here present how these field-counteracting properties can be incorporated into semi-local DFT on the meta-GGA level. Thereby we show that by utilizing the kinetic-energy-density, it is possible to model ultranonlocal effects in the Kohn-Sham potential by virtue of a semi-local energy expression.

HL 40.6 Tue 12:00 GER 38

(De)stabilizing dispersion interactions via external electric charges — •Andrii Kleshchonok[1] and Alexandre Tkatchenko[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg

Van der Waals (vdW) or dispersion interactions play a central role in the structure, stability, and reaction mechanisms in large variety of molecules and materials. However, in many situations of interest in material science and biophysics, vdW interactions should account for the coupling with external (in)homogeneous electric fields. In this work we address the effect of external static charge field on long-range electron correlations. By using the quantum Drude oscillator model, we derive analytical expressions of the charge induced dipole-quadrupole dispersion energy, that is accounted neither in standard DFT methods, nor in popular vdW correction schemes. Analysing the scaling laws of

this dispersion term, we conclude that positive charge stabilizes dispersion interactions, while a negative charge has an opposite effect. Benchmark over S22 molecular dataset estimates the induced dispersion to be in the range of 20-300 % of conventional electrostatic energy. Our findings could have broad potential implications, including exfoliation of 2D materials, chemical reaction rates in charged droplets, and biological membranes.

HL 40.7 Tue 12:15 GER 38

An optimisability proof for self-consistent constrained DFT, and its implications for constraint-based self-interaction error correction — Glenn Moynihan[1], Gilberto Teobaldi[2,3], and •David D. O'Regan[1] — [1]School of Physics, CRANN and AMBER, Trinity College Dublin, Ireland. — [2]Stephenson Institute for Renewable Energy and Department of Chemistry, The University of Liverpool, U.K. — [3]Beijing Computational Science Research Center, China.

We develop the connection between constrained DFT energy derivatives and response functions, providing a rigorous assessment of the uniqueness and character of cDFT stationary points while accounting for electronic interactions and screening [1]. In particular, we provide a non-perturbative proof that stable stationary points of linear density constraints occur only at energy maxima with respect to their Lagrange multipliers, generalizing the proof of Ref. [2]. We demonstrate that multiple solutions, hysteresis, and energy discontinuities may occur in cDFT, and we provide necessary conditions for the optimizability of multi-constraint cDFT. We show that the applicability of cDFT in automating symmetry-preserving self-interaction error corrections is limited by a fundamental incompatibility with non-linear constraints. We circumvent this by utilizing separate linear and quadratic correction terms, which may be interpreted either as distinct constraints, each with its own Hubbard U type Lagrange multiplier, or as the components of a generalized, two-parameter DFT+U functional [3]. [1] Phys. Rev. B **94**, 035159 (2016). [2] Phys. Rev. A **72**, 024502 (2005). [3] Phys. Rev. B Rapid Comms., Accepted (2016), arXiv:1608.07320.

HL 40.8 Tue 12:30 GER 38

Density-based local hybrid functional for interfaces — •Pedro Borlido[1], Silvana Botti[1], and Miguel Marques[2] — [1]Institu für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743, Jena, Germany — [2]Instiut für Physik, Martin-Luther-Universität Halle Wittenberg, D-06099 Halle, Germany

Hybrid functionals in density functional theory have become the state-of-the-art for the calculation of electronic properties of solids. The key to their performance is how and in which amount a part of Fock exchange is mixed with semi-local exchange-correlation functionals. We propose here a material dependent and local mixing parameter which is a functional of the electron density alone, through an estimator of the local dielectric function inspired by the work done in *Phys. Rev. B* 83, 035119 (2011). This new functional is by construction an approximation of the *GW* self-energy and it enables therefore calculations of quasiparticle energy levels of comparable quality as *GW*, but at the reduced cost of a hybrid density functional. In contrast with other recent self-consistent schemes for the mixing parameter, our approach does not require to calculate the dielectric function and leads to a negligible increase of the computation time.

HL 40.9 Tue 12:45 GER 38

On the hunt for better functionals in DFT: a new quantum embedding scheme — •Uliana Mordovina[1], Teresa E. Reinhard[1], Heiko Appel[1], and Angel Rubio[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain

We propose a new systematic technique to derive functionals for standard density functional theory (DFT) in an ab-initio fashion. This technique origins in the recently developed density-matrix embedding theory (DMET) [1]. DMET is a quantum-in-quantum embedding method, which is based on finding a projection between the high-dimensional wave function of the full system and a lower-dimensional wavefunction living in the active space of the embedded system, which is then solved exactly. In the original DMET scope, the projection is improved via optimization of the reduced one-body density matrix. We replace this optimization by a density inversion, exploiting the one-to-one mapping between electronic density and Kohn-Sham potential.

Not only the DMET scheme is improved by the uniqueness of the density-potential mapping, the proposed density-embedding also allows for finding accurate Kohn-Sham potentials. Moreover, unlike in usual DFT, we can systematically improve the description by increasing the size of the active space.

We show benchmark results of our method for molecules in 1D.

[1] G. Knizia, G. K.-L Chan, Phys. Rev. Lett 109, 186404, (2012)

HL 41: Nitrides: Preparation

Time: Tuesday 11:45–13:00 Location: POT 06

HL 41.1 Tue 11:45 POT 06

Molecular beam epitaxy and characterization of InGaN nanowires on Si (111) — •Saskia Weiszer[1], Maximilian Kolhep[1], Maria de la Mata[2], Jordi Arbiol[2], and Martin Stutzmann[1] — [1]Walter Schottky Institut and Physics Department, TUM, 85748 Garching, Germany — [2]Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and The Barcelona Institute of Science and Technology (BIST), UAB, 08193 Bellaterra, Spain

InGaN has a variable band gap that covers nearly the entire solar spectrum. Combined with Si, theoretical considerations show that an InGaN/Si solar cell could be an optimal implementation of a double-junction cell. In particular at an In content of around 50%, it is expected that a resonant tunnel junction is formed between both materials. Furthermore, the cell efficiency could be increased by growing nanowires instead of thin films to make use of the fact that nanowires act as a natural anti-reflection coating and to reduce structural defects. InGaN nanowires on Si (111) are grown via molecular beam epitaxy. Different growth series with varying III/V ratio, substrate temperature and Ga/In ratio are characterized by EDX, HRXRD and Raman scattering. EELS elemental maps of single nanowires confirm a strong fluctuation of In content within the InGaN nanowires. Despite the compositional inhomogeneity of InGaN nanowires, electrical characterization of nominally intrinsic InN nanowires grown on differently doped Si (111) substrates has been performed. With regard to device fabrication, first results of selective area growth of InN nanowires with different mask materials are discussed.

HL 41.2 Tue 12:00 POT 06

Growth Analysis of GaN Quantum Dots using Cathodoluminescence Microscopy — •Hannes Schürmann, Christoph Berger, Sebastian Metzner, Gordon Schmidt, Peter Veit, Frank Bertram, Armin Dadgar, Jürgen Bläsing, André Strittmatter, and Jürgen Christen — Institute of Experimental Physics, Otto-von-Guericke-Universitity Magdeburg, Germany

GaN quantum dots in AlN are grown by MOVPE applying a growth interruption after the deposition of a thin GaN film. The impact of this growth interruption on the formation of quantum dots is comprehensively analyzed using highly spatially and spectrally resolved cathodoluminescence (CL) microscopy. Structural properties were investigated using scanning transmission electron microscopy. The CL investigation reveals a drastic reduction of the spatial and spectral width of emission with the formation of GaN quantum dots. Time delayed CL spectra show further evidence of successful quantum dot growth.

HL 41.3 Tue 12:15 POT 06

Investigation of MBE grown AlN and InN layers under the effect of additional Ga acting as a surfactant — •Christopher Hein, Andreas Kraus, Heiko Bremers, Uwe Rossow, and Andreas Hangleiter — Institut für Angewandte Physik, Technische Universität, Braunschweig , Deutschland

Heteroepitaxial growth is always accompanied by misfit strain which, above a certain thickness, leads to relaxation and deterioation of the grown layer. In our work we investigate the surfactant effect of Ga on MBE growth of InN and AlN layers. Templates were 2.5μm thick GaN layers grown in our AIX-200 RF MOVPE on c-oriented sapphire. The 16 nm InN layers were grown at 490°C substrate temperature

in a double pulsed growth scheme (10s In deposition, 15s nitridation). The AlN samples consist of a previously grown MBE GaN buffer layer, followed by a low temperature AlN interlayer and finally the AlN epilayer in Al pulsed mode. Growth temperatures were 745°C for the GaN buffer and AlN epilayer whereas the interlayer was grown at 500°C. The comparison samples had an additional Ga flux during their metal pulses. In case of InN using surfactant Ga led to a reduced RMS surface roughness from 4.4 nm down to 2.2 nm ($16\mu m^2$ area) which was accompanied by a remarkable increase of surface coalesence. An increase of structural quality for the AlN layers was observed, as indicated by (0002) and ($10\bar{1}0$) ω-FWHM reductions from 817" to 766" and 2736" down to 2160" respectively. XRD shows no incorporation of Ga into the epilayers. We will elaborate on the consequences for growth of quantum dot structures on surfaces grown under the influence of a surfactant effect.

HL 41.4 Tue 12:30 POT 06

high quality Al films grown by molecular beam epitaxy — •Bowen Sheng[1], Yixin Wang[1], Zhaoying Chen[1], Ping Wang[1], Frank Bertram[2], Jürgen Christen[2], and Xinqiang Wang[1] — [1]SKLAMMP, School of Physics, Peking University, Beijing, China — [2]IEP, Otto-von-Guericke-University Magdeburg, Magdeburg, Germany

With the development of plasmonic devices in the past decade, various plasmonic applications such as plasmonic nanolasers[1], plasmon enhanced single photon emission etc.,[2] attracted much attention. However, nanoscale plasmonic devices are extremely sensitive to the metal and interface quality. Among those three metals used frequently to generate plasmons–gold, silver, aluminum (Al), Al is the most promising metal for ultraviolet plamonics devices, due to the interband transition or absorption of gold and silver in UV regime.[3]

In this work, we demonstrate the successful growth of atomic flat single crystalline Al thin films on Si(111) substrates by molecular beam epitaxy (MBE). The growth temperature and Al flux have been modified to optimize the crystalline quality and surface morphology of Al film, and finally we get high-quality Al film with mirror-like surface. The surface morphology was measured by AFM, revealing a root-mean-square roughness of 0.395nm. The FWHM of the XRD rocking curve is 564 arcsec, which indicates the realization of high-quality Al films. Other detailed analysis will be reported as well.

[1] Lu et al.Science 2012, 337(6093), 450-453; [2] Gong et al. Proc. Nat. Ac. Sci. 2015, 112(17), 5280-5285; [3]Chou et al. Sci Rep 2016, 6.

HL 41.5 Tue 12:45 POT 06

MOVPE-growth of GaN quantum dots on deep UV AlN/AlGaN distributed Bragg reflectors — •Christoph Berger, Hannes Schürmann, Sebastian Metzner, Gordon Schmidt, Jürgen Bläsing, Armin Dadgar, Frank Bertram, Jürgen Christen, and André Strittmatter — Otto-von-Guericke-Universität Magdeburg

GaN quantum dots are potential candidates to realize single photon emitters at room temperature due to their large exciton binding energy and zero-dimensional confinement potential. We observe sharp emission lines from quantum dot states in single GaN islands. These islands are realized by growing a thin GaN layer on an AlN buffer. Applying a subsequent growth interruption allows formation of GaN islands by material desorption. For cavity enhancement of the spontaneous emission, the quantum dots are embedded in an AlN cavity on a highly reflective AlN/AlGaN DBR. Adapted to the QD emission, the DBRs are designed for the deep UV spectral region at wavelengths around 270 nm. Growing 50 pairs of $AlN/Al_{0.7}Ga_{0.3}N$ on a thin AlN buffer, crack-formation could be prevented on large wafer areas and reflectivities above 90 % are realized. Structural and optical properties of the DBRs and quantum dots are investigated by XRD, AFM, TEM and cathodoluminescence performed in a SEM and in a transmission electron microscope (STEM-CL).

HL 42: Fundamentals of Perovskite Photovoltaics IV (joint session CPP/DS/HL)

Time: Tuesday 14:00–16:00 Location: ZEU 222

Invited Talk HL 42.1 Tue 14:00 ZEU 222

Ultrafast transient absorption spectroscopy of organic-inorganic hybrid perovskites on mesoporous titanium dioxide in contact with hole transport materials — •Thomas Lenzer — Universität Siegen, Physikalische Chemie, Adolf-Reichwein-Str. 2, 57076 Siegen

Organic-inorganic hybrid perovskites, such as methylammonium lead iodide, are particularly promising for applications in solar light harvesting and optoelectronics. We present our recent results on the carrier dynamics of such materials using ultrafast pump - supercontinuum probe spectroscopy in the 260-1600 nm range. The perovskite systems are investigated over a wide range of carrier densities. Slow carrier recombination processes, "phonon bottlenecks" during carrier cooling and confinement effects in low-dimensional perovskite structures are identified. We investigate electron injection processes from the perovskite into the mesoporous titania scaffold and estimate the relative contributions of electron transport pathways in the perovskite and titanium dioxide. We also discuss the hole transfer from the perovskite into triarylamine-based hole transport materials (HTMs).

HL 42.2 Tue 14:30 ZEU 222

Identification of charge transport limiting factors in perovskite-based solar cells by Time-of-Flight measurements — •Irene Grill[1,2], Meltem Aygüler[1,2], Nadja Giesbrecht[1,2], Pablo Docampo[1,2], Thomas Bein[1,2], Matthias Handloser[3], and Achim Hartschuh[1,2] — [1]Department of Chemistry & CeNS, LMU Munich — [2]Nanosystems Initiative Munich (NIM) — [3]Toptica Photonics AG

Hybrid perovskites represent one of the most promising absorber materials for future photovoltaic applications due to the recently achieved high PCE values [1]. In this work, we determine the transport time of photoinduced charges in between the top- and bottom-electrode in perovskite thin film solar cells upon pulsed laser excitation, using Time-of-Flight (ToF) photocurrent measurements. To extract the influence of the individual layers on the transport characteristics and to identify limiting factors we carried out additional ToF studies on the respective absorber layer of the photovoltaic device in a lateral architecture. The results of the single film measurements are discussed in terms of crystal size and orientation. The direct comparison of the data obtained for the individual layers and the photocurrent transients of the final device under working conditions permits the identification of limiting factors for inter-facial and intra-film charge transport simultaneously to allow for the optimization of both the fabrication techniques [2,3] and device architecture. [1] M. Saliba et al., Energy Environ. Sci. 2016, 9, 1989. [2] I. Grill et al., Sol. Energ. Mat. Sol. Cells 2016, accepted. [3] A. Binek, I. Grill et al., Chem. Asian J. 2016, 11, 1199.

HL 42.3 Tue 14:45 ZEU 222

Fill factor optimization strategies in efficient, stable triple cation perovskite solar cells — •Martin Stolterfoht, Christian Wolff, Yochai Amir, Andreas Paulke, and Dieter Neher — Institute of Physics and Astronomy, University of Potsdam, Potsdam-Golm, Germany

Perovskite solar cells (PSCs) now compete with their inorganic counterparts in terms of power conversion efficiency. To advance this technology even further, more insights into the physical mechanisms that define the bias dependence of the photocurrent are required. In this work, we varied the organic electron/hole transport layers (ETL/HTL) thickness in efficient triple cation PSCs and studied the charge carrier recombination and transit through the device. Using resistance dependent photovoltage (RPV), we identify the transit time through the transport layers as key figure of merit for maximizing the fill factor (FF) and the overall photovoltaic performance. The results are complemented by intensity dependent photocurrent measurements which elucidate the role of the HTL thickness on the bias dependence of the recombination losses and recombination order. By optimizing the transit time through the HTL (undoped PTAA) we demonstrate efficiencies under solar AM1.5G conditions of up to 20.4% with high FFs of 80%. The reported cells also exhibit excellent stability under light illumination and stability in air, even without encapsulation. However, further improving the FF via a continuous reduction of the HTL leads

to significant open-circuit voltage losses which highlights the challenge to simultaneously optimize the FF and open-circuit voltage.

HL 42.4 Tue 15:00 ZEU 222

Optical phonons in methylammonium lead halide perovskites and implications for charge transport — •Michael Sendner[1,2], Pabitra K. Nayak[3], David A. Egger[4], Sebastian Beck[1,2], Christian Müller[1,2,5], Bernd Epding[2,5], Wolfgang Kowalsky[1,2,5], Leeor Kronik[4], Henry J. Snaith[3], Annemarie Pucci[1,2], and Robert Lovrincic[2,5] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg — [2]InnovationLab, Heidelberg — [3]Clarendon Laboratory, University of Oxford — [4]Department of Materials and Interfaces, Weizmann Institute of Science — [5]Institut für Hochfrequenztechnik, TU Braunschweig

Recent reports indicated that the mechanical and electronic properties of lead-halide perovskites are strongly affected by the lattice vibrations. Herein we report far-infrared spectroscopy measurements of $CH_3NH_3Pb(I/Br/Cl)_3$ thin films and single crystals at room temperature (RT) and a detailed quantitative analysis of the spectra. We find strong broadening and anharmonicity of the lattice vibrations for all three halide perovskites, which indicates dynamic disorder of the lead-halide cage at RT. We determine the frequencies of the transversal and longitudinal optical phonons, and use them to calculate, via appropriate models, the static dielectric constants, polaron masses, electron-phonon coupling constants, and upper limits for the phonon-scattering limited charge carrier mobilities. Within the limitations of the model used, we can place an upper limit of 200 $cm^2V^{-1}s^{-1}$ for the RT charge carrier mobility in $MAPbI_3$ single crystals.
See also: Sendner et al., Materials Horizons, 3, pp 613-620, 2016.

HL 42.5 Tue 15:15 ZEU 222

Advances in Vapour Deposition of Metal-Halide Perovskite Thin-Films for Solar Cells — •Juliane Borchert, Jay B. Patel, Henry J. Snaith, and Michael B. Johnston — Department of Physics, University of Oxford, Clarendon Laboratory, Parks Road, Oxford, OX13PU, UK

Hybrid metal-halide perovskite materials are promising absorber materials both for use in single junction and tandem solar cells. A particular focus in recent research has been on the fabrication of perovskite absorber layers from solution. Alternatively, perovskite thin-films can also be deposited using co-evaporation in vacuum. This method offers several benefits. The obtained films show high uniformity over large surface areas. Thus the technique is well suited to the fabrication of large-area planar heterojunction solar cells. Additionally, the uniform film thickness makes the evaporated films ideal for precision characterisation of the optical properties of metal halide perovskite materials. Furthermore, the vapour deposition is solvent-free, which makes it compatible with a wide range of substrates and interlayers. This is for example advantageous in the fabrication of tandem solar cells. Here we present current advances in the understanding of the influence that different process variables have on the quality of the obtained films, as well as the application of co-evaporated perovskite absorber layers in devices.

HL 42.6 Tue 15:30 ZEU 222

Carrier Recombination Analysis in Perovskites Using Time-Resolved Photoluminescence — •Liudmila Kudriashova[1], Philipp Rieder[1], Kristofer Tvingstedt[1], Andreas Sperlich[1], Georgy Astakhov[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), 97074 Würzburg

Despite the incredible progress of perovskite-based photovoltaics, many aspects of charge carrier recombination in organometal halide perovskites still remain unclear, inhibiting the targeted production of high-performance solar cells. Under solar cell operating conditions photoluminescence (PL) in perovskites is mainly caused by recombination of free photogenerated charge carriers. Hence the time-resolved photoluminescence (TRPL) is a powerful tool to reveal the complex charge carrier behaviour in perovskite films. Here, we implement the combination of several kinetic models for TRPL in $CH_3NH_3PbI_3$ and $CH_3NH_3PbI_{3-x}Cl_x$ films to extract the characteristic recombination rates and estimate the trap concentration. We obtain trap densities in the range of $10^{15} - 10^{16}$ cm^{-3} and show that PL decay drastically depends on interfaces between the perovskite and conducting layers. Currently controversial aspects, such as different recombination pathways, origin of trap states, and the effect of photon recycling, are discussed. In summary, TRPL analysis enables the calculation of trap density and clarifies the origin of defects, which is crucial for the further development of perovskite-based photovoltaics.

HL 42.7 Tue 15:45 ZEU 222

Monolithic serial interconnection of perovskite solar cells using laser ablation — •Felix Schneider[1], Christof Schultz[1], Rutger Schlatmann[1,2], Steve Albrecht[3], and Bert Stegemann[1] — [1]HTW Berlin - University of Applied Sciences, Wilhelminenhofstr. 75a, 12459 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, PVcomB, Schwarzschildstr. 3, 12489 Berlin, Germany — [3]Helmholtz-Zentrum Berlin, Institut für Silizium-Photovoltaik, Kekuléstraße 5, 12489 Berlin, Germany

Based on recent work on serial interconnection of thin film solar cells by laser ablation, the proper laser parameters for scribing planar, inverted perovskite solar cell samples were determined. A device design with the layer sequence ITO/PTAA/perovskite/PCBM/Ag was used in which the P1 scribes the ITO, the P2 separates the perovskite and the selective contact layers and the P3 the metal electrode. As a result, successful P1 to P3 laser scribes with sufficiently small area losses, i.e. small dead areas, were obtained. Degradation due to humidity of the perovskite layer during laser scribing was avoided by complete laser processing in nitrogen atmosphere. Detailed characterization of the sample composition by energy dispersive x-ray spectroscopy, the morphology by atomic force microscopy as well as of the electrical functionality of the P2 scribes will be provided. The influence of laser-induced material modifications in the vicinity of the laser scribes on the module performance will be discussed.

HL 43: Plasmonics and Nanooptics V: Light-Matter Interaction

Time: Tuesday 14:00–16:00 Location: TRE Ma

HL 43.1 Tue 14:00 TRE Ma

Scanning near-field optical microscopy with inline-homodyne detection — •Jens Brauer, Jinxin Zhan, Petra Gross, and Christoph Lienau — Carl von Ossietzky University, Oldenburg, Germany

Aperturelss near-field optical microscopy is a good choice when it comes to optically investigating nanostructures with a size of only a few nanometer and is nowadays widely used in different geometries.

For most of the setups there remains the challenge of distinguishing the desired near-field signal from the very large optical background. To overcome this problem the tip-sample distance often is modulated at some tens of kilohertz and the detection signal is demodulated at higher harmonics. As Knoll & Keilmann [1] have shown theoretically the ratio of near-field to optical background improves with increasing demodulation frequency. However, also the signal amplitude at higher harmonics is decreasing dramatically. Therefore the use of interferometers, either in a homodyne or heterodyne detection scheme, is often used to amplify the near-field signal [2].

As a downside the contrast in the SNOM images critically depends on the stability of the interferometer. Here we present how to disentangle near field from background radiation in the 1st to 4th harmonic signal by measuring approach curves in an inherently stable in-line homodyne detection scheme and we give an outlook to ongoing spectroscopically resolved SNOM measurements.

[1] B. Knoll & F.Keilmann, Optics Communications, 182(4) (2000)
[2] Ocelic et al.,Applied Physics Letters, 89(10) (2006)

HL 43.2 Tue 14:15 TRE Ma

Vectorial near-field coupling on the nano scale — •M. Esmann, S.F. Becker, J. Witt, G. Wittstock, R. Vogelgesang, and C. Lienau — Carl von Ossietzky Universität, 26111 Oldenburg, Germany

Dipole-dipole coupling is ubiquitous in nanoscale systems [1,2] leading to optical modes and coherent dynamics which sensitively depend on

dipole configuration. To simultaneously study such systems on 5nm length scales and over a wide spectral range, we implemented a novel type of Scanning Near-Field Optical Microscope (SNOM): Grating-coupled Surface Plasmon Polaritons (SPPs) are adiabatically nanofocused [3] at the 10nm sized apex of a metallic nanotaper resulting in a bright, spatially isolated and spectrally broad nano light source, which acts as a probe for background-free near-field spectroscopy.

Here, we apply this technique to a prototypical system formed by dipolar coupling of the nanotaper apex to small 10×40nm gold nanorods. Upon systematic variation of coupling strength we find clear signatures of coupling-induced spectral shifts and broadening of plasmonic resonances with dramatic variations on few-nanometer length scales. We argue that our approach presents a fundamentally new way to interrogate dipole-dipole coupling in nanosystems in the spatial-, spectral- and temporal domain providing full access to coupling energies, mode profiles and the associated coherent dynamics.

[1] Zhang, Y. et al., Nature 531, 623 (2016). [2] Scholes, G.D., et al., Nature Chemistry 3, 763 (2011). [3] Stockman, M.I., PRL 93, 137404 (2004). [4] Esmann, M. et al., BJNANO 4, 603 (2013). [5] Becker, S.F. et al., ACS Photonics 3, 223 (2016).

HL 43.3 Tue 14:30 TRE Ma

Modulation of extraordinary optical transmission through nanohole arrays using ultrashort laser pulses — Kellie Pearce[1,2], Benjamin Duschner[1], Robin Dehde[1], Florian Richter[1], and •Ulf Kleineberg[1,2] — [1]Ludwig-Maximilians-Universität München, Am Coulombwall 1, 85748 Garching, Germany — [2]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching, Germany

We perform pump-probe measurements of the transmission through subwavelength hole arrays in a gold film on ITO using 16-fs laser pulses. By tuning the delay between the pulses, we can modify the contribution from different transmission resonances, and observe plasmon dephasing and decay. Simulations using a 3D FDTD solver show that the modulation of the transmission is due to the change in the intensity and distribution of fields on both interfaces.

HL 43.4 Tue 14:45 TRE Ma

Non-linear imaging of individual plasmonic nanostructures using phase-shaped femtosecond laser pulses — •Veit Giegold, Richard Ciesielski, Alexander Biewald, Tobia Mancabelli, Alberto Comin, and Achim Hartschuh — Department Chemie and CeNS, LMU Munich, 81377 Munich

We studied the second harmonic (SH) and near-degenerate four-wave (FWM) mixing response of individual plasmonic nanostructures using a confocal femtosecond pulse shaping setup. We find that the two different signals are maximized for different spectral phases of the laser pulse. We attribute this to different phase terms in the second- and third-order susceptibility of the nanostructures, respectively. We show that by using optimized phase profiles, the contrast of confocal SH and FWM images can be manipulated. This phase-enhanced nonlinear imaging can provide further insight into properties of plasmonic nanostructures.

HL 43.5 Tue 15:00 TRE Ma

Modeling of higher harmonic generation with the Fourier modal method using adaptive coordinates — •Josselin Defrance, Martin Schäferling, Maxim L. Nesterov, and Thomas Weiss — 4th Physics Institute and Research Centers SCoPE, University of Stuttgart, Germany

Metallic nano-structures can concentrate light into sub-wavelength volumes resulting in strong nonlinear responses. The influence of the geometry of such nano-systems, however, is not fully understood. Modeling these effects will not only help to optimize the nonlinear response of plasmonic nano-structures, but will also provide a better understanding of these phenomena. Nowadays, different numerical methods to model the interaction of electromagnetic fields with matter exist. The so-called Fourier modal method offers a fast and highly accurate calculation of far-field responses.

It has been shown that the Fourier modal method can be extended in order to calculate the generation of higher harmonics [1]. We have combined this method with adaptive spatial resolution and adaptive coordinates [2], thus providing an efficient and accurate numerical method for the precise analysis of the nonlinear optical responses of complex plasmonic geometries.

[1] T. Paul et al., J. Opt. Soc. B, Vol. 27, Issue. 5, pp. 1118 (2010).
[2] T. Weiss et al., Opt. Express 17, 8051 (2009).

HL 43.6 Tue 15:15 TRE Ma

Tracking Plasmon Propagation by Terahertz-Streaking at Metal Nanotips — •Lara Wimmer, Benjamin Schröder, Murat Sivis, Georg Herink, and Claus Ropers — IV. Physical Institute - Solids and Nanostructures, University of Göttingen, Germany

We resolve the propagation time of surface plasmon polaritons (SPP) traveling along the shaft of gold nanotips [1] employing Terahertz (THz) near-field streaking spectroscopy [2, 3]. Surface plasmon polaritons are launched by femtosecond near-infrared (NIR) pulses in a grating coupler at the shaft of the nanostructure, 50 *m from the tip end. At the apex, the nanofocused SPPs induce the (multiphoton) emission of photoelectrons [1], which are streaked in the locally enhanced near-field of a THz transient incident on the tip. Reference spectrograms are obtained by direct NIR-excitation of the apex. The observed temporal shift between both streaking spectrograms provides a direct measure of the group delay [4] in SPP propagation from the grating to the tip apex.

[1] Schröder et al., Phys. Rev. B 92, 085411 (2015).
[2] Wimmer et al., Nature Physics 10, 432-436 (2014).
[3] Herink et al., New Journal of Physics 16, 123005 (2014).
[4] Kravtsov et al., Opt. Lett. 38, 1322-1324 (2013)

HL 43.7 Tue 15:30 TRE Ma

Relaxation dynamics of plasmonic hot-carriers in gold nanoparticles — •Emanuele Minutella[1,2], Florian Schulz[1], and Holger Lange[1,2] — [1]Physikalische Chemie, Universität Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, CUI

Using light to drive or control chemical or physical processes is a very interesting field of research. One problem is to guide the light's energy to the specific place where reaction takes place. Due to their plasmonic properties noble metal nanoparticles have the ability to collect very efficiency photons and convert them into hot-electron-hole-pairs. As a result of size and photon energy dependent transient absorption measurements we found a binary kinetic for the relaxation times of the hot electrons. Depending on the photon energy either interband or intraband excitations are possible. We found faster decay rates for the intraband relaxation than for the interband. These results can help to improve possible hot-carrier devices.

HL 43.8 Tue 15:45 TRE Ma

Coherent phase-resolved near-field spectroscopy of single gold nanorods enabled by self-interference in an ultrasharp gold taper — Martin Esmann, Simon F. Becker, •Abbas Chimeh, Ralf Vogelgesang, and Christoph Lienau — University of Oldenburg

Plasmonic nanofocusing of light on an ultrasharp gold taper enables spectroscopic analysis of optical near-fields around individual metallic nanoparticles [1]. In order to characterize the ultrafast time-dynamics of these near-fields, the scheme should be extended to include the measurement of phase-resolved spectra. To this end, a stable inline interferometer is implemented in such a taper and plasmonic-nanofocusing spectroscopy is combined with spectral interferometry. In this method, surface plasmon polaritons are launched by a coupler on a pyramidal metallic taper and propagate towards the taper apex where they form a confined nanometer-scale light source [1]. After optical interaction with a sample, a part of the incident field is reflected backwards to the taper and interferes with the incident field on it. The interference signal is then collected from a scatterer on the shaft and spectrally resolved. Here, we implemented this method for the first time and use it to record local broadband optical spectra of single gold nanorod with 10x40 nm dimensions. We demonstrate phase-coherent mapping of optical near-field with sub-10 nanometer spatial resolution and provide a detailed analysis how near-field spectra are generated in this novel and highly sensitive interferometric measurement scheme.

[1] S. Schmidt et al., ACS Nano 6, 6040 (2012).

HL 44: Quantum Dots: Optical Properties II

Time: Tuesday 14:45–16:00 Location: POT 81

HL 44.1 Tue 14:45 POT 81

Quantum Light Sources based on Quantum-Dot Biexcitons — •Dirk Heinze, Dominik Breddermann, Artur Zrenner, and Stefan Schumacher — Department of Physics and CeOPP, Warburger Strasse 100, Paderborn, Germany

Quantum dot biexcitons show great potential as sources of quantum light. In this work we study the possibilities of two photon emission from a biexciton to generate both polarization-entangled photon pairs and all optically controllable single photons. Using a high-Q cavity we show theoretically that biexcitons can decay by simultaneously emitting two degenerate and polarization-entangled photons. The degree of entanglement is insensitive to the fine-structure splitting of the excitons due to the nature of the two-photon decay of the biexciton[1]. We demonstrate that this process is robust against phonon-assisted cavity feeding at low temperatures[2]. A partly stimulated partly spontaneous two photon emission from the biexciton can further be used to generate single photons with all optically tailored properties, such as polarization, frequency and time of emission [3],[4]. Here, the first photon is stimulated by a classical light field which drives the system into an intermediate virtual state from which the second single photon is emitted as the system relaxes into its ground state. This scheme does not rely on cavity enhancement, however the probability of emitting the single photon can be enhanced if the photon is emitted into a cavity. [1] S. Schumacher et al., Opt. Express 20, 5335-5342 (2012). [2] D. Heinze et al., arXiv:1611.04328 (2016). [3] D. Heinze et al., Nat. Commun. 6,8473 (2015). [4] D. Breddermann et al., Phys. Rev. B 94, 165310 (2016).

HL 44.2 Tue 15:00 POT 81

Strain tuning of deterministic quantum dot devices — •Esra Burcu Yarar Tauscher, Sarah Fischbach, Alexander Schlehahn, Arsenty Kagansky, Sven Rodt, Tobias Heindel, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany

Quantum light sources (QLSs) are building blocks for future quantum communication technologies. In recent years, significant progress has been achieved in this field, however, still most of the realized structures are based on spatially and spectrally random distributions of quantum emitters. In this regard, it is highly attractive to develop advanced technology platforms ensuring the precise control of the emitter's properties in deterministically fabricated devices. Self-assembled semiconductor quantum dots (QDs) integrated by in-situ electron-beam lithography into monolithic microstructures are very promising candidates to realize such high performance single photon sources. In this work we report on external strain tuning of deterministically fabricated single-QD devices. For this purpose, we apply voltage control to a ferroelectric material bonded to the single-QD microstructure via thermo-compression gold bonding. This allows us to reproducibly tune the optical properties of QDs, i.e. the emission and binding energies of excitonic complexes. Furthermore, we employ active electric feedback-control enabling long term stability of the emission energy of individual QDs. Our approach, which combines for the first time a deterministic device technology with piezo-tuning capabilities, offers high potential for the realization of bright QLSs with a complete control of their optical properties.

HL 44.3 Tue 15:15 POT 81

Wigner time delay — •Max Strauss[1], Christian Schneider[2], Martin Kamp[2], Sven Höfling[2,3], Janik Wolters[4], and Stephan Reitzenstein[1] — [1]TU Berlin — [2]Universität Würzburg — [3]University of St Andrews — [4]Universität Basel

The Heitler regime of resonance fluorescence, i.e. the low power regime of optical excitation of a two-level system (TLS), has recently been an active field of research because it offers single photons with intriguing properties. Here, we report on the first experimental study of the Wigner time delay on a semiconductor quantum dot, a solid state TLS. We show experimentally that in the Heitler regime, pulses long compared to T_1, the lifetime of the emitter, are scattered almost undistortedly while being delayed in time with respect to the exciting pulse. This time delay, also called the Wigner time delay, can reach a maximum value of T_2, the dephasing time of the quantum emitter, and is closely connected to the phase lag induced by the TLS.

HL 44.4 Tue 15:30 POT 81

Light-trapping and Waveguide Characteristics of Selective Area Grown GaN Nanowires on Transparent Substrates — •Richard Hudeczek, Julia Winnerl, and Martin Stutzmann — Walter Schottky Institut, Garching bei München, Germany

During the last decade group-III-nitride nanowires (NWs) have attracted increasing interest for device fabrication due to their high crystalline quality, e.g. for optoelectronic devices. Their large surface-to-volume ratio is advantageous for sensing or catalysis applications. Another interesting aspect is that NWs constitute intrinsic waveguides because of their one-dimensional geometry. The control of the NW density and diameter is essential for the reproducible fabrication of NW-based devices. The position-controlled growth of GaN NWs by molecular beam epitaxy can be achieved by using a patterned Ti mask as already reported by several groups [1,2].

Here, we present optical measurements of selective area grown GaN NWs on transparent substrates, e.g. c-plane sapphire and GaN based light emitting diode substrates. This allows backside illumination of as-grown NW arrays through the growth substrate. In particular, the dependence of the light trapping on the NW diameter (ranging from 70 to 220 nm), NW period which is varied between 300 and 2000 nm and the illumination wavelength (in the range of 400 to 620 nm) is investigated. Moreover, the experimental findings are compared to numerical simulations.

[1] K. Kishino, et al., J. Crystal Growth 311, 2063 (2009)
[2] F. Schuster, et al., Nano Lett. 15, 1773 (2015)

HL 44.5 Tue 15:45 POT 81

Ion-induced interdiffusion in self-assembled surface GaN quantum dots — •Charlotte Rothfuchs[1], Fabrice Semond[2], Marc Portail[2], Olivier Tottereau[2], Aimeric Courville[2], Andreas D. Wieck[1], and Arne Ludwig[1] — [1]Angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum — [2]CNRS-CRHEA, F-06560 Valbonne

In the growing field of quantum communication, there is a great demand for spin qubits and single photon sources, for which single electrically and optically active quantum dots (QDs) are prospering candidates. Providing high stability and room-temperature operation, GaN self-assembled QDs have a great appeal for these quantum technology applications. One possible pathway towards the realization of single QDs could be a top-down process using focused ion beam (FIB) implantation to post-select self-assembled molecular beam epitaxy-grown QDs. It is based on the disabling of all QDs around an intentional one by a creation of non-radiative defects. Further, magnetic impurities could be incorporated by FIB with low fluences in the non-disabled QDs for spin control. Here, we present a study on hexagonal surface GaN QDs subjected to a 100 keV gallium and a 210 keV erbium ion beam. The QDs morphology is analyzed by atomic force and scanning electron microscopy concerning their size and density. Strong diffusion processes upon ion impact at the interfaces are observed and described by a fluence-dependent model. Besides, cathodoluminescence measurements are discussed in order to investigate the ion impact on the optical properties of the QDs, influenced by the quantum confined Stark effect.

HL 45: Transport: Quantum Coherence and Quantum Information Systems - Experiment (jointly with MA, HL)

Time: Wednesday 9:30–13:00 Location: HSZ 03

HL 45.1 Wed 9:30 HSZ 03

Adiabatic two-qubit state preparation in a superconducting qubit system — •Marc Ganzhorn[1], Daniel Egger[1], Andreas Fuhrer[1], Nikolaj Moll[1], Peter Mueller[1], Marco Roth[2], Sebastian Schmidt[3], and Stefan Filipp[1] — [1]IBM Schweiz, Rueschlikon, Schweiz — [2]Department fuer Physik, RWTH Aachen, Deutschland — [3]Institut fuer Theoretische Physik, ETH Zuerich, Schweiz

The adiabatic transport of a quantum system from an initial eigenstate to its final state while remaining in the instantaneous eigenstate of the driving Hamiltonian can be used for robust state preparation. With control over both qubit frequencies and qubit-qubit couplings this method can be used to drive the system from initially trivial eigenstates of the uncoupled qubits to complex entangled multi-qubit states. In the context of quantum simulation, the final state may encode a non-trivial ground-states of a complex molecule, or the solution to an optimization problem in the context of adiabatic quantum computing. Here we present experimental results on a system comprising fixed-frequency superconducting transmon qubits and a tunable coupler to adjust the qubit-qubit coupling via parametric frequency modulation. We realize different types of interaction terms by adjusting the frequency of the modulation. A slow variation of drive amplitude and phase leads to an adiabatic steering of the system to its final state showing entanglement between the qubits.

HL 45.2 Wed 9:45 HSZ 03

Second-order decoherence mechanisms of a transmon qubit probed with thermal microwave states — •Frank Deppe[1,2,3], Jan Goetz[1], Peter Eder[1,2,3], Michael Fischer[1,2,3], Stefan Pogorzalek[1,2,3], Edwar Xie[1,2,3], Kirill G. Fedorov[1,2], 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), 80799 München, Germany

Using thermal microwaves as a probe, we identify three second-order decoherence mechanisms of a superconducting transmon qubit. First, we quantify the efficiency of a resonator filter in the dispersive Jaynes-Cummings regime and find evidence for parasitic loss channels. Second, we probe second-order noise in the low-frequency regime and demonstrate the expected T^3 temperature dependence of the qubit dephasing rate. Finally, we show that qubit parameter fluctuations due to two-level states are enhanced under the influence of thermal microwave states. In particular, we present experimental evidence for a model based on noninteracting two-level states.

The authors acknowledge support from DFG through FE 1564/1-1, the doctorate program ExQM of the Elite Network of Bavaria, and the IMPRS 'Quantum Science and Technology'.

HL 45.3 Wed 10:00 HSZ 03

Probing broadband engineered and residual environments with a transmon qubit — •P. Eder[1,2,3], F. Deppe[1,2,3], T. Le Anh[1,2], J. Goetz[1,2], M. Fischer[1,2,3], E. Xie[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, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), 80799 München, Germany

Microwave beam splitters and transmon qubits are important components in circuit quantum electrodynamics (QED). Arranging two beam splitters in the form of an interferometer, we engineer a non-trivial broadband on-chip environment. We place the transmon qubit as a sensitive probe inside this environment and perform resonance fluorescence measurements. When comparing the experimental results with predictions from the spin-boson model, we find good agreement. Small deviations between experiment and theory indicate the presence of spurious electromagnetic modes. In general, our results demonstrate how to design and scale up complex circuits for experiments on propagating quantum microwaves.

The authors acknowledge support from DFG through FE 1564/1-1, the doctorate program ExQM of the Elite Network of Bavaria and the IMPRS 'Quantum Science and Technology'.

HL 45.4 Wed 10:15 HSZ 03

Chains of nonlinear and tunable superconducting resonators — •M. Fischer[1,2,3], P. Eder[1,2,3], J. Goetz[1,2], S. Pogorzalek[1,2], E. Xie[1,2,3], K. Fedorov[1,2], 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, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), 80799 München, Germany

We present the theoretical analysis and experimental study of a quantum simulation system of the Bose-Hubbard Hamiltonian in the driven dissipative regime in the realm of circuit QED. The system consists of series-connected, capacitively coupled superconducting resonators which are both nonlinear and tunable. The nonlinearity is achieved by galvanically coupled SQUIDs. They are placed in the current antinode of each resonator and can be tuned by external coils and on-chip antennas.

The authors acknowledge support from DFG through FE 1564/1-1, the doctorate program ExQM of the Elite Network of Bavaria and the IMPRS 'Quantum Science and Technology'.

HL 45.5 Wed 10:30 HSZ 03

Towards a scalable 3D quantum memory — •Edwar Xie[1,2,3], Frank Deppe[1,2,3], Daniel Repp[2], Peter Eder[1,2,3], Michael Fischer[1,2,3], Jan Goetz[1,2,3], Kirill G. Fedorov[1], 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), 80799 München, Germany

For superconducting qubits dispersively coupled to 3D cavity resonators both T_1-and T_2-times in excess of 100 μs have been achieved. However, the 3D cavities are bulky in comparison with their (slightly less coherent) 2D counterparts. A more scalable device can be built by exploiting the multi-mode structure of the 3D cavity. Here, we present an experimental study on such a device: a transmon qubit capacitively coupled to two distinct modes of a single 3D cavity. We engineer the fundamental and the first harmonic mode of a single cavity in such a way, that the former one couples well to the external feedline, whereas the latter does not. The qubit is dispersively coupled to both modes with a rate $g/2\pi \simeq 60$ MHz. Using a second-order coupling protocol, we observe an enhancement in qubit lifetime by a factor of 3 compared to the pure qubit lifetime and find that this value is not limited by fundamental constraints.

The authors acknowledge support from DFG through FE 1564/1-1, the doctorate program ExQM of the Elite Network of Bavaria and the IMPRS 'Quantum Science and Technology'.

HL 45.6 Wed 10:45 HSZ 03

Finite-time correlations of balanced two-mode squeezed microwave states — •Kirill Fedorov[1,2], Stefan Pogorzalek[1,2], Patrick Yard[1,2], Peter Eder[1,2,3], Michael Fischer[1,2,3], Jan Goetz[1,2], Edwar Xie[1,2,3], Achim Marx[1], Frank Deppe[1,2,3], 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), 80799 München, Germany

Generation of balanced two-mode squeezed states is a key task in quantum communication and illumination with continuous variables, as it enables distribution of quantum entanglement between distant parties. For this reason, the investigation of such states is of high interest in the field of propagating quantum microwaves. In our work, we perform tomography of balanced two-mode squeezed microwave states which are created by the means of two flux-driven Josephson parametric amplifiers generating orthogonally squeezed states at the inputs of a 50 : 50 microwave beam splitter. We study finite-time correlations in order to measure a characteristic time of entanglement decay in quantum channels. Our studies show that quantum communication and illumination protocols with continuous-variable propagating microwaves are experimentally feasible.

The authors acknowledge support from DFG through FE 1564/1-1, the doctorate program ExQM of the Elite Network of Bavaria, and the IMPRS 'Quantum Science and Technology'.

HL 45.7 Wed 11:00 HSZ 03

Impact of noise on entanglement of two-mode squeezed microwave states — •S. Pogorzalek[1,2], K. G. Fedorov[1,2], P. Yard[1,2], P. Eder[1,2,3], M. Fischer[1,2,3], J. Goetz[1,2], E. Xie[1,2,3], A. Marx[1], F. Deppe[1,2,3], and R. 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), 80799 München, Germany

Propagating quantum signals in the form of microwave two-mode squeezed states (TMSSs) can be generated by utilizing Josephson parametric amplifiers (JPAs). In our experiments, we employ two flux-driven JPAs at the inputs of an entangling hybrid ring in order to generate TMSSs between the hybrid ring outputs. This allows us to generate quantum entangled propagating microwave signals suitable for quantum communication and sensing applications such as quantum teleportation and quantum radar. However, the performance of these schemes may drastically depend on the amount of environmental noise in the communication channels. We study this dependence experimentally by controlling the amount of excess noise in different parts of the setup. Finally, we investigate the robustness of entanglement to thermal and shot noise via a negativity criterion and determine fundamental negativity-versus-noise limits.

The authors acknowledge support from DFG through FE 1564/1-1, the doctorate program ExQM of the Elite Network of Bavaria, and the IMPRS 'Quantum Science and Technology'.

15 min. break.

HL 45.8 Wed 11:30 HSZ 03

Tailoring coupling in artificial superconducting quasi-spins — •Alexander Stehli, Jochen Braumüller, Andre Schneider, Hannes Rotzinger, Martin Weides, and Alexey V. Ustinov — Physikalisches Institut, Karlsruhe Institute of Technology

Due to their intrinsic coherence and easy accessibility, superconducting circuits are a promising platform for building a universal quantum computer. Such devices could solve virtually any quantum problem, however many qubits are required in order to achieve quantum supremacy. A more direct, alternative approach is provided by analog quantum simulation. By synthesizing the Hamiltonian of a quantum system with a simulator, the eigenstates and time evolution are investigated without accessing the original system.

In this work, we explore the properties of two coupled concentric transmon qubits. We show strong XX-interaction with a coupling strength of 12 MHz between the qubits. This value is extracted from spectroscopy measurements and confirmed by vacuum Rabi oscillations, in good agreement with electrodynamic calculations.

These results pave way towards future experiments on the quantum dynamics of larger systems with multiple artificial quasi-spins. The concentric transmon is expected also to feature ZZ-coupling, when biased at frequencies away from the flux sweet spot. Depending on the accessible parameter range, the simulation of the Fermi-Hubbard model is offered by a theoretical model. In this contribution, we will show our experimental and numerical data and provide an outlook on performing quantum simulation with concentric transmon qubits.

HL 45.9 Wed 11:45 HSZ 03

Probing the strong coupling regime between microwave resonators and YPc_2 molecule ensembles — •Yannick Schön[1], Eufemio Pineda[2], Hannes Rotzinger[1], Marco Pfirrmann[1], Andre Schneider[1], Julius Krause[1], Sebastian T. Skacel[1], Mario Ruben[2], Alexey V. Ustinov[1], and Martin Weides[1,3] — [1]Karlsruhe Institute of Technology, Institute of Physics — [2]Karlsruhe Institute of Technology, Institute of Nanotechnology — [3]Johannes Gutenberg-University Mainz, Institute of Physics

We investigate magnetic molecule ensembles with microwave signals in the low GHz range. This offers a measurement and manipulation framework, which can reliably be integrated into hybrid quantum systems, and facilitates joint applications of magnetic molecules in the rapidly growing field of quantum information processing.

The studied material family of lanthanide or metal Phtalocyanine 2 compounds exhibits a wide range of splittings between their electronic states, as well as molecular anisotropy, depending on the central ion. Our setup facilitates probing dynamics of different molecules with a 3d cavity in dependence of temperature, power or magnetic field.

In particular, the strong coupling of Yttrium Pc2 (YPc_2) to microwave resonators has been investigated between 25 mK and 20 K, and compared to simulation based on input-output theory. The extracted parameters contain information about the sample transitions, their linewidth, and coupling strength down to the quantum regime. Furthermore, on-chip integration of molecule ensembles with superconducting niobium 2d resonators is demonstrated.

HL 45.10 Wed 12:00 HSZ 03

A pulsed electron paramagnetic resonance spectrometer operating at millikelvin temperatures — •Stefan Weichselbaumer[1,2], Christoph W. Zollitsch[1,2], Kai Müller[1,2], Petio Natzkin[1,2], Sebastian T. B. Goennenwein[1,2,3], Martin S. Brandt[2,4], Rudolf Gross[1,2,5], and Hans Huebl[1,2,5] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, Technische Universität München, Garching, Germany — [3]Institut für Festkörperphysik, Technische Universität Dresden, Dresden, Germany — [4]Walter Schottky Institut, Technische Universität München, Garching, Germany — [5]Nanosystems Initiative Munich, Munich, Germany

Electron paramagnetic resonance (EPR) is an ubiquitous spectroscopy tool which is employed in many areas of research. One critical aspect for any application is the sensitivity of the spectrometer which scales with the degree of spin polarization in the sample. In the paramagnetic case, this spin polarization is determined by the ratio of magnetic field and temperature, B/T. Here, we report on the implementation of a pulsed EPR spectrometer using superconducting microwave resonators, operating at millikelvin temperatures. We investigate a spin ensemble of phosphorus donors embedded in an isotopically purified nuclear spin free ^{28}Si environment, which exhibits a thermal spin polarization close to unity at 50 mK. Our high sensitivity allows for single-shot measurements with an exceptional signal-to-noise ratio SNR $\gg 1$ for approximately 10^8 spins.

This work was supported by the DFG via SPP 1601 (HU1861/2-1).

HL 45.11 Wed 12:15 HSZ 03

Engineering the parity of light-matter interaction in superconducting circuits — •J. Goetz[1], C. Besson[1,2], P. Eder[1,2,3], M. Fischer[1,2,3], S. Pogorzalek[1,2,3], E. Xie[1,2,3], K.G. Fedorov[1,2], 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, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), 80799 München, Germany

In physics, parity describes the symmetry properties of quantum states and operators under spatial inversion. It has manifold applications in the standard model, quantum information and field theory. We present a novel technique for the in-situ control of the interaction operator parity in superconducting quantum circuits. Using a tunable-gap gradiometric flux qubit, which exhibits both a dipole and a quadrupole moment, we can precisely engineer the interaction parity with spatially shaped microwave fields. Our highly symmetric sample architecture enables a complete parity inversion and the observation of transparency induced by longitudinal coupling. In a second step, we couple the qubit to a resonator and, in this way, activate quadrupolar transitions similar to those in multi-electron atoms. Our work paves the way towards parity based quantum simulation and physical applications based on longitudinal light-matter interaction.

The authors acknowledge support from DFG through FE 1564/1-1, the doctorate program ExQM of the Elite Network of Bavaria, and the IMPRS 'Quantum Science and Technology'.

HL 45.12 Wed 12:30 HSZ 03

Near quantum-limited amplification and conversion based on a voltage-biased Josephson junction — •Salha Jebari[1,2], Florian Blanchet[1,2], Romain Albert[1,2], Dibyendu Hazra[1,2], and Max Hofheinz[1,2] — [1]CEA, Grenoble,France — [2]Université Grenoble Alpes, Grenoble, France

Recent experiments with superconducting circuits consisting of a DC voltage-biased Josephson junction in series with a resonator have shown that a tunneling Cooper pair can emit one or several photons with a total energy of 2e times the applied voltage. We present microwave reflection measurements on the device in , indicating that amplification is possible with a simple DC voltage-biased Josephson junction. We also show that this amplification adds noise close to the limit set by quantum mechanics for phase preserving amplifiers. For low Josephson energy, transmission and noise emission can be explained within the framework of P(E) theory of inelastic Cooper

pair tunneling and are related to the fluctuation dissipation theorem (FDT). We also experimentally demonstrate, by controlling the applied DC voltage, that our device can act as both an amplifier and a frequency converter. Combined with a theoretical model, our results indicate that voltage-biased Josephson junctions might be useful for amplification near the quantum limit, being powered by simple DC voltage and providing a different trade-off between gain, bandwidth and dynamic range, which could be advantageous in some situations.

HL 45.13 Wed 12:45 HSZ 03

Josephson-photonics devices as source of non-classical microwave radiation — •Björn Kubala[1], Joachim Ankerhold[1], Chloe Rolland[2], Marc P. Westig[2], Iouri Moukharski[2], Daniel Esteve[2], and Fabien Portier[2] — [1]Institute for Complex Quantum Systems and IQST, Ulm University, Ulm, Germany — [2]CEA Saclay, Gif-sur-Yvette, France

Sources of non-classical photons have important applications in quantum communication and sensing technologies. With non-classical microwave sources these are extended to circuit-QED setups extensively used for various quantum information tasks.

Here, we report recent experimental result, demonstrating that a dc-biased Josephson junction embedded in a carefully engineered electromagnetic environment constitutes a new source of bright non-classical radiation. We will explain, why in such a "Josephson-photonics" device with a single mode of large impedance strongly anti-bunched photons are produced, opening the path to a single-photon source in the microwave range. A Cooper-pair crossing a junction, which is coupled to two resonators, under the proper dc-bias emits a pair of photons into the two resonators and thus produces correlated light with strongly reduced noise [1]. Measurements of this noise reduction factor demonstrate the non-classical nature of the light source.

[1] A. D. Armour, B. Kubala, and J. Ankerhold, Phys. Rev. B **91**, 184508 (2015)

HL 46: Transport: Molecular Electronics and Photonics (jointly with CPP, HL, MA, O)

Time: Wednesday 9:30–12:45 Location: HSZ 201

HL 46.1 Wed 9:30 HSZ 201

Negative differential conductance in single-molecule junctions with ferromagnetic electrodes — •Peter Hasch, Yuxiang Gong, Li Jiang, Carlos-Andres Palma, Joachim Reichert, and Johannes V. Barth — Physics Department E20, Technische Universität München, Germany

Scaling down logic operations to the level of single molecules might be considered the next frontier in computation. One approach is to electrically control single spin states in a molecule, trapped between two electrodes.

Here we report the observance of a negative differential conductance (NDC), measured in a single-molecule junction. The investigated NDC could be explained by a single-spin phenomenon, arising when the molecule gets charged due to voltage-induced depopulation of the highest occupied molecular orbital. This oxidation is monitored by Raman spectroscopy, which allows to analyze chemical and electronical structures with a single-molecule sensitivity. By (anti)ferromagnetic coupling of the unpaired spin on the molecule to one of the electrodes, the molecule might act as a spin-valve, blocking charge transport of the opposite spin direction.

Single-molecule NDC elements bear considerable potential for logical crossbar architectures, and could shrink the actual state of the art devices significantly in size.

HL 46.2 Wed 9:45 HSZ 201

Single-molecule junctions with oligoynes and epitaxial graphene nanoelectrodes — •Konrad Ullmann[1], Susanne Leitherer[2], Maximilian Krempe[3], Rik Tykwinski[3], Michael Thoss[2], and Heiko Weber[1] — [1]Lehrstuhl für Angewandte Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [3]Organische Chemie I, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Single molecule junctions using graphene as electrode material have drawn considerable attention in recent years [1,2]. Due to their open access architecture, their transparency and robustness, they are well suited for a variety of unprecedented experiments. The electrode material graphene also allows for new anchor groups which connect the molecule to the electrode, e.g. via Pi-interaction.

We report on experiments using an oligoyne molecular wire with platinum termination, being contacted with epitaxial graphene nanoelectrodes. I-V characteristics show a linear behavior with a conductance close to the conductance quantum. Furthermore we present an experimental setup which uses electrospray ionisation to bring the molecules in contact with the graphene electrodes.

[1] K. Ullmann et al., Nano Lett. 15, 3512, 2015
[2] F. Prins et al., Nano Lett. 11, 4607, 2011

HL 46.3 Wed 10:00 HSZ 201

Visualizing the role of molecular orbitals in charge transport through individual diarylethene Isomers — •Gaël Reecht[1], Christian Lotze[1], Dmytro Sysoiev[2], Thomas Huhn[2], and Katharina J. Franke[1] — [1]Freie Universität Berlin , Berlin ,Germany — [2]Universität Konstanz, Konstanz, Germany.

Diarylethene molecules are prototype molecular switches with their two isomeric forms exhibiting strikingly different conductance, while maintaining similar length. With a scanning tunneling microscope (STM) we investigate the electronic structure and the transport properties of the open and closed isomers of a sulfur-free diarylethene. The electronic structure is determined with scanning tunneling spectroscopy (STS) for the molecule lying on the surface. Between the two isomers, intriguing differences of the energy and the spatial extend of the molecule orbitals are observed. We then lift the two isomers with the tip of the STM and measure the current passing through the individual molecules. We observe an important difference of conductance between the two forms. With a simple analytical model of transport based on the results of the STS measurements, we show that the previously determined orbital characteristics are essential ingredients for the complete understanding of the transport properties.

HL 46.4 Wed 10:15 HSZ 201

Electronic transport properties of a tripodal molecular platform — •safa golrokh bahoosh, amin karimi, elke scheer, and fabian pauly — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

Intensive studies on single-molecule junctions have been performed to explore the implementation of molecular-scale devices and to understand how the molecules transport charges[1]. While molecules with delocalized π-systems are the ideal compounds to form wires for electronic applications due to their expected high conductance, tripodal molecular platforms that points almost perpendicular to the surface, appear as promising candidates to establish a conducting path between two electrodes. To take into account these aspects, a 9,9'-spirobifluorene (SBF) platform has been introduced. By combining experimental and theoretical investigations of elastic and inelastic charge transport, we show that the current proceeds through the molecular "backbone" and identify a binding geometry that is compatible with the experimental observations in mechanically controlled break junctions[2]. The conductive molecular wire on the platform features a well-defined and relatively high conductance despite the length of the current path of more than 1.7 nm. If time permits, the possibility to use these molecules as a molecular toggle switch, as observed in subsequent studies with a scanning tunneling microscope, will be discussed.

[1] S. Aradhy, and L. Venkataraman, Nature Nanotechnol. 8, 399 (2013)
[2] M. A. Karimi, S. G. Bahoosh, M. Valášek, M. Bürkle, M. Mayor, F. Pauly, and E. Scheer, Nanoscale 8, 10582 (2016)

HL 46.5 Wed 10:30 HSZ 201

Analysis of local current through molecular wires in open quantum systems — •Daijiro Nozaki, Andreas Lücke, and Wolf Gero Schmidt — Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn, Germany

The understanding of the local electronic flows in single molecules is

of fundamental importance in the design of functional molecules as well as molecule-based electronic devices [1-4]. The charge transport through molecular wires connected between contacts is investigated using non equilibrium Green's function formalism combined with Landauer formula. Energy-dependent and total current through a series of molecular junctions are calculated in real space representation. The influence of contact positions, functional groups, and the replacement of atoms as defects on the transport properties are examined systematically. The static current-induced local magnetic field is also investigated in carbon-based molecular wires. It is shown that even in the same bias directions the direction of the magnetic field is easily reversed depending on the molecular topologies and the positions of electric contacts.

[1] M. Walz, J. Wilhelm, and F. Evers Phys. Rev. Lett. **113**, 136602 (2014)
[2] J. Wilhelm, M. Walz, and F. Evers Phys. Rev. B **92**, 014405 (2015)
[3] G. C. Solomon, C. Herrmann, T. Hansen, V. Mujica, and M. A. Ratner Nat. Chem. **2**, 223 (2010)
[4] T. Ono and K. Hirose, Phys. Rev. Lett. **98**, 026804 (2007)

HL 46.6 Wed 10:45 HSZ 201

Controlling the conductance of graphene-molecule junctions by proton transfer — •Dominik Weckbecker, Pedro B. Coto, and Michael Thoss — FAU Erlangen-Nürnberg, Institut für Theoretische Physik, Staudtstrasse 7/B2, 91058 Erlangen, Germany

The possibility of using single-molecule junctions as components of nanoelectronic devices has motivated intensive experimental and theoretical research on the underlying transport mechanism in these systems [1]. In this contribution, we investigate from a theoretical perspective intramolecular proton transfer reactions as a mechanism for controlling the conductance state of graphene-based molecular junctions. Employing a methodology that combines first-principles electronic structure calculations with nonequilibrium Green's function transport theory [1], we show that the proton transfer reaction proceeds via a two-step mechanism and gives rise to several states of the junction with different conductance properties. In addition, we demonstrate that the relative stability of the different conductance states and the energy barriers for the interconversion reactions can be controlled by means of an external electrostatic field. The possibility of using this mechanism for the design of nanomolecular devices such as diodes or switches is also discussed [2,3].

[1] Cuevas, J. C. and Scheer, E., Molecular Electronics, World Scientific Pub. Co., Singapore, 2010
[2] Hofmeister, C. *et al.*, J. Mol. Model. **20**, 2163 (2014)
[3] Hofmeister, C. *et al.*, arXiv: 1611.01027v1 (2016)

15 min. break.

HL 46.7 Wed 11:15 HSZ 201

Hierarchical Quantum Master Equation Approach to Vibrationally Coupled Nonequilibrium Charge Transport in Single-Molecule Junctions — •Christian Schinabeck[1], André Erpenbeck[1], Rainer Härtle[2], and Michael Thoss[1] — [1]Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany. — [2]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany.

We investigate vibrationally coupled transport in single-molecule junctions using the hierarchical quantum master equation (HQME) approach [1-3]. This method allows a systematic convergence of the reduced dynamics of open quantum systems beyond the traditional perturbative master equations. We demonstrate the importance of vibrational nonequilibrium effects for a model molecular junction consisting of an electronic level coupled to fermionic leads as well as a vibrational mode. In particular, in the off-resonant transport regime, the inelastic cotunneling signal is analyzed for a vibrational mode in full nonequilibrium, revealing a complex interplay of different transport processes and deviations from the commonly used $G_0/2$ rule of thumb [3]. Moreover, an extension of the HQME approach is presented, which allows the calculation of the full counting statistics. Using this method, the influence of higher-order cotunneling processes on the current fluctuations is analyzed.

[1] Y. Tanimura *et al.*, J. Phys. Soc. Jpn. **75**, 082001 (2006).
[2] J. Jin *et al.*, J. Chem. Phys. **128**, 234703 (2008).
[3] C. Schinabeck *et al.*, Phys. Rev. B **94**, 201407 (2016).

HL 46.8 Wed 11:30 HSZ 201

Theoretical study of current-induced bond rupture in molecular junctions — •André Erpenbeck, Christian Schinabeck, Lukas Götzendörfer, and Michael Thoss — Institut für Theoretische Physik und Interdisziplinäres Zentrum für Molekulare Materialien (ICMM), Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany

Electronic-vibrational coupling in charge transport through single molecule junctions may result in current-induced bond rupture and is thus an important mechanism for the stability of the junction. In this contribution, we demonstrate how the hierarchical quantum master equation (HQME) theory in combination with the quasi-classical Ehrenfest approach for the nuclear degrees of freedom can be used to simulate current-induced bond rupture in single molecule junctions. Employing generic models for molecular junctions with dissociative nuclear potentials, we analyze the underlying mechanisms. In particular, we investigate the dependence of the current, the population and the dissociation probability on the model parameters. In addition, we validate the quasi-classical Ehrenfest approach using numerically exact results obtained by the HQME method [1] for a model comprising one harmonic vibrational mode.

[1] C. Schinabeck, A. Erpenbeck, R. Härtle, M. Thoss, Phys. Rev. B 94, 201407(R) (2016)

HL 46.9 Wed 11:45 HSZ 201

Spin Transport in Helical Systems — •Matthias Geyer[1,2], Rafael Gutiérrez[1], Stefan Siegmund[3], and Gianaurelio Cuniberti[1,2] — [1]Institute for Materials Science, TU Dresden, 01062 Dresden, Germany — [2]Dresden Center for Computational Materials Science, TU Dresden, 01062 Dresden, Germany — [3]Center for Dynamics, TU Dresden, 01062 Dresden, Germany

Various experiments have shown strong spin selectivity in chiral molecules like DNA at room temperature. Since atomic spin orbit coupling alone is insufficient to explain the effect's magnitude, a relation to the helical geometry has been suggested. We want to provide a better understand of the underlying mechanisms by analytically and numerically investigating suitable models for electrons in helical systems with spin orbit coupling.

We follow two complementary approaches: a generic and simplified model to study the bare influence of the helical geometry and a more realistic one to calculate the effect for specific molecules. The former starts with a 3D continuum model with helix-shaped confinment from which an effective 1D Hamiltonian is derived using adiabatic perturbation theory. For the ladder an effective tight-binding model is derived from the microscopic Hamiltonian of a specific molecule. Incoherent transport calculations are performed for both models using master equations with dephasing, accounting for decoherence due to the coupling to vibrational degrees of freedom arising from structural fluctuation.

HL 46.10 Wed 12:00 HSZ 201

Charge Carrier Dynamics in κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl: From Mott Insulator to Quantum Spin Liquid — •Jana-Isabelle Polzin[1], Benedikt Hartmann[1], Takahiko Sasaki[2], and Jens Müller[1] — [1]Institute of Physics, Goethe University Frankfurt, Germany — [2]Institute for Materials Research, Tohoku University, Sendai, Japan

The organic charge transfer salts κ-(ET)$_2$X are model systems for studying strongly-correlated charge carriers and the Mott metal-insulator transition in reduced dimensions. Recently, the influence of quenched disorder attracted considerable attention. Conducting layers of ET molecules are separated by thin, insulating sheets with anions X, resulting in a quasi-2D electronic band structure. Within the ET layers the molecules are arranged in dimers forming a triangular lattice. One free charge carrier exists per dimer, its spin being geometrically frustrated. The Mott insulator κ-(ET)$_2$Cu[N(CN)$_2$]Cl shows antiferromagnetic ordering at $T_N \approx 27\,K$. It has been shown that increasing disorder induced by X-ray irradiation drives the Mott insulating state with long-ranged antiferromagnetic order into a quantum spin liquid state [1]. Here, we discuss comparative measurements of fluctuation spectroscopy on pristine and irradiated samples in order to investigate the changes in electronic transport mechanism and low-frequency charge carrier dynamics [2] when tuning the Mott insulator to the spin liquid ground state. This results in a decrease of both resistivity and the current or voltage fluctuations after irradiation.

[1] PRL 115, 077001 (2015)
[2] PRL 114, 216403 (2015)

HL 46.11 Wed 12:15 HSZ 201

Charge Carrier Dynamics at the Mott transition in κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br — •Tatjana Thomas[1], Benedikt Hartmann[1], Takahiko Sasaki[2], and Jens Müller[1] — [1]Institute of Physics, Goethe University Frankfurt, Germany — [2]Institute for Materials Research, Tohoku University, Sendai, Japan

The organic charge transfer salts κ-(ET)$_2$X are considered as model systems for studying the Mott metal-insulator transition – a key phenomenon in the physics of strongly correlated electrons – in reduced dimensions. In particular, the influence of disorder on the criticality of the Mott transition recently has been a matter of debate. Partially deuterated κ-[(H$_8$-ET)$_{0.2}$(D$_8$-ET)$_{0.8}$]$_2$Cu[N(CN)$_2$]Br, which is located in the critical region of the phase diagram, can be fine-tuned through the Mott transition by utilizing a glass-like structural ordering transition of the ET molecules' terminal ethylene groups. By applying different thermal relaxation protocols, both the ratio of W/U and a small degree of quenched disorder can be set at will, the former corresponding to changes in hydrostatic pressure of ~ 200 bar. We employ fluctuation (noise) spectroscopy as a powerful tool to study the charge carrier dynamics at low frequencies. When crossing the S-shaped Mott transition line, surprisingly we observe a step-like increase of the resistance fluctuations in the metallic region. We discuss our results in terms of critical slowing down of the order parameter fluctuations [1] and electronic phase separation, and an extended region of the phase diagram where the fluctuations are non-Gaussian.

[1] B. Hartmann et al., *Phys. Rev. Lett.* **114**, 216403 (2015).

HL 46.12 Wed 12:30 HSZ 201

Thermal conductance of Teflon and Polyethylene: Insight from an atomistic, single-molecule level — •Marius Buerkle and Yoshihiro Asai — AIST, Tsukuba, Japan

The thermal transport properties of teflon (polytetrafluoroethylene) and its polyethylene counterparts are, while highly desirable and widely used, only superficially understood. Here, we aim therefore to provide rigorous insight from an atomistic point of view in context of single-molecule devices. We show that for vinyl polymers adsorbed on metal-surfaces the thermal transport strongly depends one the properties of the metal-molecule interface and that the reduced thermal conductance observed for teflon derivatives originates in a reduced phonon injection life time. In asymmetric molecules phonon blocking on the intra molecular interface leads to a further reduction of thermal conductance. For hetrojunctions with different electrode materials we find that thermal conductance is suppressed due to a reduced overlap of the available phonon modes in the different electrodes. A detailed atomistic picture is thereby provided by studying the transport through perfluorooctane and octane on a single-molecule level using first principles transport calculations and nonequilibrium molecular dynamic simulations.

HL 47: Organic Photovoltaics and Electronics I (joined session with CPP)

Time: Wednesday 9:30–12:45 Location: POT 81

HL 47.1 Wed 9:30 POT 81

Controlling Tamm-plasmons for organic narrowband NIR photodetectors based on intermolecular charge transfer — •Andreas Mischok, Bernhard Siegmund, Dhriti Ghosh, Johannes Benduhn, Donato Spoltore, Hartmut Fröb, Christian Körner, Koen Vandewal, and Karl Leo — Dresden Integrated Center for Applied Physics and Photonic Materials, Technische Universität Dresden, Dresden

Combining a periodic distributed Bragg reflector (DBR) with a thin metal film leads to the formation of Tamm-plasmon-polaritons (TP) as sharp resonances at the DBR-metal interface. Here, we utilize such TP states to realize cavity-enhanced near infrared photodetection using an organic donor-acceptor bulk heterojunction. In such blend films, intermolecular charge transfer states play an important role during the separation of excitons. Furthermore, they can also be directly optically excited, albeit exhibiting only weak absorption coefficients and a broad linewidth. The weak extinction typically makes these states uninteresting for direct photocurrent generation, however they provide an ideal base for cavity-enhanced devices. Controlling the formation of TP resonances in a DBR-solar cell stack, we create a high-Q microcavity in the near-infrared, targeting the CT state energy. These tunable Tamm-plasmon-charge-transfer (TPCT) resonances enable direct photodetection of light well below the bandgap of the organic absorbers at zero bias and facilitate detector external quantum efficiencies of 17 % as well as a linewidth below 25 nm for spectroscopic applications.

HL 47.2 Wed 9:45 POT 81

Field-induced exciton separation in organic solar cells: Quantifying binding energies via luminescence quenching studies — •Marina Gerhard[1], Andreas P. Arndt[2], Uli Lemmer[2,3], Ian A. Howard[3], and Martin Koch[4] — [1]Department of Chemical Physics, Lund University, 22100 Lund, Sweden — [2]Light Technology Institute, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [3]Institute of Microstructure Technology, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany — [4]Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, 35032 Marburg, Germany

In this contribution we investigate the field- and temperature-dependence of luminescence quenching in organic solar cells (OSCs) employing a streak camera. We study the prototypical system PTB7:PC$_{71}$BM, where different emissive species i.e. singlet and CT states can be identified by choosing appropriate excitation conditions.[1] The quenching behavior and PL dynamics are satisfactorily reproduced by a kinetic model based on exciton dissociation via a hopping mechanism,[2] allowing us to take the important influence of disorder into account. Moreover, our experimental and simulative approach suggests that the binding energy of the emissive CT state (ca. 50 meV) is about one order of magnitude below that of singlet states. The absence of strongly bound CT states acting as 'deep' traps could essentially contribute to the high efficiency of the studied OSCs.

[1] M. Gerhard et al., J. Phys. Chem. C 119 (51), 2015, p. 28309
[2] O. Rubel et al., Phys. Rev. Lett. 100 (19), 2008, p. 196602

HL 47.3 Wed 10:00 POT 81

Dissipative Charge Transfer Dynamics at an Oligothiophene/ZnO Interface — •Thomas Plehn and Volkhard May — Institute of Physics, Humboldt University Berlin, Germany

A combined theoretical study of the entire "light to free charge carrier" kinetics on hybrid organic/inorganic interfaces describes a huge challenge, owing to the manifold of interdependent subprocesses. While studies of short time quantum dynamics demand for expensive methods including e.g. electron-phonon interaction, the long time scale kinetics, however, are very sensitive to a realistic size of the model systems. In order to meet both grades, we set up an open system dynamics study based on a stochastic Schrödinger equation method.

After an introducing overview of the organic/inorganic hybrid system under consideration we present the aspired excitation energy and charge transfer processes. The presentation gives insight into the combined coherent and dissipative kinetics in a huge organic oligothiophene cluster. An initial study has the focus on solely the organic part. Then we attend to the actual hybrid interface system by placing the molecular cluster on a ZnO surface. By means of an installed electronic excess charge distribution in the inorganic counterpart, the hole motion inside the cluster becomes subject to a realistic Coulomb attraction across the interface. In order to clarify the principles of the aspired electron-hole pair separation across such interfaces, it is fundamental to understand how the hole overcomes this existing barrier.

HL 47.4 Wed 10:15 POT 81

Charge carrier dynamics in polar organic metal-insulator-semiconductor diodes — •Alexander Hofmann[1], Simon Züfle[2], Theresa Linderl[1], Thomas Zechel[1], Lars Jäger[1], Stephane Altazin[2], Beat Ruhstaller[2], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]ZHAW School of Engineering, Technikumstrasse 9, 8401 Winterthur, Switzerland

Polar organic materials such as tris-(8-hydroxyquinolate) aluminum (Alq_3), whose strong permanent dipole moment leads to a pronounced accumulation of charge carriers at the interface, can take the role of an insulator in a metal insulator semiconductor (MIS) diode. Thus,

classic wide-bandgap insulators are replaced with polar organic materials. MIS diodes in conjunction with impedance spectroscopy (IS) and charge extraction experiments (e.g. CELIV), however, represent an established device geometry to investigate charge carrier dynamics and dielectric material properties. From temperature dependent MIS-CELIV and IS on organic MIS diodes with different hole transport materials, we are able to independently determine the activation energy of hopping transport as well as the barrier for charge injection.

HL 47.5 Wed 10:30 POT 81

Fast Organic Near-Infrared Photo-Detectors Based on Charge-Transfer Absorption — •Sascha Ullbrich, Bernhard Siegmund, Andreas Mischok, Andreas Hofacker, Donato Spoltore, Christian Körner, Karl Leo, and Koen Vandewal — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Technische Universität Dresden, Dresden, Germany

In this work, we present organic near-infrared photo-detectors based on the absorption of charge-transfer states between ZnPc as donor and C_{60} as acceptor material. By using a resonant optical cavity device architecture, we reach external quantum efficiencies above 1% at 1064nm for ZnPc:C_{60} blends, well below (>200nm) the optical gap of the neat materials. We measure transient photo-current (TPC) responses at wavelengths of 355nm, 532nm, and 1064nm, exciting dominantly C_{60}, ZnPc, or the ZnPc-C_{60} CT state, respectively, and obtain rise and fall times of a few nanoseconds at short circuit. We find that the response upon CT excitation is at least as fast as upon ZnPc or C_{60} excitation, emphasizing the possibility to generate fast free carriers by intermolecular absorption. By reducing the active area of the devices, we are able to overcome the generally high RC time limitations caused by thin organic layers. The current transients are modeled with time dependent drift-diffusion simulations of electrons and holes which reconstruct the photo-current signal, including capacitance and series resistance effects. The hole mobility of the donor material is identified as the limiting factor for the high frequency response.

HL 47.6 Wed 10:45 POT 81

Photovoltaic Performance of Organic Photodiodes Based on Homochiral Squaraine Compounds — •Manuela Schiek[1], Matthias Schulz[2], Majvor Mack[1], Oliver Kolloge[1], Dominik Höweling[1], and Arne Lützen[2] — [1]University of Oldenburg — [2]University of Bonn

The substitution pattern of non-toxic and environmentally stable dihydroxy-anilino squaraines [1] is modified with natural chiral functional groups such as a prolinol derivative. These natural compounds are available in their enantiomerically pure forms making costly separation of racemic product mixtures obsolete. Strong circular dichroism is measured in spin-casted thin films proving homo-chiral aggregation. Blended with a fullerene acceptor, these squaraines perform as light harvesting compound in a conventional bulk heterojunction photodiode. The performance depends on the blend ratio of squaraine and fullerene as well as on active layer thickness. In all cases, the devices suffer from low fill factors. Thinner layers lead to S-shaped current voltage characteristics around Voc. In addition, a thin active layer device with a high fullerene percentage is impacted by a photoshunt under illuminated reverse current conditions [2]. This becomes visible in reverse voltage biased EQE measurements showing a spectrally dependent deformation of the photocurrent response with the EQE exceeding 100% in the spectral response regime of the fullerene. [1] Schiek et al. Langmuir 32 (2016) 8533. [2] Tress et al. Phys. Stat. Solidi RRL 7 (2013) 401.

Coffee Break

HL 47.7 Wed 11:30 POT 81

Hybrid solar cells from antimony sulfide nanoparticles — •wei wang, frank strössner, eugen zimmermann, kevin wong, and lukas schmidt-mende — Department of Physics; University of Konstanz

Antimony sulfide (Sb2S3) is a promising candidate for hybrid thin film solar cells due to its various favorable properties, such as suitable optical band gap (1.75 eV), high dielectric constant and good band alignment in combination with many organic hole transport materials. In our study, amorphous Sb2S3 nanospheres were fabricated by a simple colloidial synthesis method. The Sb2S3 nanoparticles were capped by oleic acid (OA) or 1-dodecanethiol (DT) molecules. Thin film hybrid solar cells were made by using these prefabricated Sb2S3 nanoparticles as absorber material by depositing them on a TiO2 covered FTO substrate. The film was then annealed to convert the particles in a crystalline film. P3HT was deposited on top as hole transporter. The device performance of the solar cells fabricated from DT capped nanoparticles was superior to the one capped with OA ligand. Fourier transform infrared spectra (FTIR) revealed that the OA molecules were still anchored to the Sb2S3 surface after high temperature annealing, while DT molecules were almost not detectable.

HL 47.8 Wed 11:45 POT 81

Organic Light-Emitting Diodes for Optogenetic Stimulation of Neurons in *Drosophila* Larvae — •Caroline Murawski[1], Andrew Morton[1], Ifor D. W. Samuel[1], Stefan R. Pulver[2], and Malte C. Gather[1] — [1]Organic Semiconductor Centre, SUPA, School of Physics and Astronomy, University of St Andrews, North Haugh, St Andrews KY16 9SS, UK — [2]School of Psychology and Neuroscience, University of St Andrews, St Mary's Quad, South Street, St Andrews KY16 9JP, UK

Optogenetics is an emerging method in biology that enables controlling neurons non-invasively with light. Currently, however, only a small number of neurons can be controlled individually so that stimulation of neurons with light still lacks precision compared to the complexity of the brain. To overcome these limitations, we use organic light-emitting diodes (OLEDs), which enable unprecedented high-resolution optogenetic control of thousands of neurons at once. One of the challenges involves the need for very high light intensities (on the order of mW/mm^2), a brightness at which OLED efficiency typically decreases dramatically. In this contribution, we show our recent development towards achieving higher brightness OLEDs employing doped charge transport layers. Using these light sources, we demonstrate optogenetic stimulation of neurons in *Drosophila* (fruit fly) larvae and investigate subsequent behavioral changes at different light intensities.[1]

[1] A. Morton, C. Murawski, S. R. Pulver, M. C. Gather, *Sci. Rep.* 2016, **6**, 31117.

HL 47.9 Wed 12:00 POT 81

Low Voltage Losses in Cascade Organic Solar Cells by Reducing the Donor-Acceptor Interfacial Area — •Vasileios Christos Nikolis, Johannes Benduhn, Felix Holzmüller, Christian Körner, Donato Spoltore, and Koen Vandewal — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Technische Universität Dresden, Germany

High photon energy losses (E_{loss}) significantly limit the open-circuit voltage (V_{OC}) and power conversion efficiency (PCE) of organic solar cells (OSC). Reduction of E_{loss}, while keeping a high charge generation yield, can lead OSC into a new, beyond 12%, PCE regime.

In this work, we present an optimization route, which increases V_{OC} by reducing the interfacial area between electron donor (D) and acceptor (A) in planar heterojunction solar cells. Through an introduction of thin and discontinuous interlayers between D and A, we increase the V_{OC} of a cascade organic solar cell from 0.98 V to 1.16 V. Although the V_{OC} maximizes at the expense of short-circuit current and fill factor for thick interlayers, an optimum interlayer thickness for increased PCE exists. By appropriately measuring the optical gap (E_{opt}) of the device at 1.73 eV, the obtained E_{opt}-qV_{OC} losses of 0.57 eV are among the lowest observed for organic photovoltaics. Most importantly, for these devices, the external quantum efficiency (EQE) peak at the edge of the spectrum (705 nm) remains high and reaches 79%.

Our work shows that low energy losses for strongly absorbed photons can be combined with a high EQE in organic photovoltaic devices.

HL 47.10 Wed 12:15 POT 81

Flexible organic solar cell with the effects of light trapping — •Yoonseok Park[1], Koen Vandewal[1], Karl Leo[1], Jana Ber[2,3], and Andrés Fabián Lasagni[2,3] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Technische Universität Dresden, Germany — [2]Fraunhofer-Institut für Werkstoffund Strahltechnik IWS, Dresden, Germany — [3]Institute for Manufacturing Technology, Technische Universität Dresden, Germany

Organic solar cells are one of the most promising candidates for future solar power generation. They are thin and lightweight with several advantages, e. g. scalability, environmental sustainability and low cost for processing and installation. In order to set up a roll-to-roll process, flexible substrates and electrodes are required. Conventional materials, e. g. glass as substrate and ITO as electrode, are however rigid and brittle. Therefore, flexible polymer materials are investigated. Besides being flexible, polymers are much easier to process and manipulate

due to their relative softness as compared to glass and metal oxides. This gives the opportunity to easily introduce light trapping structures into these materials. In this study, we apply several light trapping approaches to organic solar cells. First, PET films structured with a direct laser patterning system as well as optical display films commercially developed to be used for LCD are examined as substrates. Moreover, since PEDOT:PSS electrode is prepared by a solution-based process, nanoparticles are added as light scattering elements. Finally, 2-D nanostructures are printed by a nano-imprinting technique onto the surface of PEDOT:PSS electrodes with PDMS stamps.

HL 47.11 Wed 12:30 POT 81

Metal-free OLEDs with organic transparent electrodes — •Irma Slowik, Axel Fischer, Paul-Anton Will, Simone Lenk, Sebastian Reineke, and Karl Leo — Technische Universität, Dresden, Deutschland

Organic light emitting devices (OLEDs) have versatile applications for flexible transparent devices as transparent displays or lightning panels. Transparent electrodes can be realized by thin metal electrodes, transparent, conducting oxides, conducting polymers, 2D materials, and metal nanowires. Organic molecular layers are mostly not suitable as electrodes due to their low conductivity, resulting in a lateral voltage drop within the organic layer and inhomogeneous emission and low efficiency of the device. However, their processing by thermal evaporation is the same as for the OLED allowing a simple fabrication process.
Here, we introduce a fully organic OLED using highly doped C_{60} as transparent electrode having a sufficiently high conductivity as well as transparency. Utilizing a tunnel junction between two highly and contrary doped semiconductors, n-doped C_{60} is suitable as top and bottom electrode, resulting in a complete organic device architecture. Although the emission decreases laterally due to the residual sheet resistance of the doped C_{60} layer, nearly uniform emission is reached within a range of several hundred microns, larger than the standard display pixel. The OLEDs provide small angular spectral shift due to the low refractive index change between electrodes and organic layers. By that approach, transparent OLEDs with bidirectional emission can be easily realized.

HL 48: Two-dimensional materials IV (joined session with TT)

Time: Wednesday 9:30–13:15 Location: POT 51

HL 48.1 Wed 9:30 POT 51

Landau-Quantized Graphene: A Tunable Nonlinear Optical Material in the THz Range — •Jacob C. König-Otto[1,2], Yongrui Wang[3], Alexey Belyanin[3], Claire Berger[4,5], Walt A. de Heer[4], Milan Orlita[6,7], 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]Texas AM University, USA — [4]Georgia Institute of Technology, USA — [5]CNRS-Université Alpes, France — [6]LNCMI, Grenoble, France — [7]Charles University in Prague, Czech Republic

Finding nonlinear optical materials for the THz and mid-infrared regimes is not straightforward. State-of-the-art devices with a high third-order optical susceptibility are often processed as complex multi-quantum-well structures designed to feature one specific resonance frequency. In our work we study Landau-quantized graphene as a tunable and simple to produce nonlinear material. To this end we perform time-integrated degenerate four-wave mixing (FWM) experiments at a photon energy of 78 meV resonant to the transitions between the Landau levels LL_{-1}, LL_0 and LL_1 at a magnetic field of roughly 4 T. We can recover expected scaling of the FWM-signal with the incident fields and the resonance behavior. The value of the third-order surface susceptibility in this material is in agreement with our calculations based on the density matrix formalism. We find the order of $\chi^{(3)}$ of Landau-quantized graphene to be competitive with more complex and elaborated solutions.

HL 48.2 Wed 9:45 POT 51

Ballistic transport in 2D periodically modulated graphene — •Andreas Sandner[1], Martin Drienovsky[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 was shown to be an efficient way of achieving a high bulk mobility. The encapsulated graphene is protected in any further top-down fabrication procedure and pronounced commensurability features could be observed in 2D antidot lattices [1].

Here, we want to introduce a new method for periodical modulation of the carrier density, employing a few layer graphene patterned bottom gate. The bottom gate is defined by etching a 2D hole array into the few layer graphene and adapts perfectly to the commonly used stacking method for van der Waals heterostructures. By tuning the local bottom gate and the global back gate voltage, we can switch between the unipolar and bipolar transport regime.

We fabricated patterned bottom gates with lattice periods down to 150 nm and observe pronounced commensurability peaks that can be nicely compared to experiments with hard-wall graphene antidot lattices. We report on the difference between the unipolar and the bipolar regime, as well as the influence of the magnitude of the imposed superlattice potential.

[1] A. Sandner et al., Nano Lett. **15**, 8402 (2015)

HL 48.3 Wed 10:00 POT 51

Commensurability oscillations in electrostatically modulated graphene — •Martin Drienovsky[1], Jonas Joachimsmeyer[1], Takashi Taniguchi[3], Kenji Watanabe[3], Ming-Hao Liu[2], Klaus Richter[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]Institut für Theoretische Physik, Universität Regensburg, Germany — [3]National Institute for Material Science, Tsukuba, Japan

We report on the first experimental observation of commensurability oscillations (COs) [1] in a 1D periodic graphene superlattice. Employing a locally acting few layer graphene patterned bottom gate (FLG PBG) and a dry van-der-Waals stacking method we prepare high mobility graphene-boron nitride heterostructures, where the ballistic length exceeds several periods of the modulation. The potential landscape can be tuned by the striped FLG PBG and a global back gate in such a way that a small, periodic and unipolar potential perturbation is generated. The magnetoresistance exhibits well pronounced COs at predicted magnetic field positions for electrostatic modulation, both for the electron and hole transport regime. Our measurements confirm strong robustness of the COs in graphene with respect to temperature [2], as they remain visible up to 155 K.

[1] D. Weiss et al., Europhys. Lett. 8, 179 (1989) [2] A. Matulis and F. M. Peeters, Phys. Rev. B 75, 125429 (2007)

HL 48.4 Wed 10:15 POT 51

Intrinsic mobility due to electron-phonon interaction in black phosphorus. — •Sergey Brener, Alexander Rudenko, and Mikhail Katsnelson — Radboud Universiteit, Niederlanden

Flexural and in-plane thermal fluctuations in crystalline membranes affect the band structure of the carriers, which has an effect on transport properties of 2D systems. I consider a specific example of one-layer black phosphorus, which is a highly anisotropic material, and present our recent results on intrinsic carrier mobility. In contrast to graphene, where the mobility is determined by two-phonon (flexural) scattering, in black phosphorus one-phonon (in-plane) processes dominate.

HL 48.5 Wed 10:30 POT 51

Strain-induced commensurability oscillations in graphene — •Jonas Joachimsmeyer[1], Martin Drienovsky[1], Takashi Taniguchi[2], Kenji Watanabe[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]National Institute for Materials Science, Tsukuba, Japan

We realized a periodic strain modulation in a graphene/hexagonal boron-nitride (hBN) heterostructure by transferring it onto a prepatterned 1D superlattice etched into hBN. The transfer was performed using a dry van-der-Waals pick-up technique. This method yields a high mobility graphene device with a mean free path exceeding the

period of the corrugation.

We conducted magnetotransport experiments in this corrugated graphene monolayer with a period of 150 nm. The modulation leads to a periodic strain which in turn gives rise to an effective periodic pseudopotential with half of the period of the corrugation [1], i.e. 75 nm. Due to the periodic potential we observe commensurability oscillations (COs) [2] in the longitudinal magnetoresistance, however superimposed by Shubnikov-de Haas (SdH) oscillations. Since both oscillations show different temperature dependences we increased the temperature up to 80 K. While the SdH oscillations get suppressed the COs still remain visible.

[1] Burgos, R., and Lewenkopf, C., arXiv:1610.04068 (preprint 2016).

[2] Ye, P. D., Weiss, D., et al., Semicond. Sci. Technol. 10, 715 (1995).

HL 48.6 Wed 10:45 POT 51

Temperature switchable type of conductivity in hybrid conjugated polyelectrolyte/graphene two-dimensional nanocomposites — •Viktor Brus[1], Marc Gluba[1], Cheng-Kang Mai[2], Stefany Fronk[2], Jörg Rappich[1], Norbert Nickel[1], and Cuillermo Bazan[2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium Photovoltaik, Kekuléstr. 5, 12489 Berlin, Germany — [2]Center for Polymers and Organic Solids, Department of Chemistry and Biochemistry, University of California at Santa Barbara, Santa Barbara, CA, 93106, USA

We found that a submonolayer of CPE-PyrBIm4 on CVD-grown graphene forms a novel two-dimensional hybrid material that exhibits preferential transport of holes or electrons as a function of temperature. Doping efficiencies increase with the increase of the temperature used to anneal the heterobilayers and a decrease of the CPE-PyrBIm4 film thickness. The switching of the conductivity type of the thin CPE-PyrBIm4/graphene heterobilayer composite occurs when graphene is not strongly overcompensated. Moreover, the conversion of the conductivity type is reversible. Doping mechanisms under consideration include charge transfer from electron rich structural units in the CPE-PyrBIm4 backbone and/or field-effect doping as a result of interfacial electrostatic effects from adjacent ionic functionalities. This effect shows the unique and complex nature of electrical properties of the novel heterobilayer hybrid organic-inorganic CPE-PyrBIm4/graphene nanocomposite material and enhances interest in further investigations.

HL 48.7 Wed 11:00 POT 51

Interlayer screening in n-doped bilayer and trilayer transition metal dichalcogenides — •Andor Kormányos[1], Viktor Zólyomi[2], and Guido Burkard[1] — [1]University of Konstanz, Germany — [2]Manchester University, United Kingdom

We derive an effective Hamiltonian based on the k.p approach that describes the dispersion at the band edges of the conduction band of bilayer and trilayer transition metal dichalcogenides (TMDCs). This model is then used to consider n-doped bilayer MoS_2 placed in uniform external electric field. We discuss the charge re-distribution between the layers due to the electric field and calculate the bandgap that opens at the K-point of the Brillouin zone in self-consistent Hartree approximation. We point out the relation between the induced band-gap and the quantum capacitance and briefly discuss the relevance of our results to recent photoluminiscence experiments in double gated bilayer MoS_2.

Coffee Break

HL 48.8 Wed 11:45 POT 51

Driven Hofstadter Butterflies — •Martin Wackerl[1] and John Schliemann[2] — [1]Institut für Theoretische Physik, Universität Regensburg — [2]Institut für Theoretische Physik, Universität Regensburg

Periodically driven quantum systems offer a great way of tuning band structures or Chern numbers. The first part will be about graphene illuminated with circular polarized light. The external driving is introduced via the Floquet formalism and the main focus will be on the deformation of the band structure of graphene. Afterwards we will give a short introduction to the Hofstadter butterfly and unify it with the Floquet formalism. We will show how the Hofstadter spectrum gets distorted when tuning the light intensity, photon energy, and polarization. The last part is about the influence of polarized light to the distribution of ground state Chern numbers of the Floquet-Hofstadter spectrum.

HL 48.9 Wed 12:00 POT 51

Resonant scattering off adatoms in monolayer graphene — •Susanne Irmer, Denis Kochan, and Jaroslav Fabian — University of Regensburg, Regensburg, Germany

We present a theoretical investigation of resonant scattering off adatoms on graphene. Resonant scattering is an important feature of adatoms as it leads to resonant enhancement of the impact of proximity effects such as local magnetic moments or spin-orbit coupling [1,2,3]. We investigate the three different adsorption positions of hollow, top, and bridge employing effective realistic tight-binding models and the T-matrix formalism. The developed resonance conditions are useful for quantum transport models as well as studies of spin relaxation in graphene with adatoms.

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] D. Kochan, M. Gmitra, and J. Fabian, Phys. Rev. Lett. 112, 116602 (2014)

[2] J. Bundesmann, D. Kochan, F. Tkatschenko, J. Fabian, and K. Richter, Phys. Rev. B 92, 081403 (2015)

[3] D. Kochan, S. Irmer, and J. Fabian, arXiv:1610.08794

HL 48.10 Wed 12:15 POT 51

Experimental realization and characterization of an electronic Lieb lattice — •Marlou Slot[1], Thomas Gardenier[1], Peter Jacobse[1], Guido van Miert[2], Sander Kempkes[2], Stephan Zevenhuizen[1], Cristiane Morais Smith[2], Daniel Vanmaekelbergh[1], and Ingmar Swart[1] — [1]Debye Institute for Nanomaterials Science, Utrecht University, Netherlands — [2]Institute for Theoretical Physics, Utrecht University, Netherlands

Geometry, whether on the atomic or nanoscale, is a key factor for the electronic band structure of materials. For example, the honeycomb geometry leads to Dirac-type bands where the charge carriers behave as massless particles. Theoretical predictions are triggering the exploration of novel 2D geometries, such as graphynes, Kagomé and the Lieb lattice. The latter is the 2D analogue of the 3D lattice exhibited by perovskites; it is a square-depleted lattice, which is characterised by a band structure featuring Dirac cones intersected by a topological flat band. Whereas photonic and cold-atom Lieb lattices have been demonstrated, an electronic equivalent in 2D is difficult to realize in an existing material. Here, we report an electronic Lieb lattice formed by the surface state electrons of Cu(111) confined by an array of CO molecules positioned with a scanning tunneling microscope. Using scanning tunneling spectroscopy and wave-function mapping, we confirm the characteristic electronic structure of the Lieb lattice. The experimental findings are corroborated by muffin-tin and tight-binding calculations. At higher energy, second-order electronic patterns are observed, which are equivalent to a super-Lieb lattice.

HL 48.11 Wed 12:30 POT 51

Interlayer Configuration in Twisted Bilayers of Folded Graphene — •Johannes C. Rode, Christopher Belke, Hennrik Schmidt, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover

Twisted bilayer graphene (TBG), i.e. stacks of two graphene sheets in arbitrary rotational misalignment, exhibit rich electronic spectra[1,2] which are highly dependent on the interlayer twist angle in general[3] as well as details in stacking configuration like lattice commensuration and corrugation[4] in particular. We here examine the latter TBG properties coming from the morphological side: TBG are prepared via Atomic Force Microscope, folding ribbons out of monolayer sheets. In the recently proposed picture of a thermally activated growth process[5], here measured quantities like interlayer distance and shape of the folded edge are found to hold novel information about angle-dependent interlayer configuration and provide insight about interaction in van der Waals bound materials.

[1] H. Schmidt; J. C. Rode; D. Smirnov; R. J. Haug, Nat. Comm. **5**, 5742 (2014).

[2] J. C. Rode; D. Smirnov; H. Schmidt, R. J. Haug, 2D Materials **3**, 035005 (2016).

[3] J. M. B. Lopes dos Santos; N. M. R. Perez; A. H. Castro Neto, Phys. Rev. Lett. **99**, 25682 (2007).

[4] E. J. Mele, Phys. Rev. B **81**, 161405(R) (2010).

[5] J. Annett; G. L. W. Cross, Nature **535**, 271-275 (2016).

HL 48.12 Wed 12:45 POT 51

Multi-scale approach for strain-engineering of phosphorene — Daniel Midtvedt[1] and •Alexander Croy[2] — [1]Department of Physics, Chalmers University of Technology, Gothenburg, Sweden — [2]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany

A multi-scale approach for the theoretical description of deformed phosphorene is presented. This approach combines a recently developed valence-force model [1] to relate macroscopic strain to microscopic displacements of atoms and a tight-binding model [2] with distance-dependent hopping parameters to obtain electronic properties. The resulting self-consistent electromechanical model is suitable for large-scale modeling of phosphorene devices. We demonstrate this for the case of an inhomogeneously deformed phosphorene drum, which may be used as an exciton funnel [3].

[1] D. Midtvedt and A. Croy, Phys. Chem. Chem. Phys. 18, 23312 (2016). [2] A. N. Rudenko, S. Yuan, and M. I. Katsnelson, Phys. Rev. B 92, 085419 (2015). [3] P. San-Jose et al, Phys. Rev. X 6, 031046 (2016).

HL 48.13 Wed 13:00 POT 51

Evolution of electronic structure of few-layer phosphorene from angle-resolved photoemission spectroscopy of black phosphorous — •Niels Ehlen[1], Boris Senkovskiy[1], Alexander Fedorov[1,2,3], Andrea Perucchi[4], Paola Di Pietro[4], Antonio Sanna[5], Gianni Profeta[6], Luca Petaccia[4], and Alexander Grüneis[1] — [1]Institute of Physics II, University of Cologne, Germany — [2]IFW Dresden, Germany — [3]St. Petersburg State University, Russia — [4]Elettra Sincrotrone Trieste, Italy — [5]Max Planck Institute of Microstructure Physics, Halle, Germany — [6]Department of Physical and Chemical Sciences/SPIN-CNR, University of L'Aquila, Italy

A complete set of tight-binding parameters for the description of the quasiparticle dispersion relations of black phosphorous (BP) and N-layer phosphorene with $N = 1 \ldots \infty$ is presented. The parameters, which describe valence and conduction bands, are fit to angle-resolved photoemission spectrocopy (ARPES) data of pristine and lithium doped BP. We show that zone-folding of the experimental three-dimensional electronic band structure of BP is a simple and intuitive method to obtain the layer-dependent two-dimensional electronic structure of few-layer phosphorene. Zone-folding yields the band gap of N-layer phosphorene in excellent quantitative agreement to experiments and *ab-initio* calculations. A combined analysis of optical absorption and ARPES spectra of pristine and doped BP are used to estimate a value for the exciton binding energy of BP.

HL 49: Quantum Dots: Optical Properties III

Time: Wednesday 9:30–12:45 Location: POT 151

HL 49.1 Wed 9:30 POT 151

A bright triggered twin-photon source in the solid state — •Tobias Heindel[1], Alexander Thoma[1], Martin von Helversen[1], Marco Schmidt[1,2], Alexander Schlehahn[1], Manuel Gschrey[1], Peter Schnauber[1], Jan-Hindrik Schulze[1], André Strittmatter[1], Jörn Beyer[2], Sven Rodt[1], Alexander Carmele[3], Andreas Knorr[3], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany — [2]Physikalisch-Technische Bundesanstalt, Abbestraße 1, 10587 Berlin, Germany — [3]Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin, Germany

We propose and experimentally demonstrate the efficient, triggered generation of photon twins using the energy-degenerate biexciton-exciton radiative cascade of a single semiconductor quantum dot (QD) [1]. For this purpose, we select a QD whose exciton's finestructure splitting equals the biexciton binding energy resulting in $E_X^H = E_{XX}^H$. Deterministically integrated within a microlens, this nanostructure emits highly-correlated photon pairs, degenerate in energy and polarization, at a rate of up to (234 ± 4) kHz. Furthermore, we directly observe the emitted twin-photon state by employing a photon-number-resolving detection system based on a transition edge sensor, which enables the reconstruction of the emitted photon number distribution.

[1] A. Thoma, T. Heindel et al., A bright triggered twin-photon source in the solid state, arXiv:1608.02768 (2016)

HL 49.2 Wed 9:45 POT 151

Optical enhancement of quantum dot emission by surface nanowires — •Sven Scholz, Rüdiger Schott, Carlo Sgroi, Yannick Raffel, Andreas D. Wieck, and Arne Ludwig — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Germany

Molecular beam epitaxy (MBE) quantum dot (QD) structures are used as fundamental research structures to investigate quantum optical phenomena. To further enhance their optical properties we use nanowires as a subwavelength waveguide. While common photonic crystal structures work with holes or micro pillars, we use focused ion beam (FIB) to catalyze nanowire growth on QD structures. The LED-QD structure is optimized regarding the optical emission. Therefore we use a methode to remove the wetting layers (WL) PL signal. To access a wide emission spectrum we use rapid-thermal annealing (RTA) and a flushing technique coupled with the WL suppression. This results in tunable and good separated QD emission peaks. The NW growth is characterized and optimized with regards to crystalline quality and morphology. The samples are characterized by photoluminescence/electroluminescence, scanning electron microscope imaging and capacitance-voltage spectroscopy.

HL 49.3 Wed 10:00 POT 151

Light holes in quantum dots — •Vlastimil Křápek — Central European Institute of Technology, Brno University of Technology, Purkyňova 123, CZ-612 00 Brno, Czech Republic — Institute of Physical Engineering, Brno University of Technology, Technická 2, CZ-616 69 Brno, Czech Republic

The valence band edge of III-V zinc-blende semiconductors is formed by heavy and light holes. In quantum dots, the lowest confined valence state is usually contributed by the heavy holes with the weight above 90 % and by the light holes with the weight below 10 %. Thus, its properties are dominated by the heavy holes. However, there are phenomena in which the light holes play equally important or even decisive role.

In my contribution I review three such phenomena: excitonic fine structure splitting tuned by external strain field [1], quantum dot molecule with a tunable tunnel coupling [2], and brightened dark exciton [3]. I explain how the light holes couple to the heavy holes due to the quantum confinement and strain field stressing the differences between both effects.

[1] J. D. Plumhof, V. Křápek, F. Ding, K. D. Jöns, R. Hafenbrak, P. Klenovský, A. Herklotz, K. Dörr, P. Michler, A. Rastelli, and O. G. Schmidt, Phys. Rev. B **83**, 121302(R) (2011).
[2] E. Zallo, R. Trotta, V. Křápek, Y. H. Huo, P. Atkinson, F. Ding, T. Šikola, A. Rastelli, and O. G. Schmidt, Phys. Rev. B **89**, 241303(R) (2014).
[3] Y. H. Huo, V. Křápek, A. Rastelli, and O. G. Schmidt, submitted.

HL 49.4 Wed 10:15 POT 151

Conductivity Spectroscopy Examination of Metastable Hole Storing — •Carsten Ebler, Simon Schlombs, Arne Ludgwig, and Andreas D. Wieck — Ruhr-Universität Bochum, Germany

Approaching the goal of a memory, storing single charge quantum, especially quantum dots are interesting. Therefore, we used epitaxial grown self-Assembled InAs QDs (SAQD) as crystalline hosts and compatibility with coupling to photons in contrast to amorphous semiconductors used in today's flash memories.

We established SAQDs in tunnel contact with an inverted GaAs, AlGaAs HEMT structure, manipulated the system with electronical and optical pulses and time resolved conductivity measurements were performed.

The experimental interaction with the device consists of a pulse train of non-resonant optical excitation of electrons and holes in the QDs and the wetting layer. The structure is appropriately biased, that the Fermi level is in electronical resonance with the X0 state in the QD to store one single hole. This hole state is read out over changes in conductivity in the HEMT in relation to carrier density in the QDs and the 2DEG.

It was possible to capture the hole state for at least 10 s and to read it out afterward. Further experimentation and different voltage pulses will give information about tunneling processes of the hole and electron states, dynamic of non-equilibrium states and time resolved exciton behavior.

HL 49.5 Wed 10:30 POT 151

Time reordering of paired photons in a dressed three-level cascade — •Samir Bounouar, Max Strauss, Alexander Carmele, Peter Schnauber, Alexander Thoma, Manuel Gschrey, Jan-Hindrik Schulze, André Strittmatter, Sven Rodt, Andreas Knorr, and Stephan Reitzenstein — Technische Universität, Berlin, Deutschland

We present the two-photon coherent control over a ladder-type three level system (ground state, exciton, biexciton in a quantum dot) at the level of single photons and single photon pairs through photon correlation spectroscopy. By collecting the photons coming from the different dressed states and by correlating them, we show that strong coupling of the laser field to the radiative cascade allows for the manipulation of the paired photons time ordering. Such an operation is crucial for the on-demand production of entangled photons "across" generation [1]. Moreover, two-photon Rabi oscillations of the dressed states population, due to the non-linear coherent driving of the radiative cascade, are observed. We also show that the single dressed states emission can be operated as a widely tunable single photon source without need of additional piezo-tuning techniques [2].

[1] J. E. Avron, Phys. Rev. Lett. 100, 120501 (2008), [2] S. Bounouar et al., arXiv:1610.08268v1 (2016).

Coffee Break

HL 49.6 Wed 11:15 POT 151

Optical and theoretical investigation of fluorescence spectral diffusion of CdSe/CdS dotrods — •Sven-Hendrik Lohmann, Christian Strelow, Tobias Kipp, and Alf Mews — Institut für Physikalische Chemie, Universität Hamburg, Grindelallee 117, 20146 Hamburg, Deutschland

Here we investigate the photoluminescence properties of individual chemically-synthesized dotrods, which consist of a spherical CdSe core enclosed by an elongated CdS shell. Time- and wavelength-resolved data were collected at low temperature to analyze the spectral diffusion of the emission. We observe a correlation between the energy and the decay time of the emission. This trend was modelled by theoretical calculations, which include migrating surface charges to describe the fluorescence jittering. Our model calculations show good agreement with our experimental studies.

HL 49.7 Wed 11:30 POT 151

Implementation of single quantum dots into photonic structures for enhanced light extraction efficiency — •Marc Sartison[1], Simone Luca Portalupi[1], Timo Gissibl[2], Michael Jetter[1], Harald Giessen[2], and Peter Michler[1] — [1]IHFG, IQST Center and SCoPE, University of Stuttgart — [2]4th Physics Institute and Research Center SCoPE, University of Stuttgart

Semiconductor quantum dots (QDs) have demonstrated their strength in being ideal candidates for quantum information purposes. However, the amount of light extracted from the semiconductor matrix is severely limited by the refractive index contrast at the semiconductor-to-air interface. Several successful efforts were made to overcome this limitation by fabrication of light extraction enhancing structures, such as micro-pillars or micro-lenses. To enhance the fabrication yield of such devices, deterministic techniques of randomly grown Stranski-Krastanov QDs were established. We present a novel approach for the deterministic placement of single QDs into light extraction enhancing structures with a fabrication yield close to 100%. The QDs are spatially and spectrally pre-selected and characterized in micro-photoluminescence, followed by a low-temperature photolithography step to define precisely placed alignment markers which are then clearly visible under the optical microscope at room temperature and allow performing further fabrication steps. Based on these markers, a 3D direct laser writing machine is aligned and micrometric-sized broadband solid immersion lenses are printed to enhance the extraction efficiency.

HL 49.8 Wed 11:45 POT 151

Far-field and quality factor optimized GaAs-based photonic crystal cavities with high collection efficiencies — •Stefan Hepp, Simone L. Portalupi, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology IQST and Research Center SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

The optical properties of semiconductor quantum dots (QDs) integrated in photonic crystal cavities can be further improved via cavity quantum electrodynamic effects. Therefore the realization of cavities with both high quality factor Q and small modal volume V are from interest to achieve a large enhancement factor. Efforts have been made to optimize the Q-factor that in some cases turns out to be detrimental for the collection efficiency because the related strong light confinement can lead to an inferior directivity for the out-of-plane emission. Here we present theoretical and experimental studies on the simultaneous optimization of the Q-factor and the far-field emission profile of the frequently utilized L3-photonic crystal cavity. We fabricated, characterized and compared cavities with different degree of optimization via μ-PL and back focal plane imaging and show that the out-of-plane radiation profile can be optimized to an almost Gaussian distribution making the light collection effective and the efficient coupling to fibers available. Despite the far-field optimization, the Q-factors still reach values as high as 6x10^3 showing that a good compromise between a high Q-factor and a near optimal emission profile can be achieved.

HL 49.9 Wed 12:00 POT 151

Spectroscopic Properties of CdTe Quantum Wires at Cryogenic Temperatures — •Svenja Patjens, Andreas Nielsen, Philip Harder, Tobias Kipp, and Alf Mews — Institut für Physikalische Chemie, Universität Hamburg, Grindelallee 117, 20146 Hamburg, Germany

One-dimensional semiconductor quantum wires grown by the solution-liquid-solid (SLS) mechanism or similar methods typically consist of alternating segments of zinc blende and wurtzite phases. [1] Here, we investigate the optical properties of near phase-pure and polytypic cadmium telluride nanowires via confocal microscopy. The wurtzite phase distribution in the wires, prepared by the solution-solid-solid (SSS) method [2], was analyzed by means of high resolution transmission electron microscopy (HRTEM). Photoluminescence spectroscopy of single specimens at cryogenic temperatures (T <9 K) revealed several distinct features and spectral shifts with respect to measurements at room temperature. Low-temperature fluorescence spectra of WZ-phase and polytypic wires were compared in order to get an insight into the effect of phase-alternations and domain sizes. We gratefully acknowledge financial support by the DFG vie KI 1257/2 and ME 1380/16-3.

[1] D. Franz et al., Nano Lett., 2014, 14 (11), pp 6655-6659
[2] F. Wang et al., Nano Lett., 2016, 16 (2), pp 889-894

HL 49.10 Wed 12:15 POT 151

Analyzing solid-state single-photon sources utilizing photon-number-resolving detectors — •Marco Schmidt[1,2], Alexander Thoma[2], Martin von Helversen[2], Manuel Gschrey[2], Peter Schnauber[2], Jan-Hindrik Schulze[2], André Strittmatter[2], Jörn Beyer[1], Sven Rodt[2], Tobias Heindel[2], and Stephan Reitzenstein[2] — [1]Physikalisch-Technische Bundesanstalt, Abbestraße 1, 10587 Berlin, Germany — [2]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany

Non-classical light sources are versatile resources for applications in various research fields ranging from quantum communication to quantum metrology. In this context, a comprehensive knowledge of the quantum optical properties of the utilized sources is highly desirable. In this work, we employ a photon-number-resolving detection system based on a transition edge sensor (TES) [1] to analyze the photon statistics emitted by deterministic solid-state single-photon source. Our measurements enable us to reconstruct the photon number distribution emitted by the single-photon sources. The obtained results are compared with standard coincidence measurements using Si-based click-detectors.

[1]Lita, Adriana E. et al., Counting near-infrared single-photons with 95% efficiency, Optics Express, vol. 16, issue 5, p. 3032 (2008)

HL 49.11 Wed 12:30 POT 151

Temperature influence on the behaviour of 1D, 2D and 3D quantum confined system — •Parva Chhantyal[1,3], Laszlo Sajti[1], Carsten Reinhardt[1,3], Suraj Naskar[2,3], Dirk Dorfs[2,3], Nadja Bigall[2,3], and Boris Chichkov[1] — [1]Nanotechnology Department, Hollerithallee 8, D-30419 Hannover, Germany — [2]Leibniz

University Hannover, Physical Chemistry, Callinstrae 3a, 30167 Hannover, Germany — [3]Laboratory for Nano and Quantum Engineering, Schneiderberg 39, 30167 Hannover, Germany

Semiconductor nanoparticles with size less than 10 nm have an interesting property, called quantum confinement, which represents the introduction of new properties to the materials by tuning their size and composition. In this research, an influence of temperature change on the behaviour of CdSe/CdS semiconductor nanoparticles is investigated. Initially, a comparative study of amplified spontaneous emission of these nanoparticles based on different sizes, such as dots, rods and platelets at room temperature is performed. The study is compared with respect to their sizes that provoke different absorption and emission spectra. The nanoparticles are spin coated on glass slides to make continuous films and then optically pumped by a 355 nm nanosecond laser. The fluorescence and laser emission spectra are measured and compared. Afterwards, the sample is heated up to different temperatures and subsequently, the influence of temperature on their emission spectra is compared for all three nanoparticles. Upon the observation of temperature influence on these nanoparticles, this approach can be adopted in real-life application as a temperature sensor.

HL 50: Nitrides: Preparation and Characterization

Time: Wednesday 9:30–13:00 Location: POT 251

Invited Talk HL 50.1 Wed 9:30 POT 251

Photoactivated chemical processes on group III-nitride nanostructures and nanohybrids — Paula Neuderth[1], Sara Hölzl[1,6], Pascal Hille[1,6], Jörg Schörmann[1], Christian Reitz[2], Mariona Coll[3], Jordi Arbiol[3,4], Roland Marschall[5], and •Martin Eickhoff[1,6] — [1]I. Physikalisches Institut, JLU Gießen, 35392 Gießen, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Germany — [3]ICMAB-CSIC, Bellaterra, CAT, Spain — [4]ICN2, Bellaterra, CAT, Spain — [5]Physikalisch-Chemisches Institut, JLU Gießen, 35392 Gießen, Germany — [6]Institut für Festkörperphysik, Universität Bremen,, 28359 Bremen, Germany

The photoluminescence (PL) emission properties of group III-nitride nanowires and nanowire heterostructures sensitively respond to changes in the chemical environment in gaseous and liquid atmospheres. At the same time, the presence of photogenerated charge carriers on their surfacecan trigger chemical processes by charge transfer into electronic levels/molecular orbitals of adsorbed gas molecules or surrounding electrolytes, as employed in photo-electrochemical water splitting. Hence, monitoring of the PL and controlling the photocurrent allows for analyzing and initiating photoactivated chemical surface processes as well as establishing new principles for opto-chemical nanosensors. We demonstrate these strategies by discussing different examples such as optical pH-sensing, detection of water adsorption or Performance enhancement of oxide-coated InGaN/GaN nanowire photoanodes. We show that part of these concepts can also be transferred to two dimensional semiconductor materials.

HL 50.2 Wed 10:00 POT 251

Effective electron mass in cubic GaN — •Elias Baron[1], Martin Feneberg[1], Rüdiger Goldhahn[1], Michael Deppe[2], and Donat J. As[2] — [1]Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg, Germany — [2]Department Physik, Universität Paderborn, Germany

Ge-doping has been proven a very efficient way to achive free electron concentrations n above $10^{20}\mathrm{cm}^{-3}$ in wurtzite GaN layers while maintaining excellent structural properties of the films. Recently, we demonstrated that similar high n values can also be obtained in cubic GaN layers by germanium doping. The films were deposited by plasma-assisted molecular beam epitaxy on 3C-SiC substrates. Here, we present a comprehensive characterization of those films covering a wide range of n values by spectroscopic ellipsometry from which the complex dielectric function (DF) is deduced. The analysis of the DFs in the mid-infrared yields the transverse-optical phonon frequency and the plasma frequencies. From the latter, the dependence of the effective electron mass on n is obtained indicating a strong non-parabolicity of the conduction band. Studies around the fundamental absorption edge indicate the superposition of carrier-density dependent Burstein-Moss effect and band gap shrinkage. Excellent agreement between theory and experiment is achieved for the energetic position of the absorption edge when applying the experimentally determined dependence electron mass dependence on n.

HL 50.3 Wed 10:15 POT 251

Hydrogen-induced modifications of N-polar InN surface properties — •Anja Himmerlich, Stefan Krischok, and Marcel Himmerlich — Institut für Physik and Institut für Mikro- und Nanotechnologien, TU Ilmenau, Germany

Indium nitride (InN) is a III-V semiconductor with controversially discussed surface electronic properties. Especially the normally observed high surface electron concentration is under debate. In contrast to In-polar InN, as-grown N-polar InN shows a reduced surface electron accumulation, that however significantly changes during storage in ambient conditions [1]. Here we present investigations on the interaction of atomic hydrogen, a dissociation product of different ambient molecules, with as-grown N-polar InN using in situ photoelectron spectroscopy. Within this study changes in the surface electronic properties, including band alignment and work function, as well as chemical bonding states of the substrate and adsorbates are characterized. We demonstrate that hydrogen preferentially bonds to the surface nitrogen atoms, resulting in the disappearance of nitrogen dangling-bond-related occupied surface state close to the valence band edge and the formation of new occupied electron states at the conduction band edge. The decrease in work function during adsorption and the increase in surface downward band bending confirm that hydrogen is acting as electron donor at N-polar InN surfaces and therefore has to be considered as one main reason for the increased electron accumulation observed for samples exposed to ambient conditions [2]. [1] Appl. Phys. Lett. 102, 231602 (2013); [2] Phys. Rev. B 91, 245305 (2015).

HL 50.4 Wed 10:30 POT 251

Improving lateral current spreading of InGaN LEDs by MOVPE grown GaN tunnel junctions — •Silvio Neugebauer, Andreas Lesnik, Florian Hörich, Hartmut Witte, Jürgen Bläsing, Armin Dadgar, and André Strittmatter — Institute of Experimental Physics, Otto-von- Guericke-University Magdeburg, Germany

Improving current injection into nitride-based p/n-junction devices is an important task for further enhancement of the efficiency of light-emitting diodes (LEDs) and vertical cavity surface emitting lasers. GaN-based homoepitaxial p/n tunnel junctions could be an effective means to improve lateral current spreading and still maintain high optical transparency. However, the effectiveness of the tunnel junction is limited due to the achievable maximum donor and acceptor concentrations as well as the activation of hydrogen passivated Mg acceptors buried beneath an n-type GaN layer. In this study, we have grown heavily doped GaN:Mg/GaN:Ge tunnel junctions on top of conventional LED structures using exclusively metal-organic vapor phase epitaxy (MOVPE). In particular, the activation process of the Mg-doped GaN layer is critical for device performance. We will compare post-growth thermal annealing schemes applied to LED mesa structures with thermal annealing of the p-type GaN:Mg layer during growth with regard to the efficiency of the activation. Furthermore, we currently investigate the potential of MOVPE regrowth of the GaN:Ge layer on top of an an ex-situ activated GaN:Mg layer.

HL 50.5 Wed 10:45 POT 251

Capacitance-voltage spectroscopy of charge-tunable GaN quantum dot ensembles at room temperature — •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, Rue Bernard Grégory, 06560 Valbonne, France

We present capacitance voltage (CV) measurement at room temperature of charge-tunable self-assembled wurtzite GaN quantum dots (QDs) in an AlxGa1-xN matrix grown by MBE. GaN and its alloys have excellent properties which makes them an ideal candidate for high power and high temperature microelectronic and QD devices, such as their thermal stability, high thermal conductivity and wide bandgap

energies.

Due to polarization effects in wurtzite GaN/AlxGa1-xN heterostructure layers the band structure is deformed. Band structure simulations were run to calculate a decent tunneling barrier and to estimate the quantum dot minimum to be close to the Fermi energy level with a sufficient lever arm to bring the QD energy levels in resonance with the Fermi energy. The length of the blocking barrier influences the position of the QDs in the energy level. Therefore, the thickness of this layer is crucial for QD position on the energy scale.

We used the known CV spectroscopy technique adapted to the GaN properties and measured the s-states of the QDs at room temperature. The Coulomb blockade energy for the electrons was calculated to be as huge as 142 meV.

Coffee Break

HL 50.6 Wed 11:30 POT 251

Impact of strain and valence band structure on radiative and non-radiative recombination in m-plane GaInN/GaN quantum wells — •Philipp Henning, Torsten Langer, Manuela Klisch, Fedor Alexej Ketzer, Philipp Horenburg, Heiko Bremers, Uwe Rossow, and Andreas Hangleiter — Institut für Angewandte Physik, Technische Universität Braunschweig

Even for thin c-plane quantum wells (QWs), where the polarization field is negligible, we observe longer room-temperature radiative lifetimes compared to m-plane structures. We use time-resolved photoluminescence spectroscopy to measure the radiative and non-radiative carrier lifetimes in GaInN/GaN QW structures grown by MOVPE, where we find room-temperature radiative lifetimes between 1ns and 200ps for m-plane QWs and minimum values around 2ns for c-plane structures. The difference amounts up to one order of magnitude and can partly be explained by an increased exciton binding energy for non-polar QWs. As confirmed by simulations, another major contribution to the shorter radiative lifetimes stems from a modified valence band structure, which results in reduced effective hole masses for non-polar QWs. A change of the strain state in the QW, as it is present for higher indium contents, has further impact on the valence band structure. By introducing a metamorphic AlInN buffer layer we aim to reduce the strain in the QW, which allows for a more detailed study of the impact of the valence band structure on the radiative lifetimes. Moreover, we find increasing non-radiative lifetimes as a consequence of the reduced strain state and lower defect formation in the QW.

HL 50.7 Wed 11:45 POT 251

Strain and compositional fluctuations in AlInN/GaN heterostructures — •Verena Portz[1], Michael Schnedler[1], Martial Duchamp[1,2], Fei-Man Hsiao[1,3], Holger Eisele[4], Jean-François Carlin[5], Raphael Butté[5], Nicolas Grandjean[5], Rafal E. Dunin-Borkowski[1,2], and Philipp Ebert[1] — [1]Peter Grünberg Institut, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Ernst Ruska-Centrum, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [3]Department of Physics, National Sun Yat-sen University, Kaohsinung 80424, Taiwan — [4]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany — [5]Institute of Physics, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

The strain and compositional fluctuations of nearly lattice-matched AlInN/GaN heterostructures are investigated by cross-sectional scanning tunneling microscopy and selected area electron diffraction measurements in scanning electron transmission microscopy. The presence of strain induces height modulations governed by different roughness components at the cleavage surfaces. The surface height modulations are compatible with a relaxation of alternatingly compressive and tensile strained domains, indicating compositional fluctuations. Changes of the a lattice constant are traced to interface misfit edge dislocations. The dislocations induce steps increasing the roughness within the AlInN layers.

HL 50.8 Wed 12:00 POT 251

Surface properties of p-type, n-type, and semi-insulating GaN layers on sapphire — •Aqdas Fariza, Andreas Lesnik, Silvio Neugebauer, Matthias Wieneke, Jürgen Bläsing, Hartmut Witte, Armin Dadgar, and André Strittmatter — Otto-von-Guericke University Magdeburg, Magdeburg, Germany

GaN and related heterostructures have been the subject of intensive research in recent years for optoelectronics and high power as well as high frequency devices. However, the large lattice constant mismatch between heterosubstrate and GaN epitaxial film leads to the generation of a high threading dislocation (TD) density which degrades device performance. Understanding the electrical activity of these dislocations and their surface potentials is very important to enhance the reliability of power electronics devices. Therefore, we have investigated defects in Mg-, Si-, C- and Fe-doped GaN samples with a focus on the local electronic properties of the material in the vicinity of dislocations. Dislocation densities are estimated from tilt and twist x-ray measurements using omega-scans of the (0002) reflection and in grazing incidence in-plane geometry of the (10-10) reflection. The surface topography, contact potentials and electronic charge states of dislocations are explored by performing atomic force microscopy, bias dependent electric force microscopy and scanning surface potential microscopy in tapping mode. The conductive layers exhibit a low contact potential whereas the enhanced contact potential difference for resistive GaN layers might be associated not only to the Fermi-level position but also to surface band bending and surface charges.

HL 50.9 Wed 12:15 POT 251

Conoscopic study: Influence of birefringence on the state of polarization in GaN samples — •Ines Trenkmann, Lukas Uhlig, Matthias Wachs, and Ulrich T. Schwarz — Chemnitz University of Technology, Experimental Sensor Science, Reichenhainer Str. 70, 09126 Chemnitz, Germany

GaN with its wurtzite crystal structure is an optical anisotropic material. In a conoscopic setup, the birefringent sample is placed between two crossed polarizers and the state of polarization of the emerging beam is compared to the polarization of the initial ray. Fringes and the typical black bands of the isogyre characterize the obtained conoscopic interference pattern, which depend on the sample thickness, the cone of the incident light ray and the difference between both refractive indices $\Delta n = n_e - n_o$. We compare experimental obtained pattern with simulated images using refractive indices from various studies that are obtained by variable angle spectroscopic ellipsometry [1, 2] and prism coupling technique [3]. The observed differences are discussed considering growth induced crystal strain. Additionally measurements of epitaxial GaN on sapphire show the influence of the sapphire substrate on the observed changes of the state of polarization [4].

References: [1] S. Shokhovets, R. Goldhahn and W. Richter, J. Appl. Phys. 94, 307 (2003). [2] S. Ghosh, P. Waltereit and K. H. Ploog, Appl. Phys. Lett. 80, 413 (2002). [3] G. Yu, H. Ishikawa and M. Umeno, Jpn. J. Appl. Phys. 36, L1029 (1997). [4] I. Trenkmann, L. Uhlig, M. Wachs, C. Mounir, U. T. Schwarz, submitted.

HL 50.10 Wed 12:30 POT 251

Anisotropic dielectric function of nonpolar AlGaN up to 20eV — •Michael Winkler[1], Shigefusa F. Chichibu[2], Ramon Collazo[3], Zlatko Sitar[3], Maciej D. Neumann[4], Norbert Esser[4], Rüdiger Goldhahn[1], and Martin Feneberg[1] — [1]Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg — [2]Institute of Multidisciplinary Research for Advanced Materials, Tohoku University — [3]Department of Materials Science and Engineering, North Carolina State University — [4]Leibniz-Institut für Analytische Wissenschaften - ISAS

The linear optical response of nonpolar $(10\bar{1}0)$ $Al_xGa_{1-x}N$ epitaxial films is analyzed quantitatively for the full composition range. The samples were grown by metal-organic vapor phase epitaxy and molecular beam epitaxy on m-plane freestanding GaN and AlN substrates. Their optical properties were measured by spectroscopic ellipsometry up to 20eV performed at the synchrotron Metrology Light Source (MLS) of the PTB in Berlin for two different configurations: One with the [0001]-direction parallel and one perpendicular to the plane of incidence. By modeling the multilayer samples including surface roughness and anisotropy the ordinary and extraordinary dielectric functions were obtained. High energy interband transitions are thus traceable as function of x in the $Al_xGa_{1-x}N$ system allowing assignments of features to certain parts of the band structure.

HL 50.11 Wed 12:45 POT 251

Photon statistics of high-β gallium 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, Hardenbergstr. 36, D-10623 Berlin — [2]École Polytechnique Fédérale de Lausanne, CH-1015 Lau-

sanne, Switzerland

The search for an ultimate nanolaser is a central goal in nanophotonics, and has led to cutting edge research at the crossroads between device physics and quantum optics. Such nanolasers employ cavity-enhanced light-matter coupling in order to greatly reduce the lasing threshold, desirable for future on-chip nanophotonic applications. Nitride nanobeam cavities grown on silicon present an ideal system to study such high spontaneous emission coupling factor (β) lasers under realistic device conditions (room temperature & ambient atmosphere) [1]. In a detailed, temperature dependent optical and quantum-optical characterization we show that classical lasing indicators are at best ambiguous for high-β devices, while photon statistics remain a sensitive indicator of the lasing transition. By analysing the temperature dependent carrier confinement in the gain medium, we can explain thresholdless lasing by the temperature- and excitation power dependent interplay of 0D and 2D gain contributions [2].

[1] Triviño et al. Nano Lett. 15(2), 2015
[2] Jagsch et al. arXiv:1603.06447

HL 51: Focus Session: Hybrid Quantum-Dot / Atom Systems

Time: Wednesday 9:30–13:00 Location: POT 112

Invited Talk HL 51.1 Wed 9:30 POT 112

Coupling atomic and solid state quantum systems — •Val Zwiller — KTH, Stockholm, Sweden — TU Delft, Netherlands

Devices based on single quantum dots enable us to efficiently generate non classical states of light at frequencies in resonance with atomic transitions. We will report on the development of devices based on GaAs/AlGaAs quantum dots tuned in resonance with Rb transitions with the aim of demonstrating a hybrid quantum memory where single photons generated in the solid state are stored in atomic memories.

HL 51.2 Wed 10:00 POT 112

An atomic memory suitable for semiconductor quantum dot single photons — •Janik Wolters, Lucas Beguin, Andrew Horsely, Jan-Philipp Jahn, Richard Warburton, and Philipp Treutlein — Universität Basel

Quantum networks will consist of many quantum memory nodes that are interconnected via photonic links, transporting single photons carrying quantum information. In the future, such quantum networks may enable: high-speed quantum cryptography for unconditionally secure communication; large scale quantum computers; and quantum simulators that will allow for exponential speed-up in solving specific complex problems. A promising route towards functional quantum networks is the heterogeneous approach, where different and separately optimized physical systems are used for single photon generation and storage. For example semiconductor quantum dots may be used as efficient, fast and deterministic single photon sources, while atomic ensembles allow for efficient storage of these photons.

We demonstrate a photonic memory in hot Rb vapor with on-demand storage and retrieval. In principle the memory is suitable for storing single photons emitted by an GaAs droplet quantum dot. Operation of the memory is demonstrated using attenuated laser pulses. For pulses with a bandwidth of ~ 100 MHz $\sim 0.5\mu$eV we achieve $\sim 25\%$ storage and retrieval efficiency, while the storage time approaches 1 μs. The developed quantum memory might become a cornerstone for future hybrid quantum dot-atom based quantum networks.

HL 51.3 Wed 10:15 POT 112

Generation of single photons with tailored waveforms using a quantum dot emitting at the Rb D2 line — •Jan-Philipp Jahn[1], Lucas Béguin[1], Janik Wolters[1], Mathieu Munsch[1], Yongheng Huo[2], Fei Ding[3], Rinaldo Trotta[2], Markus Reindl[2], Oliver G. Schmidt[3], Armando Rastelli[2], Philipp Treutlein[1], and Richard J. Warburton[1] — [1]University of Basel, CH-4056 Basel, Switzerland — [2]Johannes Kepler University Linz, A-4040 Linz, Austria — [3]IFW Dresden, D-01069 Dresden, Germany

Semiconductor quantum dots are excellent single photon sources, providing triggered single photon emission at a high rate and with 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. We have recently demonstrated the emission of high quality photons from a single droplet quantum dot emitting at the Rb D2 transition [1]. However, there is a significant mismatch between the large bandwidth of the quantum dot photons and the relatively small bandwidth of a Rb ensemble. We present here a route to creating photons with a tailored waveform by exploiting a long-lived hole spin in a droplet quantum dot. The quantum dot spin is prepared in one of the spin states and is then driven into the other spin state by a control laser whose waveform determines the waveform of the photon. We demonstrate the creation of $10-100$ ns duration waveforms with single-photon character thereby overcoming the bandwidth mismatch.

[1] J.-P. Jahn *et al.*, Phys. Rev. B **92**, 245439 (2015)

HL 51.4 Wed 10:30 POT 112

Electrically-pumped wavelength-tunable GaAs quantum dots interfaced with rubidium atoms — •Huiying Huang[1], Rinaldo Trotta[1], Yongheng Huo[1], Thomas Lettner[1], Johannes Wildmann[1], Javier Martín-Sánchez[1], Daniel Huber[1], Marcus Reindl[1], Jiaxiang Zhang[2], Eugenio Zallo[3], Oliver Schmidt[2], and Armando Rastelli[1] — [1]Institute of Semiconductor and Solid State Physics, Johannes Kepler University, Linz, Altenbergerstraße 69, 4040, Austria — [2]Altenbergerstr. 69 — [3]Paul-Drude-Institut für Festkörperelektronik Hausvogteiplatz 5-7, 10117 Berlin, Germany

The combination of semiconductor quantum-dots (QDs) and natural atoms may allow storing the state of single photons emitted from a QD in atomic vapors, which has the potential to become crucial ingredients for building up a quantum repeater. To achieve such interface, the QD emission has to be precisely tuned to atomic lines. In this talk, I will introduce the first light-emitting-diode based on single GaAs/AlGaAs QDs and demonstrate its operation as an energy-tunable source of photons with wavelength in resonance with the D2 transitions of 87Rb atoms. This device is a compact and completely electrically-driven source of non-classical light in which both the excitation and tunability are provided on-chip. By feeding the emitted photons into a 75-mm-long cell containing warm 87Rb atom vapor, we observe slow-light with a temporal delay of up to 3.4 ns. In view of the possibility of using 87Rb atomic vapors as quantum memories, this work makes an important step towards the realization of hybrid-quantum systems for future quantum networks.

Invited Talk HL 51.5 Wed 10:45 POT 112

Strain-tunable quantum dots interfaced with atomic vapors — •Rinaldo Trotta — Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, Linz, Altenbergerstrasse 69, 4040, Austria

The development of quantum networks for the distribution of quantum information among distant parties will bring about a revolution in communication science and technology. Addressing this task successfully will most likely require merging different quantum systems, where the advantages of the different constituents are combined. Hybrid natural-atomic interfaces between semiconductor quantum dots (QDs) and atomic vapors are currently emerging as a promising route for quantum networking. However, coupling the two physical systems requires several outstanding challenges to be overcome. One challenge is to match the energy of the single and entangled photons emitted by QDs to absorption lines of the atomic vapors. In this talk, I will discuss how external strain fields provided by piezoelectric actuators can be used to address this task successfully [1,2,3]. In particular, I will show how full control over the QD in-plane strain tensor allows the energy of the entangled photons emitted by QDs to be precisely controlled in the spectral range in which a cloud of natural atoms behaves as a slow-light medium.

[1] J. S. Wildmann et al., Phys. Rev. B 92, 235306 (2015) [2] H. Huang et al., arXiv:1602.02122 [3] R. Trotta et al., Nature Comm. 7, 10375 (2016).

Coffee Break

Invited Talk HL 51.6 Wed 11:45 POT 112

Atomic-vapor-enabled variable optical delay for triggered

single-photons from a semiconductor quantum dot — •Hüseyin Vural[1], Jonas Weber[1], Markus Müller[1], Simon Kern[1], Julian Maisch[1], Matthias Widmann[2], Robert Löw[3], Jörg Wrachtrup[2], Ilja Gerhardt[2], Simone Portalupi[1], Michael Jetter[1], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]3. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart — [3]5. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart

Beside their enormous flux, quantum dots (QDs) allow for high photon indistinguishability and photonic entanglement generation, and their use as flying qubits for the quantum communication of the future. One limitation of QDs is the missing long lasting quantum memory. Here, we focus on the approach of storing light in an cesium (Cs)-vapor by slowing down single photons. High dispersion between ground-state hyperfine resonances of Cs-vapors enables lower group velocities, while maintaining transmission. Using a Cs-vapor as slow light-medium, we present a variable delay up to several ns for photons from resonantly excited QD's. Increasing the temperature in the vapor changes the dispersion, which allows us to control the amount of delay experienced by the photons. Eventually we investigate and compare the single-photon emission and two-photon interference of delayed and undelayed photons.

HL 51.7 Wed 12:15 POT 112

Relaxation of gate-controlled donor qubits in silicon — Peter Boross[1], Gabor Szechenyi[1], and •Andras Palyi[2] — [1]Eotvos University, Budapest, Hungary — [2]Budapest University of Technology and Economics, Hungary

Gate control of donor electrons near interfaces is a generic ingredient of donor-based quantum computing. Here, we address the question: how is the phonon-assisted qubit relaxation time T_1 affected as the electron is shuttled between the donor and the interface? We focus on the example of the 'flip-flop qubit' (Tosi et al arXiv:1509.08538v1), defined as a combination of the nuclear and electronic states of a phosphorus donor in silicon, promising fast electrical control and long dephasing times when the electron is halfway between the donor and the interface. We theoretically estimate that the flip-flop qubit relaxation time can be of the order of 100 μs, 8 orders of magnitude shorter than the value for an on-donor electron in bulk silicon, and a few orders of magnitude shorter (longer) than the predicted inhomogeneous dephasing time (gate times). This relaxation process is boosted by (i) the nontrivial valley structure of the electron-phonon interaction, and (ii) the different valley compositions of the involved electronic states. Reference: P. Boross et al., Nanotechnology 27, 314002 (2016)

Invited Talk HL 51.8 Wed 12:30 POT 112

Correlating independent spins via single-photon projections — •Mete Atature — Cavendish Laboratory, University of Cambridge, JJ Thomson Ave., Cambridge CB3 0HE UK

Optically active spins confined in solids provide interesting and rich physical systems. Their inherently mesoscopic nature leads to a multitude of dynamics within the solid state environment of spins, charges, vibrations and light. Implementing a high level of control on these constituents and their interactions with each other creates exciting opportunities for realizing stationary and flying qubits within the context of spin-based quantum information science. In particular, coherent single photon generation together with improving spin coherence allows for generating nonlocal correlations between distant spins at a very high rate. I will provide a snapshot of the progress and challenges for quantum optically interconnected solid-state spins.

HL 52: Devices

Time: Wednesday 9:30–11:30 Location: POT 06

HL 52.1 Wed 9:30 POT 06

Full Range Electrothermal Modeling of Organic Light-emitting Diodes — •Axel Fischer, Koen Vandewal, Simone Lenk, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), TU Dresden

Organic light-emitting diodes (OLEDs) are now considered for lighting and signaling in the automobile sector, but the requirements are harsh. Moreover, cars have to operate at different ambient conditions, but the appearance of the lighting should remain the same. For tail and break lights, extreme brightness is needed ($> 10.000\,\mathrm{cd/m^2}$) in order to ensure good visibility. As a consequence, high current and power densities are applied which lead to self-heating and unpleasant inhomogeneities of the light emission, neutralizing the benefits of OLED technology such as extraordinary designs. These issues arise due to the fact that OLEDs show a strong dependence between conductivity and temperature, leading to nonlinear electrothermal feedback [Fischer *et al.*, Adv. Funct. Mater., 2014, 24]. Thus, developing accurate electrothermal models for OLEDs is of great interest to establish a future thermal management strategy, holding the brightness as well as its lateral homogeneity constantly high. Here, we present an electrothermal model for OLEDs which nicely matches the full operational range, regarding voltage and temperature and by that is able to reproduce experimentally observed "S"-shaped current-voltage characteristics upon Joule self-heating. Besides that, our approach considers recombination and drift related phenomena, giving valuable insights to the physics of OLEDs.

HL 52.2 Wed 9:45 POT 06

Detection of Terahertz radiation with a graphene-based Schottky Diode — •Maria Schlecht[1], Christian Müller-Landau[1], Alexander Glas[1], Sascha Preu[2], Stefan Malzer[1], and Heiko B. Weber[1] — [1]Lehrstuhl für Angewandte Physik, FAU Erlangen-Nürnberg (FAU), Erlangen, Germany — [2]Dept. of Electrical Engineering and Information Technology, Technische Universität Darmstadt, Germany

We report on the design, fabrication and characterization of a graphene-based Schottky diode for detection of Terahertz (THz) radiation. With epitaxially grown graphene on n-type silicon carbide one can define ohmic and Schottky contacts side-by-side on a silicon carbide wafer, forming a lateral Schottky diode [1]. Due to the nonlinearity of the IV-curve THz radiation is rectified and one measures a DC current proportional to the amplitude of the THz radiation. The responsivity scales with the second derivative of the IV-curve. Furthermore, we detected THz radiation from 70 GHz to 350 GHz using a nipnip-THz source [2]. We achieved a maximal responsivity of 30 mA/W, i.e. 1200 V/W at 78 GHz. The ability of the device to rectify THz radiation is strongly limited by the RC-roll off [2]. In order to increase the 3dB roll off frequency, we compared the nitrogen-implanted Schottky diodes with phosphor-implanted ones which have a much lower serial resistance. [1] S. Hertel et al. Nature comm. 3:951 (2012) [2] S. Preu, et al. J. Appl. Phys. 109, 061301 (2011)

HL 52.3 Wed 10:00 POT 06

Cognitive and memory devices based on Debye length modulation — •Kai-Uwe Demasius — Max Planck Institut für Mikrostrukturphysik, Halle (Saale)

By using a modulation of the screening length in semiconducting and metal-to-insulator transition materials we might reach much higher data storage densities and acess times for ferroelectric memories. A metal-insulator-semiconductor-insulator-metal (MISIM) stack might act as a switch for electric fields, which is interesting to switch and read out the polarization of a ferroelectric material. Furthermore the field transmission through through MISIM-structure shows a hyperbolic tangent behaviour which is interesting as an activation function for artificial neuronal networks.

HL 52.4 Wed 10:15 POT 06

Single-Emitter Regime and Lasing in High-Q Micropillars with Site-Controlled Quantum Dots — •Arsenty Kaganskiy, Tobias Heuser, Jan Grosse, Alexander Schlehahn, Sören Kreinberg, Fabian Gericke, Xavier Porte, Tobias Heindel, Sven Rodt, André Strittmatter, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, D-10623

We report on the realization of quantum dot (QD) - micropillar cavities based on a technology platform called buried stressor approach

[1]. This method allows for the site-controlled growth and device integration of QDs with high optical quality. In addition, this approach has the important advantage that the number of site-controlled QDs in the cavity can be controlled by the design of the buried stressor. By fine tuning the gain, one can operate these devices as few-QD microlasers or even in the single quantum dot regime. Moreover, the buried-stressor approach ensures that the ensemble with a controlled number of QDs is located in the electric field maximum in the center of the micropillars. The fabricated micropillars exhibit Q-factors up to 30000 at an emission wavelength of 932 nm. Single-QD Purcell-enhancement of the emission is investigated via temperature-induced resonance-tuning. The lasing action of the micropillars is proven by power dependent measurements.

[1] A. Strittmatter et al., Appl. Phys. Lett. 100, 093111 (2012)

Coffee Break

HL 52.5 Wed 10:45 POT 06

Heterostructures of 2D carbon materials for pH-sensing — •David Kaiser[1], Andreas Winter[1], Christof Neumann[1], Thomas Weimann[2], and Andrey Turchanin[1] — [1]Institute for Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany — [2]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany

Chemical functionalization of single-layer graphene (SLG) is of key importance for applications in functional electronic devices such as, e.g., field effect transistor (FET) based nanosensors. However, the electronic quality of graphene is typically degraded after the functionalization, which significantly restricts the applications. Here, we employ a route to non-destructive chemical functionalization of graphene via engineering of novel carbon nanomembrane (CNM)/SLG hybrids to build an electrolyte-gate FET sensor which can detect the pH value. We employ SLG grown by methane CVD on Cu foils and amino-terminated 1 nm thick CNMs generated by electron-beam induced crosslinking of aromatic self-assembled monolayers to engineer hybrid CNM/SLG FETs. We show that the intrinsically high electronic quality of pristine SLG is preserved in the amino-functionalized hybrids and that sensing of pH is possible with high sensitivity.

HL 52.6 Wed 11:00 POT 06

Ionic Liquid Gating of Solution Processed MoS2 Thin Film Transistors — •Francis Oliver Vinay Gomes[1,2], Xiaoling Zeng[2], Marko Marinkovic[1], Torsten Balster[2], and Veit Wagner[2] — [1]Evonik Resource Efficiency GmbH, Paul-Baumann-Strasse 1, 45772 Marl, Germany — [2]Jacobs University Bremen, Department of Physics & Earth Science, Campus Ring 1, 28759 Bremen, Germany

Ionic liquid (IL) gating of thin film transistors (TFTs) based on solution processed MoS2 obtained from Mo-precursor solution on various substrates has been investigated. Chemical conversion of the deposited films on silicon and sapphire substrates to MoS2 were obtained by annealing in presence of sulfur. Films deposited on amorphous Si/SiO2 substrates showed random grain orientation. However, improved film growth with oriented grains was observed on crystalline sapphire substrates. Raman and XPS, and TEM measurements revealed formation of polycrystalline MoS2 films with grain size of 100 nm.

TFTs fabricated from MoS2 implementing IL gating through electrostatic carrier accumulation exhibited ambipolar transport with dominant n-type behaviour. TFT performance was observed for films thinner than 9 nm due to gate-channel control and the threshold voltage is dependent on the ratio of IL to host polymer mixture. Sapphire in contrast to silicon substrates demonstrated ten times higher ON/OFF ratio attributed to the improved film growth. The efficient use of IL gating achieved in this wet-chemical MoS2 can be extended to quantitatively study other dichalcogenides for future nanoelectronic devices.

HL 52.7 Wed 11:15 POT 06

Cognitive computing with mem-circuits — •Alessandro Fumarola and Stuart Parkin — Max Planck Institute for Microstructure Physics, Halle (Saale), Sachsen-Anhalt, Germany

The time and energy spent transporting information between memory and processor in standard computers (across the so-called 'Von-Neumann bottleneck') has become problematic for data-centric applications such as real-time image recognition and natural language processing[.

Non-VN systems, such as the human brain, are capable of full on-line learning and could be designed moving from reliable but binary devices to dense and analog (but less reliable) nanoscale elements. Previous work has been carried out, for example,with phase-change devices and other non-volatile memories, obtaining high machine learning performance in large-scale hardware/software systems.

In this work, we assess the suitability and advantages of other circuit elements with memory, namely memcapacitors, used as synaptic devices in such Non-VN configurations. Simulated power and performance benchmarks are provided. Possible solid-state implementation of binary and analog memcapacitors are also proposed and characterized.

HL 53: Fundamentals of Perovskite Photovoltaics V (joint session CPP/DS/HL)

Time: Wednesday 10:15–12:45 Location: ZEU 250

Invited Talk HL 53.1 Wed 10:15 ZEU 250

Light-induced degradation of methylammonium and formamidinium PbI3 perovskites — •Norbert H. Nickel, Felix Lang, Victor V. Brus, and Jörg Rappich — Helmholtz-Zentrum Berlin für Materialien und Energie, Institut für Silizium Photovoltaik, Kekuléstr. 5, 12489 Berlin

We investigate the stability of methylammonium (CH3NH3+ - MA) and formamidinium (HC(NH2)2+ - FM) lead iodide perovskite films using visible and ultra violet light in oxygen atmosphere and in vacuum. Insight into the degradation mechanisms was obtained from in-situ Fourier-transform infrared absorption (FT-IR), photoluminescence, and gas effusion measurements. We revisited the light-induced degradation of MAPbI3 in the presence of oxygen. Illumination in O2 atmosphere results in a swift degradation. Isotope experiments clearly show that O2 acts as a catalyst decomposing MA ions into CH3NH2 and hydrogen. In case of FMPbI3 perovskites illumination in the presence of O2 results in a more complex reaction; decomposition of the FM ions occurs at the N-C-N bonds and as a result CO2 and C = O molecules are formed that rapidly diffuse out of the crystalline lattice.

In addition, we present experimental evidence of a hitherto unknown but fundamental degradation mechanism of MAPbI3 and FMPbI3 perovskite layers due to exposure to visible and ultra violet light. This degradation mechanism does not require the presence of oxygen or other constituents. Our data indicate that the molecular orbitals of the organic ions are not in resonance with the energy bands of the perovskite.

HL 53.2 Wed 10:45 ZEU 250

Degradation Studies of Methylammonium Lead Iodide under Controlled Exposure to Oxygen and Light — •Paul Fassl, Qing Sun, David Becker-Koch, Alexandra Bausch, and Yana Vaynzof — Kirchhoff-Institute for Physics / Centre for Advanced Materials, Heidelberg University, Germany.

Despite the remarkable increase in the power conversion efficiency of hybrid organometal-halide perovskite solar cells reaching 22% to date, the low environmental stability of the material remains only partly understood. While the instability of methylammonium lead iodide (CH3NH3PbI3) in humid atmospheres has been studied experimentally as well as theoretically, degradation in the presence of oxygen and light has just recently been reported.

In this work, planar pinhole-free perovskite films are degraded under dry conditions with precisely controlled exposure to various oxygen levels and simulated sunlight using our environmental stability testing rig and then characterized by multiple techniques such as XPS, PDS, PL, AFM and SEM. These results are then correlated to the efficiency decay of photovoltaic devices (ITO/PEDOT:PSS/CH3NH3PbI3/PCBM/BCP/Ag), where the bare perovskite film has been first degraded under identical conditions.

Our results show that exposure to oxygen and light is one of the major reasons for the fast degradation of unencapsulated perovskite solar cells at ambient conditions and that the morphology and defect

density of the pristine perovskite film has a considerable impact on the rate of degradation.

HL 53.3 Wed 11:00 ZEU 250

Real-Time Observation of Iodide Ion Migration in Methylammonium Lead Halide Perovskites — •Cheng Li[1], Antonio Guerrero[2], Yu Zhong[1], Anna Gräser[1], Carlos Andres Melo Luna[3], Jürgen Köhler[3], Juan Bisquert[2], Richard Hildner[3], and Sven Huettner[1] — [1]Macromolecular Chemistry I, Universität Bayreuth, Universitätstr. 30, 95447 Bayreuth, Germany — [2]Institute of Advanced Materials (INAM), Universitat Jaume I, 12006 Castell, Spain — [3]Experimental Physics IV and Bayreuth Institute of Macromolecular Research, Universität Bayreuth, Universitätstr. 30, 95447 Bayreuth, Germany

To investigate the origin of current-voltage (J-V) hysteresis characteristic in perovskite solar cells (PSC), we utilize correlated time-resolved photoluminescence (PL) microscopy and impedance spectroscopy (IS) on perovskite films to in-situ investigate both the spatial and temporal evolution of these PL inactive areas under external optical/electrical fields. We attribute the formation of PL inactive domains to the migration and accumulation of iodine ions under external electrical fields. Furthermore, we fabricate and characterize PSC incorporating phenyl-C61-butyric acid methyl ester (PCBM) and PCBM polymer to investigate the influence of diffusions of PCBM molecules on the hysteretic behavior. Following that, the step-wise temperature dependent J-V measurement demonstrates the reduction of migration with the aid of PCBM molecules. Hence, it is proposed that the elimination/alleviation of J-V curve hysteresis is ascribed to the diffusion of PCBM molecules, which passivate the iodide related defects.

HL 53.4 Wed 11:15 ZEU 250

Polarization of Methylammonium Lead Halide Perovskite Films on Microstructured Arrays — •Martina Stumpp[1,3], Raffael Ruess[1,3], Jan Muessener[2,3], and Derck Schlettwein[1,3] — [1]Justus-Liebig-University Giessen, Institute of Applied Physics — [2]Justus-Liebig-University Giessen, 1st Physics Institute — [3]Justus-Liebig-University Giessen, Laboratory for Materials Science

Despite the great advances of methylammonium lead halide perovskites in photovoltaics, many properties such as the I-V hysteresis of such films are not fully understood and, therefore, need detailed investigation. In the current study, $CH_3NH_3PbI_3$ and $CH_3NH_3Pb(I_{3-x}Cl_x)_3$ films were prepared on microstructured gold or platinum electrode arrays on SiO_2/Si wafers in order to use symmetric contacts and widely inert substrates. The perovskite films were poled with high voltages and the current was measured under variation of ambient parameters and analyzed in detail. Following the poling of the samples, voltage sweeps were performed. The I-V characteristics during these sweeps showed clearly that the perovskite films were polarized and that the polarization had a persistent character. Additionally, different hysteresis characteristics were observed. The origin of regular and inverted characteristics will be discussed.

15 min break

HL 53.5 Wed 11:45 ZEU 250

Characterization of the perovskite solar cells containing atomic layer deposited Al_2O_3 buffer layer. — •Małgorzata Kot[1], Konrad Wojciechowski[2], Henry Snaith[2], and Dieter Schmeisser[1] — [1]BTU Cottbus-Senftenberg, Konrad-Wachsmann-Allee 17, 03046 Cottbus, Germany — [2]Clarendon Laboratory, University of Oxford, Parks Road, Oxford, OX13PU, UK

Hybrid perovskites have potential to overcome performance limits of the current solar cell technologies and achieve low cost and high versatility. Nonetheless, they are prone to degradation in presence of moisture within a couple of hours or days. In this work, we use the atomic layer deposition (ALD) of Al_2O_3 on the $CH_3NH_3PbI_3$ perovskite at room temperature in order to verify if this thin ALD layer may protect the perovskite film against moisture degradation and to check the impact of the Al_2O_3 on the solar to power conversion efficiency (PCE). Depth profiling X-ray photoelectron spectroscopy study shows that the ALD precursors are chemically active only at the perovskite surface and the film bulk is not affected. The perovskite film coated with Al_2O_3 layer has enhanced moisture stability. Solar cells with a fresh-made $CH_3NH_3PbI_3$ perovskite film have shown PCE of 15.4%, while the one with 50 days aged perovskite only 6.1%. However, when the aged perovskite is covered with RT-ALD-Al_2O_3 the PCE value is clearly enhanced.[1]

[1] M. Kot et al., Room temperature ALD impact on efficiency, stability and surface properties in perovskite solar cells, ChemSusChem, acctepted.

HL 53.6 Wed 12:00 ZEU 250

Influence of the grain size on electronic properties of methylammonium lead iodide — •Oleksandra Shargaieva, Felix Lang, Jörg Rappich, Thomas Dittrich, Bernd Rech, and Norbert Nickel — Helmholtz-Zentrum Berlin, Institute for Silicon Photovoltaics, Kekulestr. 5, D-12489 Berlin (Germany)

Recently, hybrid perovskites have drawn the attention of researchers due to huge potential as absorbers in photovoltaic devices. The biggest advantage of such materials is the ease of the preparation within low costs leading to highly efficient solar cells. However, the solution based processing often lacks a control over crystal quality of obtained material. Despite the numerous reports showed different methods to improve morphology of perovskite layer, the influence of microscopic structure on properties of the material is not fully understood.

In this work we present a new approach to tune the grain size of CH3NH3PbI3 perovskite from 150 to 1000 nm with about 100 nm step. The new method is based on solid-phase recrystallization and provides a reliable way to control the grain size and hence, systematically study the influence of the grain size on optical and electrical properties of the material. The recrystallized perovskite layers were characterized using photoluminescence spectroscopy and surface photovoltage measurements. The recrystallized samples demonstrated a pronounce increase of the PL intensity due to lower defect density in treated material. Furthermore, our study showed a direct correlation between grain size and the transport length, L, with the maximum value of 900 nm.

HL 53.7 Wed 12:15 ZEU 250

Investigation of novel material systems for hybrid photovoltaics - alternatives for the paradigm — •Nuri Hohn[1], Mike Boone[2], Eric Rivard[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]University of Alberta, Department of Chemistry, Edmonton, Alberta, Canada

Organic materials have been found to offer various, promising advantages for photovoltaic (PV) devices like flexibility and the potential of low-cost/large scale production. Hybrid devices combine these advantages with the chemical/physical stability of inorganic materials and, thus, overcome the issue of limited lifetimes of purely organic cells. Poly(styrene-block-ethylene oxide) templated sol-gel chemistry is used to synthesize high surface-to-volume ratio, mesoporous titania thin films, which allows for precise structure control and an increased amount of interface. The n-type, electron conducting titania thin film serves as a basis for novel organic material studies. The studies aim to introduce new material combinations to the field of hybrid PV and to open up pathways for enhanced efficiency in terms of energy conversion and band alignment. Thin film spectral absorption characterization is carried out via UV/Vis measurements. Furthermore, morphological characterization is realized via SEM and XRD to address to surface structure and the crystallinity of the material.

HL 53.8 Wed 12:30 ZEU 250

Water-processed hybrid solar cells: deposition of the active layer with vertical composition gradient — •Volker Körstgens[1], Florian Buschek[1], Martin Wörle[2], Hristo Iglev[2], Wiebke Ohm[3], Stephan V. Roth[3], Reinhard Kienberger[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]TU München, Physik-Department, LS Laser- und Röntgenphysik, James-Franck-Str. 1, 85748 Garching — [3]DESY, Notkestr. 85, 22607 Hamburg

Particular environmentally friendly processing of hybrid solar cells with the solvent water is feasible with an active layer consisting of laser-ablated titania and a water-soluble polythiophene [1]. One way to optimize conversion efficiencies of these devices is the introduction of a vertical compositional gradient of the two components of the active layer. Dip-coating and spray-coating have been utilized as techniques which are suitable for the cost-effective preparation of hybrid photovoltaics. We followed the development of the morphology during spray deposition 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 and the influence on photovoltaic performance with the introduction of a compositional gradient are discussed.

[1] Körstgens et al., Nanoscale 7, 2900 (2015).

HL 54: Plasmonics and Nanooptics VI: Light-Matter Interactions and Characterisation

Time: Wednesday 10:30–12:30 Location: TRE Ma

HL 54.1 Wed 10:30 TRE Ma

Remote excitation and detection of surface-enhanced Raman scattering from graphene — •Nicolas Coca Lopez, Nina Gordon, Tobia Mancabelli, Nicolai Hartmann, and Achim Hartschuh — Department of Chemistry and Center for Nanoscience, Ludwig-Maximilian-University Munich

In this contribution, we show the remote excitation and detection of surface enhanced Raman scattering (SERS) from graphene. Surface plasmon polaritons (SPPs) were launched by focused laser illumination at the termination of a metallic nanowire (NW) which served as a plasmonic waveguide. An SPP excited by the laser travels to the other end of the waveguide that is placed on top of single layer graphene, resulting in the remote excitation of Raman scattering. In the reversed direction, locally excited Raman scattering from graphene is coupled to an SPP traveling along the NW and scattering out at its end. By projecting the sample scattered light onto a CCD camera mounted on a spectrometer we quantified the SPP contributions at different wavelengths in combination with polarization dependent measurements.

HL 54.2 Wed 10:45 TRE Ma

Helicity Sorting of Photons: A Spin Optical Device — •Enno Krauss[1], Gary Razinskas[1], Dominik Koeck[1], Swen Grossmann[1], and Bert Hecht[1,2] — [1]NanoOptics & Biophotonics Group, Experimentelle Physik 5, Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Röntgen Research Center for Complex Material Systems (RCCM), Am Hubland, 97074 Würzburg, Germany

Spin optics adds an additional degree of freedom and therefore promises new functionalities in optical nanocircuits in analogy to spintronics. Here we study experimentally and theoretically spin-optical devices, so-called photon helicity sorters, based on "birefractive" propagation in a plasmonic two-wire transmission line. We study the mechanism that leads to spin-orbit coupling in these devices including the role of a geometrical phase.

HL 54.3 Wed 11:00 TRE Ma

Optical properties of hybrid chiral plasmonic systems — •Martin Schäferling, Maxim L. Nesterov, Xinghui Yin, Harald Giessen, and Thomas Weiss — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany

Chiroptical spectroscopy is a vital technique in the life sciences. The combination of chiral media with plasmonic nanostructures offers a possibility to enhance the tiny chiroptical responses. Theoretical studies of such hybrid systems are necessary to understand the occurring interactions. A well-established method to investigate the potential interaction strength between plasmonic nanostructures and a chiral molecule is the analysis of chiral near-fields [1]. This method works for the presence of a few molecules in the limit of weak coupling. However, in systems where a sizeable amount of a chiral medium is present, additional effects beyond the capabilities of this model can occur.

In this contribution, we analyze the full hybrid system combining plasmonic nanostructures with chiral media. In one approach, we use numerical full-wave simulations where we introduced an effective chiral medium via its constitutive equations. Our results reveal the importance of coplanarity of the incident field with the generated near-field in addition to strong field enhancement [2]. Additionally, we show first results of a semi-analytical approach using perturbation theory [3] to analyze the influence of a chiral medium on plasmonic resonances.

[1] M. Schäferling et al., Phys. Rev. X **2**, 031010 (2012).
[2] M. L. Nesterov et al., ACS Photonics **3**, 578 (2016).
[3] T. Weiss et al., Phys. Rev. Lett **116**, 237401 (2016).

HL 54.4 Wed 11:15 TRE Ma

Colloid-defined Scattering Interfaces with Tailored Disorder for PV Applications — Peter Michael Piechulla[1], •Lutz Mühlenbein[1], Alexander Sprafke[1], Ralf B. Wehrspohn[1], Stefan Nanz[2], Aimi Abass[2], and Carsten Rockstuhl[2] — [1]FG Mikrostrukturbasiertes Materialdesign, MLU Halle-Wittenberg — [2]Institut für Theoretische Festkörperphysik, KIT, Karlruhe

Optical interfaces with tailored scattering properties are of interest for numerous applications, such as light management in photonic devices. In particular, thin film solar cell absorber materials exhibit long absorption lengths in the long wavelength range compared to the absorber thickness, which makes effective light trapping structures indispensable. Numerical studies reveal that interfaces with a certain degree of disorder outperform strictly periodic structures due to their improved broadband response. However, the proposed design in these studies are mostly either hypothetical in nature or rely on expensive top down fabrication methods. In our approach, we deposite a monolayer of colloidal particles onto a substrate using self-organization effects. Colloidal size distribution and manipulation of interaction potentials between particles and substrate provide effective levers to obtain desired surface profiles. The structure is then stabilized by conformal coating using atomic layer deposition and can be used as back side structure for solar cells. In this contribution, we will identify relevant fabrication parameters of these structures and present experimental data for their scattering properties. The presented experimental work is motivated by optical simulations that are specific to colloidal structures.

HL 54.5 Wed 11:30 TRE Ma

Characterization of thin-load polymethyl-methacrylate plasmonic waveguides using PEEM — •Malte Grossmann[1], Martin Thomaschewski[1], Alwin Klick[1], Elzbieta Sobolewska[2], Arkadiusz Jaroslaw Goszczak[2], Till Leissner[2], Jacek Fiutowski[2], Horst-Günter Rubahn[2], and Michael Bauer[1] — [1]Institute of Experimental and Applied Physics, University of Kiel, Leibnizstraße 19, D-24118 Kiel, Germany — [2]Mads-Clausen-Institute, NanoSYD, University of Southern Denmark, Alsion 2, DK-6400 Sønderborg, Denmark

Surface plasmon-polaritons (SPPs) are promising candidates for future signal transport applications due to their capability of bypassing the diffraction limit of light. However, for applications such as on-chip communications SPPs have to be confined laterally. This can be achieved using plasmonic waveguides. Here we present work on dielectric-loaded SPP waveguides (DLSPPW) using a thin load (30 to 50 nm) of polymethyl-methacrylate (PMMA).

PMMA DLSPPW of variable width are fabricated on gold substrates using electron-beam lithography. We investigate the waveguides using photoemission electron microscopy supported by a wavelength-tunable near-infrared laser. The dispersive characteristics of the waveguides are compared to finite-element-method calculations. We are able to determine waveguide mode effective index with quantitative agreement and mode confinement with qualitative agreement to expectations set by the finite-element-method calculations for both singlemode and multimode waveguiding.

HL 54.6 Wed 11:45 TRE Ma

Design and fabrication of metasurfaces with high polarization sensitivity on top of crystalline gold plates — •Manuel Gonçalves[1], Vaishnavi Rao[1], Gregor Neusser[2], Christine Kranz[2], Boris Mizaikoff[2], and Othmar Marti[1] — [1]Institute of Experimental Physics, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany — [2]Institute of Analytical and Bioanalytical Chemistry, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany

Metasurfaces emerged in the last 10 years as one of the most successful realizations of plasmonic metamaterials. The two-dimensional geometrical arrangement of sub-wavelength plasmonic and dielectric nanostructures permits to use metasurfaces in a variety of ways: transformation of the polarization of light beams, beam focusing, holography, generation of structural colors. The units constituting plasmonic metasurfaces are tailored based on the plasmonic properties of single, or coupled particles. Among the several lithography techniques used for fabrication, focused ion-beam (FIB) is best indicated for milling crystalline films and particles, due to the accuracy achieved.

We have investigated the optical properties of grooves milled in crystalline gold plates and have designed a metasurface to be used in reflection using several groove elements. Due to the large sensitivity of the plasmonic absorption on the polarization of the light irradiating the grooves, the metasurface can be used as a polarization sensitive optical filter for specific bands in the visible and NIR spectrum.

HL 54.7 Wed 12:00 TRE Ma

Imaging with SNOM and EELS in plasmonics — •Vlastimil Křápek[1,2], Petr Dvořák[1,2], Ai Leen Koh[3], Zoltán Édes[1,2], Michal Horák[1,2], Michal Kvapil[1,2], Lukáš Bříinek[1,2], Tomáš Šamořil[1,2], Martin Hrtoň[1,2], and Tomáš Šikola[1,2] — [1]Central European Institute of Technology, Brno University of Technology, Purkyňova 123, CZ-612 00 Brno, Czech Republic — [2]Institute of Physical Engineering, Brno University of Technology, Technická 2, CZ-616 69 Brno, Czech Republic — [3]Stanford Nano Shared Facilities, Stanford University, Stanford, California 94305, USA

Scanning near-field optical microscopy (SNOM) is a powerful tool for imaging and analysis of surface plasmon polaritons (SPPs) [1]. However, the correct interpretation of SNOM images requires profound understanding of principles behind their formation. To study fundamental principles of SNOM imaging in detail, we performed spectroscopic measurements of plasmon interference patterns by an aperture-type SNOM setup equipped with a supercontinuum laser and a polarizer. The series of wavelength- and polarization-resolved measurements, together with results of numerical simulations, then allowed us to identify the role of individual near-field components in formation of SNOM images.

Electron energy loss spectroscopy (EELS) is a technique for imaging of localized plasmon resonances with unprecedented spatial resolution. We present our EELS imaging of gold plasmonic particles suitable for the enhancement of optical processes [2].

[1] P. Dvořák *et al.*, Nano Lett **13**, 2558 (2013).
[2] V. Křápek *et al.*, Opt. Express **23**, 11855 (2015).

HL 54.8 Wed 12:15 TRE Ma

Multimodal Tip-Enhanced Microscopy — Kai Braun, •Otto Hauler, Dai Zhang, and Alfred J. Meixner — Institut für Physikalische und Theoretische Chemie, Auf der Morgenstelle 18, 72076 Tübingen

Electromagnetic coupling between plasmonic resonances of two closely spaced metal particles can lead to a strongly enhanced optical near field in the gap between. It is the leading amplification mechanism for surface- and tip-enhanced Raman scattering (SERS/TERS) or enhanced molecular luminescence and has widespread applications in nanoplasmonics. Collecting correlated signals of photoluminescence (PL) and Raman as well as topography, tip-enhanced hyperspectral imaging is able to provide a thorough map of the chemical and morphology-related optical properties in multi-component material systems. Introducing new microscope functions offer us insights into various aspects, such as morphology related photophysical and photochemical processes. Despite its attractive capabilities, developing a tip-enhanced near-field microscope providing reliable and reproducible performance is demanding. In the last years great efforts have been made in our lab to develop stable, reproducible and reliable near-field optical microscopes, which largely meet the above requirements. They successfully demonstrated their capability in high-resolution optical imaging and spectral mapping, or using the tip as local probe for enhanced coupled fields. Furthermore we demonstrate the direct manipulation and measurement of surface properties via electrical charging or injection of charge carriers

HL 55: Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - IV

Time: Wednesday 10:30–13:00 Location: GER 38

Invited Talk HL 55.1 Wed 10:30 GER 38

Electronic excitations in 2D materials and heterostructures — •Kristian Sommer Thygesen — Technical University of Denmark, Lyngby, Denmark

Atomically thin two-dimensional (2D) materials have recently emerged as a new class of materials with unique and highly tunable optoelectronic properties. Different 2D crystals can be stacked to form van der Waals heterostructures (vdWH) where the individual 2D layers are held together by weak van der Waals forces leading to atomically well-defined interfaces. This fascinating scenario opens up the possibility of designing heterostructures with tailored electronic or optical properties. I will give a general introduction to the electronic properties of 2D materials, including characteristic features of their dielectric screening and collective excitations with special emphasis on the challenges related to their ab-initio description. I will show how the dielectric function of a given 2D material can be controlled by embedding it into a vdWH, and how this in turn can be used to control the band structure, exciton binding energies or the plasmon dispersion in 2D materials.

HL 55.2 Wed 11:00 GER 38

Charge and energy transport at the nanoscale: A DFT perspective — •Florian G. Eich, Fabio Covito, and Angel Rubio — Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, D-22761 Hamburg, Germany

Understanding the interplay between charge and energy transport at the nanoscale paves the way for novel thermoelectric devices, which may prove useful for the development for sustainable energy sources. However, concepts, such as heat flow, temperature and entropy are only well-established at the macroscopic level for slow dynamics. This raises the question about whether these concepts can be employed for small length and short time scales. We will present our recent efforts to use a time-dependent density-functional theory framework, dubbed nonequilibrium thermal DFT, in order to generalize temperature and heat or energy flow to the microscopic regime. To this end we will highlight the analogy of the formally exact microscopic equations of motion for charge density and energy density in thermal DFT to the macroscopic equations of motion of hydrodynamics. Furthermore, we will present first result using our approach to compute transient energy energy currents induced by a temperature gradient and show that in the steady-state limit persistent temperature oscillations develop.

HL 55.3 Wed 11:15 GER 38

Conductance of aromatic and antiaromatic molecular circuits — Narendra P. Arasu and •Héctor Vázquez — Inst. of Physics, Academy of Sciences of the Czech Rep., CZ

Molecular structures with delocalized conjugated orbitals play an essential role in molecular transport due to their high conductance and small attenuation factors. While much work has been done on aromatic molecules, some studies have shown that conductance actually decreases with aromaticity [1].

In this talk I will discuss the effect of (anti)aromaticity on conductance. I will show results of first-principles transport calculations for an aromatic-antiaromatic pair of molecules and compare with experiment. Conductance is calculated using DFT and NEGF including corrections to the DFT level positions. The corrected conductance values are in very good agreement with experiment. We find that the conductance of the antiaromatic molecule is much higher than that of its aromatic counterpart. Calculations show this to be a consequence of the smaller HOMO-LUMO gap of the antiaromatic complex as well as on the molecular level alignment at the junction [2].

[1] W. Chen, H. Li, J.R. Widawsky, C. Appayee, L. Venkataraman, and R. Breslow, J. Am. Chem. Soc. 136 918 (2014).
[2] S. Marqués-González, S. Fujii, J.-Y. Shin, H. Shinokubo, N.P. Arasu, H. Vázquez and M. Kiguchi, (to be submitted).

HL 55.4 Wed 11:30 GER 38

Current-induced cooling of Carbene-based molecular junctions: role of electrodes structure — •Giuseppe Foti and Héctor Vázquez — Institute of Physics, Czech Academy of Sciences Cukrovarnicka 10, Prague 6

In this talk I will present our first principles calculations based on density functional theory (DFT) plus Nonequilibrium Green's functions (NEGF) of the current-induced heating and cooling dynamics

of a series of Carbene-based molecular junctions [1]. I will show how the atomistic details of electrode terminations have a strong impact on the heating dynamics of the junctions and how they can maximize the cooling of the system. In the cases where the molecule is attached to blunt leads and the electronic coupling to bulk states is strong the cooling efficiency of the most active vibrational modes decreases monotonically as bias increases. This results in the heating of the junction. On the other hand, when the molecule is connected to sharp electrode terminations such as chain-like structures, which can be formed experimentally when the metal-molecule bond is mechanically strong, and the electronic coupling to electrode states is weak, the cooling efficiency shows a non-monotonic behavior. It first decreases as a function of voltage but then increases at relatively high biases, effectively cooling down the junction [2]. These results reveal the important role of the atomistic structure of metal-molecule interface in the current-induced damping of localized molecular vibrations.

[1] Foti, G.; Vázquez, H. Nanotechnology 2016, 27, 125702.
[2] Foti, G.; Vázquez, H. submitted

HL 55.5 Wed 11:45 GER 38

DFTB-based recursive Green's function algorithms for electron transport in quasi-1D systems — •Fabian Teichert[1,2,4], Andreas Zienert[3,4], Jörg Schuster[4], and Michael Schreiber[2] — [1]Dresden Center for Computational Materials Science (DCMS), Dresden, Germany — [2]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany — [3]Center for Microtechnologies (ZfM), Technische Universität Chemnitz, Chemnitz, Germany — [4]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany

Within the last decades, quantum transport theory and density functional theory have become very important for predicting the electronic properties of new materials and future electronic devices.

We focus on the problem of improving quantum transport algorithms for large quasi-1D systems which are enormously time-consuming today. We combine the density functional tight binding (DFTB) approach with the recursive Green's function formalism (RGF), which is very effective for such systems. First, we show how to improve the RGF for the case of randomly distributed real defects. For this, we use the steps of the renormalization decimation algorithm (RDA), which is part of the electrode calculation. Second, we show how to improve the calculation of the surface Green's functions of electrodes which have a long unit cell. Here, we employ the decimation technique to reduce the dimensionality of the periodic Hamiltonian matrix, leading to effective matrices, which are treated by the RDA. Finally, we apply these algorithms to carbon nanotubes and present our results.

HL 55.6 Wed 12:00 GER 38

Conditions for formation of two-dimensional electron gas at the $LaFeO_3/SrTiO_3$ — •Igor Maznichenko[1], Sergey Ostanin[1], Arthur Ernst[2], Ingrid Mertig[1,2], Katayoon Mohseni[2], Holger L. Meyerheim[2], Eberhard K.U. Gross[2], Pengfa Xu[3], Wei Han[3], Philip M. Rice[3], Jaewoo Jeong[3], Mahesh G. Samant[3], and Stuart S.P. Parkin[2,3] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [3]IBM Almaden Research Center, 650 Harry Road, San Jose, California 95120, USA

The formation of a conducting two dimensional electron gas (2DEG) at the interface between two insulating oxide layers was explained theoretically for atomically and chemically abrupt interfaces via polar discontinuity.

Here we show that a 2DEG is formed at the interface between thin layers of lanthanum ferrite, $LaFeO_3$ (LFO), that are more than 3 unit cells thick, when grown epitaxially on $SrTiO_3$ (STO) (001). The interface property highly depends on the surface property of TiO_2 terminated STO. The interface is conducting if the STO is not annealed in an oxygen environment prior to the LFO growth, while insulating if the STO is annealed.

First principles calculations reveal that a 2DEG should be realized for an ideal interface but that modest chemical intermixing suppresses it. These calculations also show that the presence of oxygen vacancies supports 2DEG formation due to electronic doping.

HL 55.7 Wed 12:15 GER 38

Thermal Renormalization of the Electronic Structure: Trends across Chemical and Structural Space — •Honghui Shang[1], Christian Carbogno[1], Patrick Rinke[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Aalto University, Helsinki, Finland

Advances in electronic structure theory now allow us to compute the renormalization of the electronic structure due to thermal nuclear motion from first principles [1]. In this work, we present a systematic computational assessment of this renormalization for 82 octet binaries in both the zincblende and the rocksalt structure. After validating our computational approach that is based on finite-differences [2] and Fröhlich-type corrections [3] for polar materials, we discuss and analyze the observed trends: For instance, we find that most materials exhibit the expected band-gap reduction upon temperature increase; however, some materials (e.g. CuCl and CdO) do not follow this trend and exhibit the opposite behavior. We discuss the underlying electronic mechanism as well as its dependence on the chemical composition and structure of the material. In this context, also the sensitivity of such calculations with respect to the chosen basis set and exchange-correlation functional (LDA, PBE, HSE06) are critically investigated.

[1] F. Giustino, arXiv:1603.06965 (2016).
[2] G. Antonius, *et al. Phys. Rev. Lett.* **112**, 215501 (2014).
[3] J. P. Nery and P. B. Allen, *Phys. Rev. B* **94**, 115135 (2016).

HL 55.8 Wed 12:30 GER 38

Spin-wave excitations and electron-magnon scattering from 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

We study the spin excitations and the electron-magnon scattering in bulk Fe, Co, and Ni within the framework of many-body perturbation theory as implemented in the full-potential linearized augmented-plane-wave method. Starting from the *GW* approximation we obtain a Bethe-Salpeter equation for the magnetic susceptibility treating single-particle Stoner excitations and magnons on the same footing. 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 theorem and present an approach that implements the magnetic susceptibility using a renormalized Green function instead of the non-interacting one, leading to a substantial improvement of the Goldstone-mode condition [1]. Finally, we employ the solution of the Bethe-Salpeter equation to construct a self-energy that describes the scattering of electrons and magnons. The resulting renormalized band structures exhibit strong spin-dependent lifetime effects close to the Fermi energy. We also see kinks in the electronic bands, which we attribute to electron scattering with spatially extended spin waves.

[1] Müller *et al.*, Phys. Rev. B **94**, 064433 (2016).

HL 55.9 Wed 12:45 GER 38

Charged supercells revised: Small Polarons in Oxides with proper account for long-range polarization — •Sebastian Kokott, Sergey V. Levchenko, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, DE

Formation of small polarons (excess charges localized within one unit cell) often determines charge mobility and optical absorption in oxide materials. In this work, we address two important challenges in the DFT description of small polarons: sensitivity to the errors in exchange-correlation (XC) treatment and finite-size effects in supercell calculations. The polaron properties are obtained using a modified neutral potential-energy surface (PES) [1]. Using the hybrid HSE functional and considering the whole range $0 \leq \alpha \leq 1$ of exact exchange, we show that the modified PES model significantly reduces the dependence of the polaron level and binding energy in MgO and TiO_2 on the XC treatment. It does not eliminate the dependence on supercell size. Based on Pekar's model [2], we derive the proper long-range behavior of the polaron and a correction that allows to obtain the polaron properties in the dilute limit (tested for supercells containing up to 1,000 atoms). The developed approach reduces drastically the computational time for exploring the polaron PES, and gives a consistent description of polarons for the whole range of α. It allows us to find a self-trapped hole in MgO that is noticeably more stable than reported previously.—[1] B. Sadigh *et al.*, PRB **92**, 075202 (2015); [2] S.I. Pekar, ZETF **16**, 335 (1946). This work received funding from the Leibniz ScienceCampus "GraFOx".

HL 56: Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - IV

Time: Wednesday 10:30–13:00 Location: GER 38

Invited Talk HL 56.1 Wed 10:30 GER 38

Electronic excitations in 2D materials and heterostructures — •Kristian Sommer Thygesen — Technical University of Denmark, Lyngby, Denmark

Atomically thin two-dimensional (2D) materials have recently emerged as a new class of materials with unique and highly tunable optoelectronic properties. Different 2D crystals can be stacked to form van der Waals heterostructures (vdWH) where the individual 2D layers are held together by weak van der Waals forces leading to atomically well-defined interfaces. This fascinating scenario opens up the possibility of designing heterostructures with tailored electronic or optical properties. I will give a general introduction to the electronic properties of 2D materials, including characteristic features of their dielectric screening and collective excitations with special emphasis on the challenges related to their ab-initio description. I will show how the dielectric function of a given 2D material can be controlled by embedding it into a vdWH, and how this in turn can be used to control the band structure, exciton binding energies or the plasmon dispersion in 2D materials.

HL 56.2 Wed 11:00 GER 38

Charge and energy transport at the nanoscale: A DFT perspective — •Florian G. Eich, Fabio Covito, and Angel Rubio — Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, D-22761 Hamburg, Germany

Understanding the interplay between charge and energy transport at the nanoscale paves the way for novel thermoelectric devices, which may prove useful for the development for sustainable energy sources. However, concepts, such as heat flow, temperature and entropy are only well-established at the macroscopic level for slow dynamics. This raises the question about whether these concepts can be employed for small length and short time scales. We will present our recent efforts to use a time-dependent density-functional theory framework, dubbed nonequilibrium thermal DFT, in order to generalize temperature and heat or energy flow to the microscopic regime. To this end we will highlight the analogy of the formally exact microscopic equations of motion for charge density and energy density in thermal DFT to the macroscopic equations of motion of hydrodynamics. Furthermore, we will present first result using our approach to compute transient energy energy currents induced by a temperature gradient and show that in the steady-state limit persistent temperature oscillations develop.

HL 56.3 Wed 11:15 GER 38

Conductance of aromatic and antiaromatic molecular circuits — Narendra P. Arasu and •Héctor Vázquez — Inst. of Physics, Academy of Sciences of the Czech Rep., CZ

Molecular structures with delocalized conjugated orbitals play an essential role in molecular transport due to their high conductance and small attenuation factors. While much work has been done on aromatic molecules, some studies have shown that conductance actually decreases with aromaticity [1].

In this talk I will discuss the effect of (anti)aromaticity on conductance. I will show results of first-principles transport calculations for an aromatic-antiaromatic pair of molecules and compare with experiment. Conductance is calculated using DFT and NEGF including corrections to the DFT level positions. The corrected conductance values are in very good agreement with experiment. We find that the conductance of the antiaromatic molecule is much higher than that of its aromatic counterpart. Calculations show this to be a consequence of the smaller HOMO-LUMO gap of the antiaromatic complex as well as on the molecular level alignment at the junction [2].

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[2] S. Marqués-González, S. Fujii, J.-Y. Shin, H. Shinokubo, N.P. Arasu, H. Vázquez and M. Kiguchi, (to be submitted).

HL 56.4 Wed 11:30 GER 38

Current-induced cooling of Carbene-based molecular junctions: role of electrodes structure — •Giuseppe Foti and Héctor Vázquez — Institute of Physics, Czech Academy of Sciences Cukrovarnicka 10, Prague 6

In this talk I will present our first principles calculations based on density functional theory (DFT) plus Nonequilibrium Green's functions (NEGF) of the current-induced heating and cooling dynamics of a series of Carbene-based molecular junctions [1]. I will show how the atomistic details of electrode terminations have a strong impact on the heating dynamics of the junctions and how they can maximize the cooling of the system. In the cases where the molecule is attached to blunt leads and the electronic coupling to bulk states is strong the cooling efficiency of the most active vibrational modes decreases monotonically as bias increases. This results in the heating of the junction. On the other hand, when the molecule is connected to sharp electrode terminations such as chain-like structures, which can be formed experimentally when the metal-molecule bond is mechanically strong, and the electronic coupling to electrode states is weak, the cooling efficiency shows a non-monotonic behavior. It first decreases as a function of voltage but then increases at relatively high biases, effectively cooling down the junction [2]. These results reveal the important role of the atomistic structure of metal-molecule interface in the current-induced damping of localized molecular vibrations.

[1] Foti, G.; Vázquez, H. Nanotechnology 2016, 27, 125702.

[2] Foti, G.; Vázquez, H. submitted

HL 56.5 Wed 11:45 GER 38

DFTB-based recursive Green's function algorithms for electron transport in quasi-1D systems — •Fabian Teichert[1,2,4], Andreas Zienert[3,4], Jörg Schuster[4], and Michael Schreiber[2] — [1]Dresden Center for Computational Materials Science (DCMS), Dresden, Germany — [2]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany — [3]Center for Microtechnologies (ZfM), Technische Universität Chemnitz, Chemnitz, Germany — [4]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany

Within the last decades, quantum transport theory and density functional theory have become very important for predicting the electronic properties of new materials and future electronic devices.

We focus on the problem of improving quantum transport algorithms for large quasi-1D systems which are enormously time-consuming today. We combine the density functional tight binding (DFTB) approach with the recursive Green's function formalism (RGF), which is very effective for such systems. First, we show how to improve the RGF for the case of randomly distributed real defects. For this, we use the steps of the renormalization decimation algorithm (RDA), which is part of the electrode calculation. Second, we show how to improve the calculation of the surface Green's functions of electrodes which have a long unit cell. Here, we employ the decimation technique to reduce the dimensionality of the periodic Hamiltonian matrix, leading to effective matrices, which are treated by the RDA. Finally, we apply these algorithms to carbon nanotubes and present our results.

HL 56.6 Wed 12:00 GER 38

Conditions for formation of two-dimensional electron gas at the $LaFeO_3/SrTiO_3$ — •Igor Maznichenko[1], Sergey Ostanin[1], Arthur Ernst[2], Ingrid Mertig[1,2], Katayoon Mohseni[2], Holger L. Meyerheim[2], Eberhard K.U. Gross[2], Pengfa Xu[3], Wei Han[3], Philip M. Rice[3], Jaewoo Jeong[3], Mahesh G. Samant[3], and Stuart S.P. Parkin[2,3] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [3]IBM Almaden Research Center, 650 Harry Road, San Jose, California 95120, USA

The formation of a conducting two dimensional electron gas (2DEG) at the interface between two insulating oxide layers was explained theoretically for atomically and chemically abrupt interfaces via polar discontinuity.

Here we show that a 2DEG is formed at the interface between thin layers of lanthanum ferrite, $LaFeO_3$ (LFO), that are more than 3 unit cells thick, when grown epitaxially on $SrTiO_3$ (STO) (001). The interface property highly depends on the surface property of TiO_2 terminated STO. The interface is conducting if the STO is not annealed in an oxygen environment prior to the LFO growth, while insulating if the STO is annealed.

First principles calculations reveal that a 2DEG should be realized for an ideal interface but that modest chemical intermixing suppresses it. These calculations also show that the presence of oxygen vacancies supports 2DEG formation due to electronic doping.

HL 56.7 Wed 12:15 GER 38

Thermal Renormalization of the Electronic Structure: Trends across Chemical and Structural Space — •Honghui Shang[1], Christian Carbogno[1], Patrick Rinke[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Aalto University, Helsinki, Finland

Advances in electronic structure theory now allow us to compute the renormalization of the electronic structure due to thermal nuclear motion from first principles [1]. In this work, we present a systematic computational assessment of this renormalization for 82 octet binaries in both the zincblende and the rocksalt structure. After validating our computational approach that is based on finite-differences [2] and Fröhlich-type corrections [3] for polar materials, we discuss and analyze the observed trends: For instance, we find that most materials exhibit the expected band-gap reduction upon temperature increase; however, some materials (e.g. CuCl and CdO) do not follow this trend and exhibit the opposite behavior. We discuss the underlying electronic mechanism as well as its dependence on the chemical composition and structure of the material. In this context, also the sensitivity of such calculations with respect to the chosen basis set and exchange-correlation functional (LDA, PBE, HSE06) are critically investigated.
[1] F. Giustino, arXiv:1603.06965 (2016).
[2] G. Antonius, *et al. Phys. Rev. Lett.* **112**, 215501 (2014).
[3] J. P. Nery and P. B. Allen, *Phys. Rev. B* **94**, 115135 (2016).

HL 56.8 Wed 12:30 GER 38

Spin-wave excitations and electron-magnon scattering from 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

We study the spin excitations and the electron-magnon scattering in bulk Fe, Co, and Ni within the framework of many-body perturbation theory as implemented in the full-potential linearized augmented-plane-wave method. Starting from the *GW* approximation we obtain a Bethe-Salpeter equation for the magnetic susceptibility treating single-particle Stoner excitations and magnons on the same footing. 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 theorem and present an approach that implements the magnetic susceptibility using a renormalized Green function instead of the non-interacting one, leading to a substantial improvement of the Goldstone-mode condition [1]. Finally, we employ the solution of the Bethe-Salpeter equation to construct a self-energy that describes the scattering of electrons and magnons. The resulting renormalized band structures exhibit strong spin-dependent lifetime effects close to the Fermi energy. We also see kinks in the electronic bands, which we attribute to electron scattering with spatially extended spin waves.
[1] Müller *et al.*, Phys. Rev. B **94**, 064433 (2016).

HL 56.9 Wed 12:45 GER 38

Charged supercells revised: Small Polarons in Oxides with proper account for long-range polarization — •Sebastian Kokott, Sergey V. Levchenko, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, DE

Formation of small polarons (excess charges localized within one unit cell) often determines charge mobility and optical absorption in oxide materials. In this work, we address two important challenges in the DFT description of small polarons: sensitivity to the errors in exchange-correlation (XC) treatment and finite-size effects in supercell calculations. The polaron properties are obtained using a modified neutral potential-energy surface (PES) [1]. Using the hybrid HSE functional and considering the whole range $0 \leq \alpha \leq 1$ of exact exchange, we show that the modified PES model significantly reduces the dependence of the polaron level and binding energy in MgO and TiO_2 on the XC treatment. It does not eliminate the dependence on supercell size. Based on Pekar's model [2], we derive the proper long-range behavior of the polaron and a correction that allows to obtain the polaron properties in the dilute limit (tested for supercells containing up to 1,000 atoms). The developed approach reduces drastically the computational time for exploring the polaron PES, and gives a consistent description of polarons for the whole range of α. It allows us to find a self-trapped hole in MgO that is noticeably more stable than reported previously.—[1] B. Sadigh *et al.*, PRB **92**, 075202 (2015); [2] S.I. Pekar, ZETF **16**, 335 (1946). This work received funding from the Leibniz ScienceCampus "GraFOx".

HL 57: Organic Photovoltaics and Electronics II (joined session with CPP)

Time: Wednesday 14:45–17:45 Location: POT 81

HL 57.1 Wed 14:45 POT 81

singlet fission process of organic molecules attached to neon clusters — •shahareh izadnia, aaron laforge, and frank stienkemeier — Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

Charge and excitation transfer along with the corresponding decay and loss mechanism are fundamental aspects in light harvesting, organic photovoltaics, and optoelectronic devices.

In particular, singlet fission is a unique decay mechanism where a molecule excited to its singlet state can partially transfer its energy to a neighboring ground state molecule, and thereby create two molecules excited to a triplet state. As such, singlet fission can increase the efficiency of organic electronics and photovoltaic by creating multiple charge carriers from one single photon. Here, we report a systematic study of acene complexes attached to the surface of neon clusters. Depending on the system parameters, singlet fission and other lifetime reduction mechanisms are observed.

HL 57.2 Wed 15:00 POT 81

Novel Organic NIR Detector Class Based on Charge-Transfer Absorption — •Bernhard Siegmund, Andreas Mischok, Johannes Benduhn, Olaf Zeika, Sascha Ullbrich, Frederik Nehm, Donato Spoltore, Hartmut Fröb, Christian Körner, Karl Leo, and Koen Vandewal — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Technische Universität Dresden, Dresden, Germany

Blending two organic species on a molecular level can introduce interfacial states which allow to absorb far below their optical gap. Although such intermolecular charge-transfer (CT) states form an important recombination path in organic solar cells, their near-infrared (NIR) absorption properties have been unused for photo-sensitive devices up to now. In this presentation, we disclose a new resonant optical cavity device architecture enabling NIR photodetection by means of efficient CT absorption. We demonstrate tunable detection wavelengths between 810nm and 1550nm with a single material blend, far below the optical gap of both donor and acceptor. The combination of spectral narrowband detection and broad tunability make this novel, flexible and potentially visibly transparent device principle highly suitable for integrated low cost spectroscopic NIR photodetection.

HL 57.3 Wed 15:15 POT 81

Revealing the loss mechanisms in ZnO/organic hybrid solar cells — •Moritz Eyer[1], Sebastian Kickhöfel[2], Johannes Frisch[2], Sergey Sadofev[1], Joachim Puls[1], Norbert Koch[1], Emil List-Kratochvil[2], and Sylke Blumstengel[2] — [1]Institut für Physik, Humboldt-Universität zu Berlin — [2]Inst. f. Physik, Inst. f. Chemie und IRIS Adlershof, Humboldt-Universität zu Berlin

In order to study the losses of ZnO/organic hybrid photovoltaic devices a model system of ZnMgO and poly(3-hexylthiophene) (P3HT) is introduced. It allows tuning the interface band gap energy between the ZnMgO conduction band minimum and the P3HT HOMO systematically by varying the Mg content in the inorganic component. This enables a profound study of charge separation and recombination processes at the interface of inorganic/organic hybrid heterojunctions.

Prior to full charge separation electron and hole on opposite sides of the interface form hybrid charge transfer excitons (HCTX) bound by Coulomb interaction [1]. Electroluminescence measurements in the

near IR spectral range confirm the existence of HCTX and yield valuable information of their physical properties. Temperature dependent photovoltaic measurements provide the necessary information to understand the charge separation process and its influence on the parameters defining the performance of a photovoltaic device. A detailed study of the interface energetics allows quantifying the recombination losses of inorganic/organic hybrid heterojunctions in order to fully exploit their potential in solar energy.

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

HL 57.4 Wed 15:30 POT 81

Silver nanowires and polymer based transparent electrodes for Organic solar cells — •Yoonseok Park, Ludwig Bormann, Koen Vandewal, and Karl Leo — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Technische Universität Dresden, Germany

Organic photovoltaics (OPV) are prospective candidates for future renewable energy production because of their potential scalability, low cost, and flexibility. For establishing flexible organic devices, a highly transparent, conductive and flexible electrode is required, replacing ITO which is brittle and requires high temperature processes. Many alternative materials such as conductive polymers, graphene, and metal nanowires have been studied. Among these, metal nanowires, especially silver nanowire (AgNW) networks, show outstanding flexibility, conductivity, and transparency. However, AgNW network electrodes have a few basic problems: (i) a poor electrical contact between wires, resulting in a low conductivity, (ii) overlapping wires cause roughness, often resulting in electrical shorting of devices and (iii) open spaces between wires can be in the range of square micrometers. In this study, highly conductive PEDOT:PSS has been deposited on AgNW electrodes to form conductive bridges between the open spaces and to smoothen the sharp points of the network. The maximum process temperature is 120 °C. OPV cells using these AgNW / PEDOT:PSS transparent electrodes exhibit power conversion efficiencies up to 7.15%. Moreover, OPV devices on PET substrates with an alumina encapsulation and barrier adhesive show excellent mechanical flexibility.

HL 57.5 Wed 15:45 POT 81

Three-dimensional graphene-based electrodes for asymmetric supercapacitors — •Maximilian von Seckendorff[1], Simon Drieschner[1], Jörg Wohlketzetter[1], Jose A. Garrido[2], and Martin Stutzmann[1] — [1]Walter Schottky Institut und Physik-Department, Technische Universität München, Garching, Germany — [2]The Barcelona Institute of Science and Technology, Bellaterra, Spain

Three-dimensional (3D) graphene-based structures combine the outstanding physical and chemical properties of graphene such as high conductivity, mechanical stability and chemical inertness with a high surface-to-volume ratio, making them highly promising for energy storage applications in supercapacitors. Here we demonstrate the fabrication of 3D graphene-based electrodes by chemical vapor deposition using sintered copper particles and electrodeposited nickel/copper alloys as catalytic metal substrates. After selective wet chemical etching of the metal scaffold, a freestanding graphene foam of high structural quality as confirmed by Raman spectroscopy is obtained. In an asymmetric supercapacitor, this graphene foam is used as the cathode and is combined with a graphene foam coated with pseudocapacitive elements such as manganese dioxide as the anode. This combination results in an extended electrochemical potential window above 1.5 V and, therefore, a higher energy density ($>$ 5 Wh/kg) compared to symmetric supercapacitors. The electrochemical performance of this asymmetric capacitor is investigated by cyclic voltammetry, electrochemical impedance spectroscopy, and charge-discharge-measurements and confirms its great potential for energy storage applications.

Coffee Break

HL 57.6 Wed 16:30 POT 81

Semitransparent Electrodes for Evaporated Small Molecule Organic Solar Cells — •Dhriti Sundar Ghosh and Karl Leo — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), TU Dresden

Transparent Electrodes are key in novel flexible devices. We report a highly efficient microcavity assisted small molecule organic solar cell (SM-OSC), containing an indium-free semitransparent TiO2(30nm)/Ag 9nm based transparent electrode with average visible transmittance of 66.7% and sheet resistance of 6.3 Ohm/sq. The electrode also consisted of a wetting layer of polyethyleneimine which promotes the growth of ultrasmooth, and highly conductive Ag films even at very low thicknesses. The role of high index TiO2 undercoat layer is investigated in detail by optical simulations and is shown to enhance the microcavity effect, leading to increased light coupling into the photoactive layer. With comparable photocurrent, and high fill-factor values owing to much better electrical properties, the semitransparent electrode based SM-OSC outperforms the state-of-art indium tin oxide (ITO) based reference device with photon conversion efficiency of 8.1% compared to 7.7% despite having lower transmittance (˜21%) relative to ITO. This work demonstrates that a properly designed semitransparent TE is a promising alternative to ITO and can lead to more efficient photovoltaic devices.

HL 57.7 Wed 16:45 POT 81

Intereference-induced thermoelectric effects in topological states of matter — •Flavio Ronetti[1,2], Luca Vannucci[1,2], Giacomo Dolcetto[3], Matteo Carrega[4], and Maura Sassetti[1,2] — [1]Dipartimento di Fisica, Università di Genova,Via Dodecaneso 33, 16146, Genova, Italy. — [2]CNR-SPIN, Via Dodecaneso 33, 16146, Genova, Italy. — [3]Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg. — [4]NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, I-56127 Pisa, Italy.

In topological states of matter, such as edge states of quantum Hall systems and two-dimensional topological insulators, protection from backscattering guarantees phase-coherent ballistic transport, allowing for the observation of quantum interference effects. Intriguing thermoelectric properties can be achieved by exploiting the phase-coherent edge states of two quantum Hall systems coupled by tunnelling region. Considering a multiple quantum point contacts geometry, interference paths effectively break the electron-hole symmetry. Therefore, when the systems are driven out of equilibrium by a thermal gradient, a thermoelectric charge current can be induced. Correspondingly, an interference pattern in the heat current is predicted. In the case of two-dimensional topological insulators, the presence of spin degree of freedom give rise to a rich tunnelling dynamics. In a double quantum point contact geometry, the effective transmission related to spin-flipping processes acquires a functional dependence on energy in the interacting regime, thus generating a thermoelectric spin current in response to a thermal gradient.

HL 57.8 Wed 17:00 POT 81

Organic thermoelectrics based on low-dimensional molecular metals — •Alexander Steeger[1], Florian Huewe[1], and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Efficient recovery of waste heat by thermoelectric generators (TEGs) requires low-cost materials exhibiting high electrical conductivities σ and Seebeck coefficients S, but low thermal conductivities κ. The suitability of a given material for thermoelectric applications is quantified by the dimensionless figure of merit $zT = \sigma S^2 T/\kappa$. In this contribution, we propose crystalline low-dimensional molecular metals as an alternative class of organic thermoelectric materials combining the advantages of low weight, chemical variety, sustainability, high charge carrier mobility and reduced electronic dimensionality with the availability of p- and n-type conductors. For the first time, we determined all physical quantities contributing to zT on exclusively one single crystal sample of p-type TTT_2I_3 and n-type $(DMe\text{-}DCNQI)_2Cu$, revealing high power factors and promising figures of merit surpassing $zT \geq 0.15$ below 40 K. The thermoelectric performance of low-dimensional metals is affirmed by the power output per active area of a prototypical all-organic TEG reaching values of ~mW/cm^2 and could be further increased by taking full control over the amount of charge-transfer and band filling. Financial support by the DFG (Project No. PF385/6-1) and the FP7 (H2ESOT, Project No. 308768) of the European Commission is gratefully acknowledged.

HL 57.9 Wed 17:15 POT 81

Ag-segregation at dislocations and grain boundaries in annealed PbTe thermoelectric materials studied by atom probe tomography — •Yuan Yu[1], Oana Cojocaru-Mirédin[1], Yaron Amouyal[2], Ariel Sheskin[2], and Matthias Wuttig[1] — [1]I. Physikalisches Institut (IA), RWTH Aachen, 52074, Aachen, Germany — [2]Technion-Israel Institute of Technology, 32000 Haifa, Israel

PbTe-based alloys play a significant role in thermoelectric (TE) applications. The figure-of-merit, ZT, of standard PbTe is near 1, whereas

for PbTe alloys doped with Sr, Na, K, and Ag, the ZT factors are larger than 2. The large enhancement of ZT values mainly benefits from the elemental doping-induced band modification and nano-precipitation. However, the effects of these dopants on the TE properties is still not well understood mainly due to the difficulty to track the impurity redistribution in 3D with traditional characterization techniques. Here, we investigated the distribution of Ag in PbTe TE material using 3D atom probe tomography. We clearly find that the Ag is prone to form platelet-like nanostructures with diameters of ~15 nm and thickness of ~3 nm in the as-quenched state. After annealing at 380 °C for 48 h, these platelet-like nanostructures dissolve in the matrix, leading to a Ag-supersaturated matrix. Thus, the Ag tends to segregate at the dislocations and grain boundaries. These Ag-decorated dislocations and grain boundaries as well as the remaining stable Ag-rich nanoprecipitates are believed to influence the electron and phonon transport processes. Our results can help to better tailor the structures and provide more information for the theoretical calculation.

HL 57.10 Wed 17:30 POT 81

Potassium Prussian Blue Nanoparticles: A Low-cost Cathode Material for Potassium-ion Batteries — •Yang Xu, Min Zhou, Liying Liang, and Yong Lei — Institute für Physics & IMN MacroNano (ZIK), Technische Universität Ilmenau, Ilmenau 98693, Germany

Potassium-ion batteries (KIBs) in organic electrolytes hold great promise owing to the abundance of potassium, close redox potential to lithium, and similar electrochemistry with lithium system. Investigations of KIB cathodes have been scarcely reported so far. We for the first time report hydrated potassium Prussian blue K0.220Fe[Fe(CN)6]0.805 nanoparticles as a potential cathode material. The cathode exhibits a high discharge voltage of 3.1~3.4 V, high reversible capacity of 73.2 mAh g-1, and great cyclability with a very small capacity decay rate of ~0.09% per cycle. Electrochemical reaction mechanism analysis identifies the carbon-coordinated FeIII/FeII couple as redox-active site and proves structural stability of the cathode during charge/discharge. Furthermore, we present a KIB full-cell by coupling the nanoparticles with commercial carbon materials. The full-cell delivers a capacity of 68.5 mAh g-1 at 100 mA g-1 and retains 93.4% of the capacity after 50 cycles. Considering the low cost and material sustainability, this work may trigger future attention on rechargeable KIBs.

Reference

C. Zhang, Y. Xu, M. Zhou, L. Liang, H. Dong, M. Wu, Y. Yang, Y. Lei, Adv. Funct. Mater. 2016, DOI: 10.1002/adfm.201604307.

HL 58: Quantum Dots: Optical Properties IV

Time: Wednesday 14:45–18:15 Location: POT 151

Invited Talk HL 58.1 Wed 14:45 POT 151

Towards an ideal semiconductor source of polarization entangled photons — •Fei Ding — Institute for Solid State Physics, Leibniz Universität Hannover, Germany — Institute for Integrative Nanosciences, Leibniz Institute for Solid State and Materials Research Dresden, Germany

Sources of polarization entangled photons are important components for building optical quantum networks [1]. Semiconductor quantum dots (QDs) are among the most promising sources due to several undeniable advantages. However, they are far from being ideal and several critical challenges need to be solved for practical applications.

In this talk I will review our recent efforts in developing a high yield, high fidelity and wavelength-tunable entangled photon sources. A large ensemble of as-grown entangled photon emitters can be obtained with a yield close to 100% and high entanglement fidelity (up to 0.9) [2]. The wavelength mismatching between different source can be solved by using a unique strain tuning technique [3,5]. The superior properties of these sources, combined with the possibilities of electrical injection [5] and on-chip integration [6], will eventually lead to the development of an ideal semiconductor entangled photon source.

[1] J.W. Pan et al. Rev. Mod. Phys. 84, 777 (2012) [2] R. Keil, M. Zopf, F. Ding* et al. arXiv:1611.03717 (2016) [3] F. Ding* et al. Phys. Rev. Lett. 104, 067405 (2010) [4] Y. Chen, F. Ding* et al. Nature Commun. 7, 10387 (2016) [5] J. Zhang, F. Ding* et al. Nature Commun. 6, 10067 (2015) [6] Y. Zhang, F. Ding* et al. Nano Lett. 16, 5785 (2016)

HL 58.2 Wed 15:15 POT 151

Linear and nonlinear spectroscopy of excitonic complexes in single self-assembled quantum dots — •Jens Kerski[1], Annika Kurzmann[1], Amran Al-Ashouri[1], Patrick A. Labud[2], Arne Ludwig[2], Andreas D. Wieck[2], Martin Geller[1], and Axel Lorke[1] — [1]Faculty of Physics and CENIDE, Universität Duisburg-Essen, Germany — [2]Chair of Applied Solid State Physics, Ruhr-Universität Bochum, Germany

The maximum resolution of images taken with an optical setup is given by *Abbe's diffraction limit*. This can be overcome by using nonlinear processes as demonstrated by the semiconductor industry and in STED-microscopy.

In this work, we use linear and nonlinear photoluminescence spectroscopy to image a single self-assembled InAs/GaAs quantum dot (*QD*). In self-assembled QDs the recombination intensity of different excitonic radiative transitions depends nonlinearly on the excitation power. Due to this nonlinearity, we show here an increased spatial resolution of the optical imaging of a single QD. The experimental results are supported by empirical simulations, implemented for this work. This mechanism can easily be adapted to nanoparticles and other systems which exhibit a nonlinear dependence of their emitted radiation on the excitation power. Furthermore, an unexpected effect is observed indicating a specific angle dependence of the radiations of different excitonic states.

HL 58.3 Wed 15:30 POT 151

InGaAs quantum dots as light source for silicon photonics — •Norbert Witz, Matthias Paul, Jan Kettler, Michael Jetter, Simone L. Portalupi, and Peter Michler — IHFG, IQST Center and SCoPE, University of Stuttgart

One of the greatest needs of silicon photonics is an efficient light source, since many other functionalities have been already demonstrated and optimized. Indeed, being an indirect bandgap material, the photon emission in silicon is a three particle process thereby resulting in low efficient light emission. An attractive alternative is found in III/V semiconductor materials, which exhibit excellent optical properties. Especially semiconductor quantum dots (QDs) are promising candidates for this task. Adjusting the growth conditions, it is possible to tailor QD size and shape so that the emission wavelength shifts into the telecom O- or C-band at 1.3μm or 1.55μm. Because of the large lattice mismatch, monolithical growth of III/V materials on silicon substrate causes the formation of defects, which could prevent the efficient photon emission from the QDs. To evade this problem, III/V light sources grown by metal-organic vapour-phase epitaxy (MOVPE) have been directly glued onto a silicon chip. The emitted light is coupled into a single-mode waveguide by a diffractive Bragg grating, optimized for the spectral range of the glued sample. In order to fabricate a compact device, it is inevitable to excite the light source electrically. For this reason electrically pumped samples, with InGaAs QDs serving as an active medium have been developed.

HL 58.4 Wed 15:45 POT 151

Deterministic integration of quantum dots into on-chip waveguides and beamsplitters by in-situ electron beam lithography — •Peter Schnauber[1], Oliver Kirsch[1], Ronny Schmidt[1], Arsenty Kaganskiy[1], Andre Strittmatter[2], Sven Rodt[1], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany — [2]Abteilung für Halbleiterepitaxie, Otto-von-Guericke Universität, 39106 Magdeburg, Germany

On-chip waveguides and beamsplitters have proven to be suitable to realize basic quantum logic circuits. Moreover, quantum dots (QDs) can be integrated into such on-chip elements to act as quantum light sources. In order to efficiently couple the QD's emission into a waveguide, the QD's lateral position inside a thin waveguide must be precisely controlled. When integrating multiple QDs in complex waveguide circuits it is important to preselect and fine-adjust their emission

wavelength to achieve for instance two-photon interference which is necessary for quantum gate operation. A spatially and spectrally deterministic integration of QDs into waveguides can be achieved by in-situ electron beam lithography (EBL)[1]. By applying our method, QDs are preselected by means of helium-temperature cathodoluminescence spectroscopy right before waveguides and beamsplitters are patterned in-situ with the naturally high resolution of EBL. Special care is taken to optimize the surface roughness of such low-temperature-patterned structures.

[1] M. Gschrey et al., Nat. Commun. 6, 7662 (2016)

HL 58.5 Wed 16:00 POT 151

Influence of morphology on InAlGaAs quantum dots emitting at telecom wavelength — •Christian Carmesin[1], Marco Schowalter[2], Vitalii Sichkovskyi[3], Mohamed Benyoucef[3], Daniel Mourad[1], Michael Lorke[1], Tim Grieb[2], Knut Müller-Caspary[2], Johann Peter Reithmaier[3], Andreas Rosenauer[2], and Frank Jahnke[1] — [1]Institute for Theoretical Physics, University of Bremen — [2]Institute of Solid State Physics, University of Bremen — [3]Institute of Nanostructure Technologies and Analytics, University of Kassel

Self-organized quantum dots are promising candidates for the realization of deterministic single photon sources with high repetition rate and tunable emission energy due to the advantage of integrability into electrical devices. We have characterized a new and promising material system of InAs/InAlGaAs/InP based quantum dots and identified dominant contributions to the connection between morphology and optical properties. For this purpose, experimentally determined photoluminescence spectra are compared to results of atomistic tight-binding calculations using a one hundred million atom supercell. Structure und composition characteristics of the system are obtained from high-resolution scanning transmission electron microscopy of a single representative quantum dot. We have identified concentration fluctuations among different quantum dots of the ensemble as the main source of inhomogeneous broadening.

Coffee Break

HL 58.6 Wed 16:45 POT 151

Inversion of permanent exciton dipole moment in self-assembled In(Ga)As quantum dots by nonlinear piezoelectricity — Johannes Aberl[1], •Petr Klenovsky[2,3], Johannes S. Wildmann[1], Javier Martin-Sanchez[1], Thomas Fromherz[1], Eugenio Zallo[4,5], Josef Humlicek[2,3], Armando Rastelli[1], and Rinaldo Trotta[1] — [1]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, Altenbergerstraße 69, A-4040 Linz, Austria — [2]Department of Condensed Matter Physics, Masaryk University, Kotlářská, CZ-61137 Brno, Czech Republic — [3]Central European Institute of Technology, Masaryk University, Kamenice 753/5, CZ-62500 Brno, Czech Republic — [4]Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstraße 20, D-01069 Dresden, Germany — [5]Paul-Drude-Institut für Festkörperelektronik, Hausvogteilplatz 5-7, 10117 Berlin, Germany

We show tuning of the electric dipole moment of excitons confined in self-assembled In(Ga)As quantum dots by anisotropic biaxial stress up to complete erasure of its magnitude and inversion of its sign. We attribute this effect to the piezoelectricity due to applied stress, the magnitude of which we estimate using a simple model based on the piezotronic effect. Self-consistent $\vec{k}.\vec{p}$ calculations reveal that the strain-induced changes of the dipole moment in our QDs that we observe can be only accounted for by the nonlinear piezoelectric effect, the importance of which in QD-physics has been theoretically recognized but it proved to be difficult to single out experimentally.

HL 58.7 Wed 17:00 POT 151

Two-photon interference from deterministically fabricated remote quantum dot microlenses — •Peter Schnauber[1], Alexander Thoma[1], Jonas Boehm[1], Manuel Gschrey[1], Jan-Hindrik Schulze[1], Andre Strittmatter[2], Sven Rodt[1], Tobias Heindel[1], and Stephan Reitzenstein[1] — [1]Institut fuer Festkoerperphysik, Technische Universitaet Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany — [2]Abteilung fuer Halbleiterepitaxie, Otto-von-Guericke Universitaet, 39106 Magdeburg, Germany

Two-photon interference (TPI) is of fundamental importance for the realization of quantum communication schemes such as the quantum repeater. Here, we report on TPI experiments in Hong-Ou-Mandel configuration using deterministically fabricated, remote single-photon sources [1]. By using 3D in-situ electron-beam lithography, we fabricate quantum-light sources at desired wavelengths by integrating preselected semiconductor quantum dots into monolithic microlenses. Exciting the quantum dot microlenses into their p-shell at 80 MHz, the individual "single photon" sources exhibit TPI visibilities of 49 % and 22 %, respectively. When examining the TPI of photons emitted by two remote sources, we measure an uncorrected TPI visibility of 29 %. This agrees with the visibility predicted from the dephasing of the individual emitters. Due to the broadband increase in photon extraction efficiency (> 20 nm), quantum dot microlenses are a promising technology platform for future entanglement swapping experiments employing entangled photon pairs from remote biexciton-exciton radiative cascades.

[1] A. Thoma et al., arXiv:1611.06859, 2016

HL 58.8 Wed 17:15 POT 151

Coherent Control of a Photonic Crystal Microresonator with Electric Readout — Wadim Quiring[1], •Björn Jonas[1], Jens Förstner[1], Ashish K. Rai[2], Dirk Reuter[1], Andreas D. 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 coherent two pulse experiments on GaAs photonic crystal microresonators. The MBE-grown structures have a membrane, which is designed as a n-i layer with an embedded InGaAs quantum well. Metallic contacts with 50 nm dimensions have been processed by e-beam lithography in order to realize a local Schottky gate on the central part of the microresonator. The resulting structures allow for photocurrent detection of cavity excitations at Q-factors around 5000. [1] Resonant and detuned two-pulse ps-laser excitation is used for the coherent excitation and manipulation of the cavity, which is monitored by photocurrent detection via the built-in quantum well. We are able to measure the amplitude and phase of the cavity excitation as a function of the detuning. Our experimental findings are well described by an analytical theory, in which the cavity is treated as a dissipative two-level system. We further show, that our phase sensitive experiments can also be successfully performed at room temperature, which makes real-world applications of cavity based phase control and frequency discrimination feasible.

[1] W. Quiring et al., Appl. Phys. Lett. 107, 041113 (2015)
[2] W. Quiring et al., Optics Express 24, 20672 (2016)

HL 58.9 Wed 17:30 POT 151

Towards the optimization of photodetectors based on ZnO nanowires functionalized with Carbon Nanoparticles (C-Dots) — •Kseniia Zimmermann[1], Davide Cammi[1], Rene Gorny[1], Angelina Vogt[1], Frank Dissinger[2], Siegfried Waldvogel[2], and Tobias Voss[1] — [1]Braunschweig, Institut für Halbleitertechnik, Germany — [2]Johannes Gutenberg-Universität Mainz, Institut für Organische Chemie, Germany

Carbon nanoparticles (C-dots) have been first discovered in 2004 by Xu. et al. as a side product during the synthesis of single-wall carbon nanotubes. Since then, they have gained huge attention due to their tunable optical properties, low toxicity and the availability of a variety of relatively easy preparation methods. Today, C-dots are considered to be promising candidates for color conversion in LEDs, as well as further applications in pharmacy and photonic. In this work, the optical properties of different colloidal carbon dots have been investigated and it has been found, that the absorption and emission properties strongly depend on the stabilizing (ligand) molecules, the nature of the solvent and the pH-value of the solution. The C-Dots were subsequently attached to the surface of hydrothermally grown ZnO nanowires in order to study electron transfer processes in the hybrid system. Compared to unfunctionalized nanowires, we have observed enhanced photoconductivity in the hybrid devices under irradiation with photon energies below the band gap energy of the ZnO nanowires, down to 2.1 eV. Such hybrid organic/inorganic structures may be used for light-harvesting and in photodetectors.

HL 58.10 Wed 17:45 POT 151

An electrically controlled single-photon source driven by an on-chip integrated quantum dot microlaser — •Pierce Munnelly[1], Tobias Heindel[1], Martin Kamp[2], Sven Höfling[2], Christian Schneider[2], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universtität Berlin, Germany — [2]Technische Physik, Universität Würzburg, Würzburg, Germany

Quantum dot micropillar cavities are of great interest with respect the realization of high-β microlaser and non-classical light sources. Beyond this, they can also act as active elements in integrated quantum optics schemes, in which they can be monolithically fabricated together with other electro-optical components to form, for instance, compact, resonantly driven single photon sources.
In the present work, we report on an electrically triggered, monolithically integrated whispering gallery mode (WGM) laser which drives a c-QED enhanced single photon source (SPS) on a chip. In our concept, lateral emission from the WGM laser excites a quantum dot in a laterally displaced (by 10 μm) micropillar cavity which acts as an efficient, vertically emitting SPS. Via an additional electrical contact applied to the displaced micropillar, we are able to eletro-optically control the SPS via the quantum-confined Stark effect. In this configuration we demonstrate fast spectral resonance tuning and triggered single photon emission of an on-chip driven quantum dot micropillar cavity.

HL 58.11 Wed 18:00 POT 151

Degradation of semiconductor nanowire lasers upon optical pumping — •Maximilian Zapf, Robert Roeder, and Carsten Ronning — Institute of Solid State Physics, Friedrich Schiller University Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Semiconductor nanowires (NWs) are promising candidates for nanoscale coherent light sources in future optoelectronic devices, as they inherently provide the necessary compounds of a laser system such as optical gain and a resonator-like structure. The optical output intensity of a semiconductor NW follows the pump power dependency of a multimode laser system upon moderate optical pumping [Geburt et al., Nanotechnology 23, 365204 (2012)]. However, for extremely high pump powers a material degradation of the laser gain material induces an unambiguous deviation from this dependence. Yet, experiments and future applications require a degradation-free lasing operation in order to retain reliable and durable devices. Thus, we developed a method for identifying the threshold value of any degradation process and its underlying physics. Furthermore, a critical temperature for a NWs' applicability as nano laser can be determined by evaluating the temperature dependence of both the lasing and the degradation threshold.

HL 59: Nitrides: Preparation and Characterization II

Time: Wednesday 14:45–17:45 Location: POT 251

HL 59.1 Wed 14:45 POT 251

High Temperature Vapor Phase Epitaxy of GaN - Investigation of defect related UV luminescence — •Friederike Zimmermann[1], Franziska C. Beyer[1], Gleb Lukin[2], Tom Schneider[2], Olf Pätzold[2], Mykhailo Barchuk[3], and Johannes Heitmann[3] — [1]Institute of Applied Physics, TU Bergakademie Freiberg, 09599 Freiberg, — [2]Institute of Nonferrous Metallurgy and Purest Materials, TU Bergakademie Freiberg, 09599 Freiberg, — [3]Institute of Materials Science, TU Bergakademie Freiberg, 09599 Freiberg,

Compared to conventional growth techniques like hydride vapor phase epitaxy and metalorganic vapor phase epitaxy point defect formation for GaN grown by high temperature vapor phase epitaxy (HTVPE) is not yet well understood. We report on a photoluminescence study on GaN grown by HTVPE with a systematic variation of Ga temperature and growth pressure.

Photoluminescence spectra recorded at 15 K show a strong ultraviolet luminescence (UVL) with zero phonon line at 3.27 eV. The intensities of all other defect related transitions are lower by at least one order of magnitude. The high relative intensity of this donor-acceptor pair recombination can not be explained by a high concentration of acceptor impurities. Silicon and boron are the main impurities, whereas magnesium is present in the range of mid 10^{15} cm^{-3} only. Reduced Ga temperature and growth pressure result in better surface morphology and structural quality as well as a significant drop of relative UVL intensity.

HL 59.2 Wed 15:00 POT 251

Internal quantum efficiency of strain controlled semipolar GaInN/GaN quantum wells — •Fedor Alexej Ketzer[1], Philipp Horenburg[1], Heiko Bremers[1], Uwe Rossow[1], Florian Tendille[2], Philippe De Mierry[2], Philippe Vennéguès[2], Jesús Zúñiga-Pérez[2], and Andreas Hangleiter[1] — [1]Institut für Angewandte Physik, Technische Universität Braunschweig — [2]Centre de Recherche sur l'Hétéro-Epitaxie, Valbonne, France

In this contribution we report on the effect of strain manipulation on internal quantum efficiencies (IQE) of semipolar (11$\bar{2}$2) multi quantum well (MQW) structures. For strain control we use AlInN interlayers prior to the MQW structure. Due to the large range of possible lattice constants for different AlInN compositions, we can control the strain in the MQW in a wide range. Relaxation of strain in the MQW region is one of the main reasons for a lowered IQE at high indium concentrations, necessary for long emission wavelengths. We compare samples, grown via low pressure MOVPE on (11$\bar{2}$2) GaN templates grown on patterned r-sapphire substrates, with and without AlInN interlayer and different growth conditions for the MQWs. We determine the structural properties of our samples by high resolution X-ray diffraction. The IQEs are measured by temperature and excitation power dependent photoluminescence spectroscopy with resonant excitation. We observe a redshift of our strain-manipulated samples associated with an increased indium content in the quantum wells. Our samples show high IQEs of up to 44% and 30% at 300 K for emission wavelengths of 545 nm and 575 nm, respectively.

HL 59.3 Wed 15:15 POT 251

Interplay between yellow and blue luminescence bands in GaN:C — •Zahid Usman, Martin Feneberg, Andreas Lesnik, Marc P. Hoffmann, Armin Dadgar, and Rüdiger Goldhahn — Otto-von-Guericke Universität Magdeburg, Institut für Experimentelle Physik

Carbon doped GaN has attracted much attention due to its compensating nature for unintentionally introduced background electron densities. That is why a semi-insulating buffer layer of this material is often introduced in high electron mobility transistors. Photoluminescence can be a useful tool to understand the charge states of deep defects which yield different recombination channels in GaN. Here, we present photoluminescence spectra with different excitation densities, recorded on carbon and silicon co-doped GaN samples. Depending on dopant densities, the photoluminescence spectra show yellow and blue luminescence bands with different intensity ratios. For increasing pump power density the yellow luminescence band saturates at a critical excitation power density while the blue luminescence band increases further. Our results suggest that both recombination bands evolve from the deep carbon acceptor in different charge states. The yellow band is assigned to come from carbon in (-/0) state while the blue band originates from carbon in (0/+) charge state.

HL 59.4 Wed 15:30 POT 251

Time-resolved Investigation of Charge Transfer in Asymmetric Cubic $Al_{0.64}Ga_{0.36}N/GaN$ Double Quantum Wells Grown by MBE — •Tobias Wecker[1], Gordon Callsen[2], Axel Hoffmann[2], Dirk Reuter[1], and Donat Joseph As[1] — [1]Department of Physics, University of Paderborn, 33098 Paderborn — [2]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin

Non-resonant carrier transfer between quantum wells (QWs) is of high significance for many devices like quantum cascade lasers. In this study, time-resolved photoluminescence is used to investigate this effect in asymmetric double QWs for low temperatures. Asymmetric cubic $Al_xGa_{1-x}N/GaN$ double QWs with an Al content of x = 0.64 * 0.03 were grown on 3C-SiC (001) substrate by radio-frequency plasma-assisted molecular beam epitaxy. Three samples with different barrier thickness d were analyzed (1 nm, 3 nm, 15 nm). The two QWs are 2.5 nm and 1.35 nm thick, to show separated emission bands in the luminescence. Three clearly distinguishable emission bands at 3.49 eV, 3.73 eV and 4.12 eV are observed and could be assigned to the different layers. A correlation between the carrier lifetimes in the QWs and the barrier thickness is found. Exploiting rate equations the intensity ratios of both QW emissions have been calculated. Electronic coupling between the QWs is only observed for barrier thicknesses below 3 nm.

Coffee Break

HL 59.5 Wed 16:15 POT 251

Time-integrated and time-resolved luminescence studies of planar and 3D InGaN/GaN heterostructures — •Angelina Vogt[1], Jana Hartmann[1,2], Hao Zhou[1], Sönke Fündling[1,2], Hergo-Heinrich Wehmann[1,2], Andreas Waag[1,2], and Tobias Voss[1] — [1]Institute of Semiconductor Technology and Laboratory for Emerging Nanometrology, TU Braunschweig, 38092 Braunschweig — [2]Epitaxy Competence Center, ec2, 38092 Braunschweig

Three-dimensional core-shell GaN-based heterostructures with embedded InGaN quantum wells (QWs) on non-polar sidewalls are promising candidates for a novel LED architecture based on GaN material free of extended defects. In order to optimize the internal quantum efficiency (IQE) of the 3D heterostructures, a detailed knowledge of the radiative and non-radiative recombination channels and their rates is required. Here, we compare the spectrally and temporally resolved photoluminescence (PL) of InGaN/GaN 3D heterostructures with the respective data of planar InGaN/GaN structures. All heterostructures were grown by MOVPE. We used time-integrated PL measurements to analyse the homogeneity of the indium in the QWs. The luminescence dynamics of the InGaN QWs were investigated by time-resolved experiments in order to characterise the fundamental optical relaxation and recombination processes. We analyse the processes for different structures, laser photon energies and temperatures. Due to the quantum confined Stark effect (QCSE), we find a biexponential decay characteristic for the planar structures, while the 3D structures with the non-polar InGaN QWs as light-emitters show a monoexponential decay of the InGaN PL.

HL 59.6 Wed 16:30 POT 251

Depth and laterally resolved cathodoluminescence spectroscopy on Ga(In)N quatum well structures — •Matthias Hocker[1], Pascal Maier[1], Ingo Tischer[1], Tobias Meisch[2], Marian Caliebe[2], Ferdinand Scholz[2], and Klaus Thonke[1] — [1]Semiconductor Physics Group, University of Ulm — [2]Institute of Optoelectronics, University of Ulm

We present the combination of lateral and depth-resolved cathodoluminescence (CL) spectroscopy on a Ga(In)N based LED sample. It is demonstrated how the analysis of depth-resolved CL measurements can be enhanced by taking semiconductor-specific parameters such as exciton diffusion length and band gap energies into account for the corresponding Monte-Carlo simulation of the primary electron scattering. The results of the depth-resolved measurement were found to be in very good agreement with the layer thickness values expected from growth conditions. We show, how a semi-threedimensional schematic model of the sample under investigation can be reconstructed from the experimental data, and which amount of information can be obtained by this measurement method.

HL 59.7 Wed 16:45 POT 251

Photoluminescence spectroscopy of Ge-doped 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

Recently, germanium was introduced as an alternative to silicon for n-type doping of cubic GaN. We demonstrated that free carrier concentrations up to 3.7×10^{20} cm^{-3} can be obtained and the incorporation of Ge is in good agreement to the trend of the Ge vapour pressure curve in a doping range spanning several orders of magnitude [1]. In this contribution we report on the optical properties of Ge-doped cubic GaN determined by photoluminescence (PL) spectroscopy. Cubic GaN layers with nominal thicknesses of 600 nm were grown by plasma-assisted molecular beam epitaxy on 10 μm thick 3C-SiC(001)/Si(001) substrates. The Ge doping level was varied by about six order of magnitude by varying the Ge effusion cell temperature between 600 °C and 1000 °C. PL spectra were obtained for sample temperatures between 13 K and 300 K. Above a Ge concentration of approximately 2×10^{18} cm^{-3} the near band edge emission lines merge to a broad band. A donor ionization energy of about 36 meV was estimated.

[1] M. Deppe, J. W. Gerlach, D. Reuter, and D. J. As, Phys. Stat. Sol (b) (2016) (submitted)

HL 59.8 Wed 17:00 POT 251

Polarity Control of GaN Nanowires — •Max Kraut, Martin Hetzl, Theresa Hoffmann, and Martin Stutzmann — Walter Schottky Institut and Physics Department, Technische Universität München, Garching, Germany

Heteroepitaxial GaN nanowires (NWs) have gained much interest in current research. However, the nucleation process of the GaN crystals, and in particular the orientation of the polar axis of the wurtzite crystal is not fully understood yet. Inconsistent results have been reported whether N, Ga or mixed polarity is the dominant feature. This indicates a complex interplay of growth mode, substrate type and growth parameters. We have systematically investigated the polarity distribution of GaN NWs grown by molecular beam epitaxy via selective area growth (SAG). Thanks to its high chemical and physical stability, diamond (111) has been used as a model substrate to elucidate the influence of the growth parameters, namely III/V flux ratio and substrate temperature T_{sub}. The polarity of individual NWs has been identified by Kelvin Probe Force Microscopy (KPFM) which allows a statistical investigation of large NW arrays. We find that T_{sub} is the driving force for the polarity distribution of GaN NWs on diamond whereas the III/V flux ratio plays a minor role. In particular, a variation of the fraction of Ga-polar SAG GaN NWs ranging from 45% up to 90% has been achieved by adjusting T_{sub}. In the case of self-assembled NWs and a comparably elevated temperature, N polarity is found to be the dominant crystal orientation. The findings obtained on diamond are in agreement with GaN NW growth on other substrates.

HL 59.9 Wed 17:15 POT 251

Misfit strain as a control parameter in epitaxy of In-rich non- and semipolar GaInN/GaN multi quantum well structures — •Philipp Horenburg[1], Fedor Alexej Ketzer[1], Heiko Bremers[1], Uwe Rossow[1], Florian Tendille[2], Philippe De Mierry[2], Philippe Vennéguès[2], Jesús Zúñiga-Pérez[2], and Andreas Hangleiter[1] — [1]Institute of Applied Physics, TU Braunschweig, Germany — [2]Centre de Recherche sur l'Hétéro-Epitaxie, Valbonne, France

We demonstrate the role of misfit strain as an independent parameter in MOVPE growth of m-plane and (11$\bar{2}$2)-oriented, In-rich GaInN quantum wells (QWs). Reducing the misfit strain in the active zone is an essential task to improve the material quality and efficiency of light emitting structures. In order to manipulate the strain state of the QWs, we insert a metamorphic AlInN buffer layer as a growth template for the active zone. With the buffer layer being partially relaxed towards larger in-plane lattice constants, the lattice mismatch at a given In composition of the GaInN is reduced as compared to GaN as a template. As a consequence, we see a decrease of the strain energy in the QWs as compared to samples without AlInN under identical QW growth conditions. We further see evidence for an increased In incorporation efficiency up to InN mole fractions of 38% in both structural analysis by high resolution X-ray diffraction and room temperature photoluminescence spectroscopy. Thus, strain manipulation opens up an additional degree of freedom in epitaxy of GaInN QWs in addition to thermodynamic parameters such as the QW growth temperature.

HL 59.10 Wed 17:30 POT 251

Influence of electric field variation on optical properties of semipolar InGaN/GaN light emitting diodes — •Stefan Freytag[1], Michael Winkler[1], Tim Wernicke[2], Luca Sulmoni[2], Ingrid Koslow[2], Duc V. Dinh[3], Brian Corbett[3], Peter J. Parbrook[1], Martin Feneberg[1], Michael Kneissl[2], and Rüdiger Goldhahn[1] — [1]Institut für Experimentelle Physik, Otto-von-Guericke-Universität, Magdeburg, Germany — [2]Technische Universität Berlin, Institute of Solid State Physics — [3]Tyndall National Institute, University College Cork, Cork, Ireland

Semipolar InGaN/GaN quantum-well (QW) structures with the (20$\bar{2}\bar{1}$) and (20$\bar{2}$1) surface orientations have attracted a lot of interest in recent years for applications in efficient light emitting diodes. Studies revealed unexpected differences in the energy splitting of QW emission energy as well as the optical polarization degree ρ between the two orientations. We report a comprehensive electro-optical (electroreflectance) characterization of those structures embedded in p-/n-junctions. The analysis yields the optical polarization dependent absorption related transition energies between depletion and forward bias. The data are compared to bias dependent photoluminescence and electroluminescence measurements. Results have been interpreted based on k·p theoretical model calculations.

HL 60: Organic Electronics and Photovoltaics IV: OPV

Time: Wednesday 15:00–18:30 Location: ZEU 260

Invited Talk HL 60.1 Wed 15:00 ZEU 260

The role of incoherent hopping in the photogeneration of charges in organic semiconductors — •Anna Köhler — University of Bayreuth, 95400 Bayreuth, Germany

We demonstrate that efficient and nearly field-independent charge separation in organic planar heterojunction solar cells can be described by an incoherent hopping mechanism that can be modelled by kinetic Monte Carlo simulations that include the effect of on-chain delocalization. We address, first, the issue of differentiating between geminate and nongeminate recombination in solar cells.(Adv. Funct. Mater. 2016, DOI: 10.1002/adfm.201604906) We show that a reduced fill factor and the appearance of an s-shaped I-V curve even at low light intensities results from geminate recombination due to the back diffusion of holes toward their siblings at the donor-acceptor interface rather from to charge accumulation at the donor-acceptor interface. Second, we consider how optical excitation of C60 and PCBM contribute to the photogeneration of charge carriers. (J. Phys. Chem. C 2016 DOI: 10.1021/acs.jpcc.6b0847). We find that intrinsic photogeneration starts at a photon energy of about 2.25 eV, i.e., about 0.4 eV above S1. It originates from charge transfer type states that can autoionize incoherently via thermalization before relaxing to S1 state, in the spirit of Onsager's 1938 theory.

HL 60.2 Wed 15:30 ZEU 260

Charge separation and recombination in PBTT-T/fullerene blends and solar devices — •Elisa Collado Fregoso[1], Jona Kurpiers[1], Samantha Hood[2], Ivan Kasal[2], James Durrant[3], and Dieter Neher[1] — [1]Institut für Physik und Astronomie, Potsdam University, Potsdam-Golm, Germany — [2]Centre for Quantum Computation and Communication Technology, The University of Queensland, Brisbane, Australia — [3]Centre for Plastic Electronics, Department of Chemistry, Imperial College London, UK

Organic solar cells, particularly polymer/fullerene solar cells, are an important area of scientific research on the generation of sustainable and renewable energy. However, further optimization of solar device efficiency is still needed to reach commercialization.

In this talk, the relationship between active layer nanostructure and charge separation and recombination kinetics in thin films and solar devices fabricated with mixtures of PBTT-T/fullerene will be established. Via a combined theoretical and experimental kinetic study using Transient absorption spectroscopy (TAS) and Time-delayed collection field (TDCF) we clearly establish the effect of an intermixed versus a more flat interface towards the separation of bound charges and charge recombination regimes. This is further correlated with device performance, thus showing the importance of careful blend nanostructure control.

HL 60.3 Wed 15:45 ZEU 260

Electron Affinity and Charge Trapping in Ternary Fullerene-based Donor:Acceptor Films for Organic Photovoltaics — •Michael Auth[1], Michael Brendel[1], Andreas Sperlich[1], Stephan Väth[1], Jens Pflaum[1,2], 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

Fullerene materials for organic photovoltaics (OPV) are highly expensive, due to their elaborate purification. To determine if this step is necessary to a high degree, we investigate the influence of fullerene mixtures, i.e. unpurified fullerenes, in ternary OPV materials. As the molecule's electron affinity determines where charge carriers reside, it also determines if unintentional molecules act as trap sites. Since electron paramagnetic resonance (EPR) addresses localised charges, we investigate photo-induced charge transfer via EPR in correlation with solar cell parameters (V_{OC}, J_{SC}, PCE). For polymer-fullerene blends we used the conjugated polymers P3HT or PTB7, together with the soluble fullerene derivatives $PC_{70}BM$, $PC_{60}BM$ and $IC_{60}BA$. As comparison, we furthermore investigated solar cell absorbers made of various vacuum deposited mixtures of C_{70} and C_{60} fullerenes on top of Diindenoperylene (DIP). For all configurations we compare the redistribution of electrons in the fullerene phase with the corresponding stoichiometry to determine electron affinity differences. In conjunction with solar cell parameters we are then able to determine the influence of unpurified fullerenes upon OPV.

HL 60.4 Wed 16:00 ZEU 260

Role of trapped and free charges on the recombination in a low band-gap organic solar cell — •Steffen Roland[1], Antonio Facchetti[2], and Dieter Neher[1] — [1]University of Potsdam, Institute of Physics and Astronomie, Potsdam, Germany — [2]Northwestern University, Department of Chemistry, Evanston, IL-USA

While the role of traps on the transport of photogenerated charges has been analyzed in detail in the literature, the effect of energetic disorder on the rate of non-geminate recombination is yet not very clear. In this talk a new comprehensive approach of how to treat recombination in energetically disordered organic solar cells is proposed. Charge extraction techniques are used to examine the recombination dynamics of a typical organic solar cell (PMDPP3T:PCBM) in detail. While temperature dependent steady-state charge extraction experiments predict a significant amount of trapped charges, it is found that the recombination current (J_R) is dominated by a bimolecular process. A model is introduced in which free charges (outside the Fermi-gap) that contribute to J_R are discriminated from trapped charges (inside the Fermi-gap), which do not contribute to J_R. The free charge carrier recombination coefficient is determined by time delayed collection field measurements and used to accurately fit the measured JV-characteristics over a wide range of light intensities. These results prove that in this system, although charges undergo trapping, the recombination current is dominated by free bimolecular carrier recombination. This work sheds new light on the influence of trapped charges on the recombination process, a topic that has yet remained controversial within the field.

HL 60.5 Wed 16:15 ZEU 260

Recombination Dynamics and the Role of Space Charge Effects in Organic Photovoltaics — •Martin Stolterfoht[1], Ardalan Armin[2], Safa Shoaee[1], Bronson Philippa[3], Paul Meredith[2], and Dieter Neher[1] — [1]University of Potsdam, Potsdam-Golm, Germany — [2]The University of Queensland, Brisbane, Australia — [3]James Cook University, Cairns, Australia

The origin of photocurrent losses in the power-generating regime of organic solar cells (OSCs) remains a controversial topic, although recent literature suggests the importance of bimolecular recombination in determining the bias dependence of the photocurrent. Here we studied the steady-state recombination dynamics in OSCs with different hole mobilities from short-circuit to maximum power point (Adv. Energy Mater. DOI: 10.1002/aenm.201601379). We show that in this bias regime, first-order recombination outweighs bimolecular recombination of free charges. We demonstrate that the first-order losses increase with decreasing slower carrier mobility and attribute them to recombination of photogenerated and injected charges and/or geminate recombination. We also present how the competition between bimolecular recombination and extraction can be described using a simple figure of merit under consideration of space charge effects (J. Phys. Chem. Lett. DOI: 10.1021/acs.jpclett.6b02106). The experimental results obtained on 25 different OSCs represent a conclusive understanding of bimolecular recombination and allow to minimize these losses for given device parameters. Nevertheless, more work is necessary to understand the recombination losses in the power-generating regime in full generality.

HL 60.6 Wed 16:30 ZEU 260

Experimental and simulated illumination dependent conductivity changes in organic bulk hetero junction solar cells — •Arne Müller, Vladislav Jovanov, and Veit Wagner — Jacobs University Bremen,Campus Ring 1, 28579 Bremen, Deutschland

The usage of organic solar cells for indoor application or for wearable electronics requires a good functionality for a wide range of irradiated light intensities. Therefore the IV behaviour of bulk hetero junction solar cells is analysed for a large variety of illumination intensities. We find that the IV-characteristic differs from the predictions of the Shockley-model, which is attributed to the low mobility of the charge carriers. The results are compared to drift-diffusion device simulations and with a simplified device model based on the Fermi-level spitting behaviour inside the semiconductor. In addition JscVoc experiments were performed to gain an insight into the series-resistance properties

at different light intensities. As expected we found that the conductivity of the device is changed due to the light created charge carriers. The findings of the JscVoc analysis are then compared to our improved device model.

15 min break

HL 60.7 Wed 17:00 ZEU 260

Design and Application of NIR Absorbing Donator Materials for Efficient Organic Solar Cells — •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, TU Dresden — [2]Dresden Center for Computational Materials Science, TU Dresden — [3]Center for Advancing Electronics Dresden, TU Dresden

Recently, fluorene-functionalized aza-BODIPYs have been successfully applied as donor material in organic solar cells.[1] Optimized bulk heterojunction solar cells with C60 have yield power conversion efficiencies up to 4.5 %, rendering the compounds highly competitive among other NIR-absorbing small-molecule donor materials. Based on an analysis of electronic properties, internal reorganization energies, and the optical properties of more than 100 aza-BODIPYs we give guidelines for the design of further optimized materials for solar cell applications. The observed independence of most of the functionalization strategies makes them an ideal material class for tailor-made donor materials that can cover a broad range of absorption, charge transport, and energetic regimes.

[1] M. Lorenz-Rothe, K. S. Schellhammer et al. Adv. Electron. Mater. 2, 1600152 (2016).

HL 60.8 Wed 17:15 ZEU 260

Manipulating the morphology in printed organic solar cells — •Stephan Pröller[1], Daniel Moseguí González[2], Chenhui Zhu[3], Alexander Hexemer[3], Peter Müller-Buschbaum[2], and Eva M. Herzig[1] — [1]TU München, Munich School of Engineering, Herzig Group, 85748 Garching, Germany — [2]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [3]Lawrence Berkeley National Laboratory, Advanced Light Source, Berkeley, USA

The nanomorphology can strongly influence the physical properties of organic thin films. For example, polymer:fullerene blends used in organic photovoltaics vary significantly in performance depending on the inner film morphology. To allow large-scale production of these devices, control of the nanostructure during the processing of the active layer is important. This firstly needs an understanding of the processes involved during the drying of the film. Using an industrial slot-die coater implemented into a synchrotron beamline we have successfully characterized the solidification process of an active layer using grazing incidence small and wide angle X-ray scattering (GISAXS/GIWAXS). We use the gained knowledge to further manipulate the structure of printed organic thin films by external intervention while printing. With this manipulation, we are able to positively influence the morphological evolution and thus the performance of the produced devices.

HL 60.9 Wed 17:30 ZEU 260

On the Role of Triplet Excitons in Organic Solar Cells — •Andreas Sperlich[1], Stefan Väth[1], Hannes Kraus[1], 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

A strategy for increasing the conversion efficiency of organic photovoltaics has been to increase V_{OC} by tuning the energy levels of donor and acceptor components. However, this opens up a new loss pathway from an interfacial charge transfer state (CTS) to a donor triplet exciton (TE) state called electron back transfer (EBT), which is detrimental to device performance. To test this hypothesis, we study triplet formation in high performing blends of the fullerene $PC_{70}BM$ with either the polymer PTB7 [1] or the soluble small molecule p-DTS(FBTTh$_2$)$_2$ [2] and determine the impact of the morphology-optimizing additive 1,8-diiodoctane (DIO). Using photoluminescence and spin-sensitive optically and electrically detected magnetic resonance (ODMR, EDMR) measurements we find that TE formation does not only depend on the materials' energetics, but also on temperature and nano-morphology. Furthermore, we observe TEs in real devices under realistic working conditions even for the most efficient solar cells, which has implications not only for efficiency, but also for devices stability.

[1] H. Kraus, et al., Sci. Reps. 6, 29158 (2016)
[2] S. Väth, et al., Adv. Energy Mater., doi: 10.1002/aenm.201602016 (2016)

HL 60.10 Wed 17:45 ZEU 260

Watching Paint Dry: The Impact of Diiodooctane on the Kinetics of Aggregate Formation in Thin Films of Poly(3-hexylthiophene) — •Markus Reichenberger[1], Sebastian Baderschneider[2], Daniel Kroh[1], Steffen Grauf[1], Juergen Koehler[2,3], Richard Hildner[2], and Anna Koehler[1,3] — [1]Experimental Physics II, University of Bayreuth, 95440 Bayreuth, Germany — [2]Experimental Physics IV, University of Bayreuth, 95440 Bayreuth, Germany — [3]Bayreuth Institute of Macromolecular Research (BIMF), University of Bayreuth, 95440 Bayreuth, Germany

We have investigated how the addition of 1,8-diiodooctane (DIO) alters the formation of disordered and ordered phases in a film of poly(3-hexylthiophene-2,5-diyl) (P3HT). By combining in situ time-resolved absorption spectroscopy with 60 ms time resolution, optical and transmission electron microscopy and spatially resolved photoluminescence spectroscopy, we show that, in addition to the excitonic coupling, the film formation process during spin-coating as well as the subsequent long-time film drying process differ significantly when DIO is added to a solution of P3HT. During spin-coating, the addition of DIO reduces the actual time for transformation from disordered to ordered phase, even though it increases the time until the disorder-order transition sets in. In place of a solidification front, we observe an all-over solidification throughout the entire film. The phase separation between nonaggregated and aggregated phase increases when using DIO, with compositional variation in the content of aggregated phase on a micrometer scale.

HL 60.11 Wed 18:00 ZEU 260

Bicontinuous Morphologies in Ternary Blends of Molecular Glasses — •Michael Grimann, Evgeny Tatarov, and Thomas Fuhrmann-Lieker — University of Kassel, Institute of Chemistry and Center for Interdisciplinary Nanostructure Science and Technology, 34109 Kassel, Germany

We demonstrate nanoscale phase separated morphologies in organic functional materials. These glassy compounds comprise structural motifs known from OLED or organic laser materials like oligophenyls and triarylamines as electron donors. We developed electron acceptors containing perfluorinated aromatic moieties which lead to a miscibility gap with the respective donors. Binary blends thereof undergo phase separation via spinodal decomposition in equichoric compositions. Kinetics of this demixing process can be significantly slowed by addition of especially designed surfactant-like bipolar materials. The resulting bicontinuous morphologies of tuneable scale are useful for future random lasing and photovoltaic applications.

HL 60.12 Wed 18:15 ZEU 260

Controlling the aggregation of native polythiophene during in situ polymerization — •Jenny Lebert, Eva M. Kratzer, Mihael Coric, Salma Mansi, and Eva M. Herzig — TU München, Munich School of Engineering, Herzig Group, 85748 Garching, Germany

Native polythiophene belongs to the class of conjugated, semiconducting polymers which become conductive upon doping and therefore offer a broad range of potential applications in organic electronics. While polythiophene itself is insoluble, it is possible to obtain solution processed thin films by employing an in situ polymerization technique. This way, the soluble monomers are deposited to the substrate and chemically linked afterwards. Since it is well known, that the performance of polymeric electronic devices depends strongly on the molecular interactions within the thin films, understanding and controlling the crystallization and film morphology are of crucial importance.

Here, we would like to present the possibilities of influencing the aggregation of the polythiophene chains in the film formation process by varying easily changeable synthetic parameters. The synthesized polymer films are analyzed regarding their optic and electronic properties as well as their morphology to show a clear dependence of the chosen synthetic path on the final film characteristics.

HL 61: Plasmonics and Nanooptics VII: Applications and Other Aspects

Time: Wednesday 15:00–18:00 Location: TRE Ma

HL 61.1 Wed 15:00 TRE Ma

Hydrogen Sensing using Chemically Grown Plasmonic Nanorods in a Dust-on-Film Geometry — •Domenico Paone[1], Martin Mayer[2], Nikolai Strohfeldt[1], Florian Sterl[1], Tobias König[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart — [2]Institute of Physical Chemistry and Polymer Physics, Dresden

Noble metal nanostructures are able to confine electromagnetic radiation on a subwavelength nanometer scale. The resonant excitation of localized surface plasmons in such nanostructures gives rise to strong light absorption and scattering. These optical properties can be used in a rich variety of practical applications such as gas sensing. In this work, we present a dust-on-film sensing geometry by drop coating gold nanoparticles on active hydrogen absorbing films. The nanoparticles are fabricated by a seed-mediated growth method that enables the synthesis of nanorods with a wide variation of lengths. We employ these nanorods as optical antennas to investigate locally the hydrogen catalysis and absorption of palladium and magnesium films. To study our dust-on-film system, we perform single-particle dark-field spectroscopy on the individual gold nanorods. We are able to find pronounced spectral shifts upon exposure to different hydrogen concentrations, leading the way toward the development of inexpensive chemical reaction sensors with high sensitivity.

HL 61.2 Wed 15:15 TRE Ma

Directional Emission from Active Dielectric Nanoantennas — •Manuel Peter[1], André Hildebrandt[2], Christian Schlickriede[3], Thomas Zentgraf[3], Jens Förstner[2], and Stefan Linden[1] — [1]Physikalisches Institut, University of Bonn, Nußallee 12, D-53115 Bonn, Germany — [2]Department of Electrical Engineering, University of Paderborn, Warburger Strasse 100, D-33098 Paderborn, German — [3]Department of Physics, University of Paderborn, Warburger Strasse 100, D-33098 Paderborn, Germany

Here, we report on the directional light emission from an active dielectric nano antenna. The leaky-wave antennas are made from Hafnium dioxide. Colloidal semiconductor quantum dots with an emission wavelength of 780 nm are deposited with a lithographic technique from an aqueous solution into the feed gap of the antenna. Quantum dots serve as dipole sources. Their fluorescence is guided by the director that acts as a leaky waveguide which emits the light in a narrow angle distribution into the substrate. A reflector is used to increase the efficiency of the antenna. By imaging the back-focal plane of a high NA microscope objective, we can directly map the angular distribution of the fluorescence. In our experiment we observe a strong effect of the antennas with a main lobe of the fluorescence pointing into the substrate with a longitudinal angle of θ=21°. Additionally we will present results on the polarization of the directed light and the change of directivity for antennas with different dimensions. All the measured angular intensity distributions are in good agreement with the numerical calculations.

HL 61.3 Wed 15:30 TRE Ma

Plasmonic analog of electromagnetically induced absorption leads to giant thin-film Faraday rotation — •Dominik Floess, Mario Hentschel, Thomas Weiss, and Harald Giessen — 4th Physics Insitute and Research Centre SCoPE, University of Stuttgart, Stuttgart, Germany

We demonstrate the realization of a hybrid magnetoplasmonic thin film structure that resembles the classical optical analog of electromagnetically induced absorption. In transmission geometry our Au nanostructure embedded in an EuS film induces giant Faraday rotation of up to 14° for a thickness of below 150 nm for $B = 5$ T. Crucial for our achievement is the introduction of EuS as a new material for magnetoplasmonics. At low temperatures, it enables the realization of complex magnetoplasmonic structure geometries, which would not be feasible with commonly used magneto-optic materials. Our concept will lead to important, highly integrated, non-reciprocal photonic devices for light modulation, optical isolation, and magnetic field optical sensing. The simple fabrication of EuS nanostructures also enables more sophisticated and intriguing future designs of magnetoplasmonic systems and three-dimensional magneto-optic metamaterials.

HL 61.4 Wed 15:45 TRE Ma

Anderson localization in disordered plasmonic waveguide arrays — •Cherpakova Zlata, Felix Bleckmann, and Stefan Linden — Physikalisches Institut, Rheinische Friedrich-Wilhelms-Universität Bonn, Nußallee 12, 53115 Bonn, Germany

We report on the observation of Anderson localization in disordered arrays of evanescently coupled dielectric-loaded surface plasmon polariton (SPP) waveguides. The samples are fabricated by negative-tone gray-scale electron beam lithography. On-diagonal disorder is introduced to the arrays by randomly altering the waveguides effective refractive index which is a monotonous function of the waveguide height. Thus, by choosing the maximum variation of the waveguide height we can control the degree of disorder. SPPs were excited by shining a highly focused laser beam on the grating, deposited on top of the central waveguide. The spatial evolution of the SPP field intensity is monitored by real space leakage radiation microscopy (LRM). The corresponding momentum-resolved spectra which reveal the information on the energy spectrum of an equivalent condensed matter system is measured as well by making use of Fourier space LRM. With these techniques we experimentally demonstrate the transverse localization of the SPP with increasing degree of disorder both in real and Fourier space.

HL 61.5 Wed 16:00 TRE Ma

Ultrafast imaging of electric fields around nanostructures — •Jan Vogelsang, Germann Hergert, Petra Gross, and Christoph Lienau — Institut für Physik, Carl von Ossietzky Universität, 26129 Oldenburg, Germany

The combination of high spatial resolution electron microscopes and high temporal resolution laser spectroscopy promises experiments in unexplored spatio-temporal regimes. E.g., many fundamental photoinduced processes such as coherent charge and energy transport phenomena occur on few-fs time scales. However, in today's ultrafast electron microscopes the time resolution is so far limited to ~100fs: The electrons propagate over mesoscopic distances, which gives rise to electron pulse broadening due to dispersion.

Recently, we demonstrated a new, plasmon-driven electron source that tackles this challenge: Adiabatic nanofocusing of surface plasmons on sharply etched metallic tapers concentrates light in a nanometric volume and efficiently induces electron emission. Direct illumination of the emission site is avoided and hence the apex-sample-distance can be chosen arbitrarily small (Nano Lett. 15, 4685, 2015).

Here, we show first ultrafast electron micrographs with few-nm spatial and few-ten-fs temporal resolution. We record an ultrafast change of the electric field near carbon nanostructures after laser excitation. It deflects the probing electrons which directly maps the field distribution to the 2d electron detector. The results prove that the simple, but efficient working principle of a lensless point-projection microscope is ideal for maintaining the ultrashort duration of electron pulses.

HL 61.6 Wed 16:15 TRE Ma

Spectral imaging of topologically protected edge states in plasmonic waveguide arrays — •Felix Bleckmann[1], Andrea Alberti[2], and Stefan Linden[1] — [1]Physikalisches Institut, Rheinische Friedrich-Wilhelms-Universität Bonn, Nußallee 12, 53115 Bonn, Germany — [2]Institut für Angewandte Physik, Rheinische Friedrich-Wilhelms-Universität Bonn, Wegelerstr. 8, 53115 Bonn, Germany.

The Su-Schrieffer-Heeger (SSH) model, i.e., a chain of lattice sites coupled via alternating strong and weak bonds, is the prototypical one-dimensional system with nontrivial topological character. It supports two different dimerizations with distinct topological properties. At any interface between both, one topologically protected edge state exists.

We report on the observation of topologically protected edge states in evanescently coupled plasmonic waveguide arrays employed to implement the SSH model. The arrays are fabricated on top of a gold film by negative-tone grey-scale electron-beam lithography. Alternating strong and weak bonds were realized by choosing two different separations between neighboring plasmonic waveguides. We created an interface between the two dimerizations of the SSH model by repeating the larger separation twice.

Surface plasmon polaritons are excited directly at the interface. Their spatial evolution as well as their momentum-resolved spectra are measured by making use of real and Fourier space leakage radi-

ation microscopy. We demonstrate that the topologically protected edge state is localized at the interface and has a midgap position in the momentum-resolved spectrum.

HL 61.7 Wed 16:30 TRE Ma

Resonant Plasmonic Antenna-Enhanced Far-IR and Terahertz Spectroscopy — •Ksenia Weber[1], Maxim Nesterov[1], Thomas Weiss[1], Michael Scherer[2], Mario Hentschel[1], Jochen Vogt[3], Christian Huck[3], Weiwu Li[4], Martin Dressel[4], Harald Giessen[1], and Frank Neubrech[3] — [1]4th Physics Institute, University of Stuttgart, Stuttgart — [2]InnovationLab GmbH, Heidelberg, Germany — [3]Kirchhoff Institute for Physics, Heidelberg University, Germany — [4]1st Physics Institute, University of Stuttgart, Stuttgart

Terahertz spectroscopy is a technique with a vast range of sensing applications, based on material-specific absorption features of molecular vibrations. However, the low absorption cross section of these excitations strongly limits its sensitivity. The possibility to increase the sensitivity of spectroscopic methods via the enhanced electromagnetic near fields provided by plasmonic nanoantennas has been shown before for surface-enhanced infrared spectroscopy (SEIRA). In the present work we transfer the concept of SEIRA to single digit terahertz frequencies. We use plasmonic nanoantennas for the enhancement of molecular vibrations with frequencies in a spectral region from 4.5 to 45 THz We therefore fabricated arrays of rectangular gold antennas by electron beam lithography and coated them with thin layers of the fullerenes C_{60} and C_{70}, as well as the amino acid threonine. The samples were investigated with Fourier transform infrared spectroscopy using a bolometer as detector. An increased SEIRA enhancement of one two orders of magnitude is found for antennas resonant at 6.7 THz when compared to 45 THz, corresponding to a λ^3 scaling.

HL 61.8 Wed 16:45 TRE Ma

Watching hydride formation in single plasmonic magnesium nanoparticles — •Florian Sterl, Heiko Linnenbank, Nikolai Strohfeldt, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany

Magnesium (Mg) has recently demonstrated its potential for active plasmonics in the visible wavelength range via the absorption of hydrogen. We have shown that this can be achieved by using Mg nanoantennas with a catalytic palladium (Pd) capping layer. Upon hydrogenation, Mg forms non-metallic magnesium hydride (MgH_2). In this system, the plasmonic resonance can be switched off and back on via exposure to hydrogen and oxygen gas, with switching times on the order of tens of seconds. On one hand, this leads to potential applications such as tunable plasmonic displays. On the other hand, the system can be used to investigate the hydrogenation of Mg.

MgH_2 is considered a promising candidate for solid-state hydrogen storage, owing to its high hydrogen content of up to 7.6 wt%, and can also be considered a model system for other energy storage materials. We aim for a better understanding and characterization of the hydrogen diffusion in Mg at the nanoscale, using different techniques: We investigate the time dynamics of the Mg-MgH_2 phase transition using the optical far field of Mg/Pd nanoantennas, and probe the optical near field of individual Mg nanostructures to observe the evolution of hydrogenated domains during this transition. We furthermore address the mechanical deformation due to the hydrogen-induced expansion of the Mg crystal lattice.

HL 61.9 Wed 17:00 TRE Ma

Palladium Nanopatches - Size-dependent Hydrogen Kinetics — •Nikolai Strohfeldt[1], Florian Sterl[1], Ronald Griessen[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Stuttgart, Germany — [2]Faculty of Sciences, Division of Physics and Astronomy, VU University, Amsterdam, The Netherlands

Nanoparticles exhibit many potentially interesting properties that are relevant for key applications such as storage of energy in batteries or data in non-volatile memories. Especially the storage of hydrogen in nanomaterials has stimulated the development of powerful new investigation methods. Electron-beam lithography makes it possible to create essentially monodisperse ensembles of particles, which can conveniently be studied with optical and plasmonic methods. In nanoparticles, H desorption occurs fully coherently only for small crystalline nanocubes (typically smaller than 50 nm) at temperatures sufficiently close to the critical temperature. For larger particles, it is partially incoherent, where dilute α-PdH_x and high concentration β-PdH_x phases coexist. In polycrystalline particles, larger than 200 nm, the H absorption occurs at much lower pressures than in nanocubes. With a newly developed localized surface plasmon resonance method we succeeded in determining the size dependence of the hydrogen induced in-plane and out-of-plane expansion. With increasing size the in-plane expansion of these particles is increasingly hampered. The knowledge gathered with Pd-H nanoparticles is at the basis of recent developments of active plasmonic elements based on the Y-H and Mg-H systems.

HL 61.10 Wed 17:15 TRE Ma

Polaronic nature of charge carriers at the LAO/STO interface — •Vladimir N. Strocov[1], Claudia Cancellieri[2], Adrian Husanu[1], Ulrich Ashauer[3], and Andrey Mishchenko[4] — [1]Swiss Light Source, Paul Scherrer Insitute, Switzerland — [2]EMPA, Switzerland — [3]University of Bern, Switzerland — [4]RIKEN Center for Emergent Matter Science, Japan

2D electron system emergent at the paradigm buried oxide interface $LaAlO_3/SrTiO_3$ (LAO/STO) is explored with soft-X-ray ARPES, which combines resolution in electron energy and momentum with enhanced probing depth and chemical specificity [1]. Accentuated with resonant photoexcitation of the interface Ti^{3+} ions, ARPES response of the interface charge carriers resolves the manifold energy band structure of t_{2g}-derived subbands formed in the interface quantum well. The temperature dependent peak-dip-hump spectral lineshape manifests polaronic nature of the interface electrons, where the breathing-mode LO3 phonon at 118 meV limits low-temperature mobility of the interface charge carriers, and the polar TO1 one, changing its frequency from 18 to 14 meV across the antiferrodistortive phase transition, causes a dramatic mobility drop with temperature [2]. Doping with oxygen vacancies, affecting electron-phonon coupling, opens ways to tune the interfacial mobility at oxide interfaces in view of their potential device applications.

1. V.N. Strocov *et al*, Synchr. Rad. News 27, N2 (2014) 31
2. C. Cancellieri *et al*, Nature Comm. 7 (2016) 10386

HL 61.11 Wed 17:30 TRE Ma

Attosecond time-resolved photoelectron spectroscopy of hybrid nanoresonators — •Julia Hengster and Thorsten Uphues — ARS, CFEL, Luruper Chaussee 149, 22761 Hamburg

Understanding plasmons as collective oscillations of the free-electron gas density important questions related to their propagation, damping, charge and energy localization came up. Nevertheless the behaviour of hybrid nanostructures approaching the monolayer limit raises a new type of questions concerning their plasmonic behaviour in space and time, following the complex dynamics of the electromagnetic field.

Attosecond time-resolved experiments are on the way to resolve subcycle electron dynamics from plasmonic interaction of ultrashort driving pulses in surfaces and nanostructures. Our approach of attosecond photoscopy demonstrates a reliable route to extend attosecond technology to surface and nanostructure dynamics. Hybrid nanostructures exhibit complex plasmonic properties sensitive to parameters as geometrical aspect ratios or material compositions. Vertically aligned disk nano-resonators belong to a group of tailored systems demonstrating field enhancement with strong localization. We found a remarkably sensitive behaviour in the coupling of surface and bulk plasmons with respect to the outer geometry of the resonators with ultrafast subcycle dynamics.

As proof-of-concept we demonstrate attostreaking from gold films with significant deviation to gas-phase streaking. Furthermore we developed non-destructive preparation procedures for nanoparticle samples as requirement for attosecond photoscopy.

HL 61.12 Wed 17:45 TRE Ma

Monitoring of structural changes of polypeptides using resonant surface enhanced infrared spectroscopy — •Rostyslav Semenyshyn[1], Mario Hentschel[1], Jochen Vogt[2], Christian Huck[2], Christoph Stanglmair[3], Claudia Pacholski[3], Frank Neubrech[1,2], and Harald Giessen[1] — [1]4th Physics Institute, University of Stuttgart — [2]Kirchhoff Institute for Physics, University of Heidelberg — [3]Max Planck Institute for Intelligent Systems, Stuttgart

Infrared (IR) vibrational spectroscopy is a powerful tool for the identification of chemical and structural composition of molecules. Its detection limit can be improved by several orders of magnitude using surface-enhanced IR absorption (SEIRA) with resonant nanoantennas. Here, we demonstrate the capability of SEIRA for the ultra-sensitive detection of minute amounts of a polypeptide, namely poly-L-lysine (PLL). Furthermore, we applied SEIRA to monitor structural changes

of the molecules introduced by injecting sodium dodecyl sulfate as well as varying the pD value. For this purpose, we functionalized nanoantenna arrays with mercaptoundecanoic acid (MUA) and mercaptoundecanol (MUoL) in order to bind PLL molecules to the gold surface. The combination of MUA and MUoL ensures a sufficient flexibility, allowing for structural changes. Such changes are detected based on a detailed analysis of the amide-I vibrations. Hence, we tuned the plasmonic resonances of nanoantennas to the amide-I band of PLL and performed in-vitro SEIRA measurements in D_2O based solutions. Following this approach, we monitored the reversible change between α-helix and β-sheet structural states of PLL in low concentrations.

HL 62: Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - V

Time: Wednesday 15:00–18:15 Location: GER 38

HL 62.1 Wed 15:00 GER 38

First-principle Linear Response in Real Space — •Honghui Shang[1], Danilo S. Brambila[1], Christian Carbogno[1], Patrick Rinke[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Aalto University, Helsinki, Finland

Density-functional perturbation theory (DFPT) has developed into an important computational tool for assessing the linear electronic response of crystalline solids to perturbations, e.g., from electric fields or nuclear displacements [1]. In this work we present a full real-space reformulation of DFPT and its implementation [2] in the all-electron, numeric atom-centered orbital electronic structure theory code FHI-aims. We discuss the specific contributions, e.g., relativistic effects and Pulay terms, that arise in such a formulation and validate our implementation by systematically comparing with the finite-difference approach for various extended systems. The computational efficiency is then analyzed via scaling and scalability tests on massively parallel architectures (CRAY and IBM x86 clusters). Finally, we show that this real-space formalism enables an arbitrarily dense sampling of the Brillouin zone by numerically cheap Fourier transformations, which in turn facilitates an efficient evaluation of the electron-phonon coupling matrix elements. We demonstrate the efficiency by computing the relaxation time of hot carriers in Si.

[1] X. Gonze and C. Lee, *Phys. Rev. B* **55**, 10355, (1997).
[2] H. Shang, *et al.*, *Comp. Phys. Comm. (accepted)*, arXiv:1610.03756.

HL 62.2 Wed 15:15 GER 38

Anharmonic Vibrations in Solids: Why and When Going Beyond Perturbative Treatments is Necessary — •Hagen-Henrik Kowalski, Maja-Olivia Lenz, Christian Carbogno, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

In *ab initio* theory, the nuclear motion is typically assessed using a truncated second order Taylor expansion for the potential energy (harmonic approximation). Recent computational and methodological advancements [1] allow to extend this expansion to the third order so to approximately treat also anharmonic effects. Little is known, however, about the role of higher order terms. In this contribution, we systematically compare how a third-order expansion performs with respect to techniques that are able to capture higher degrees of anharmonicity, e.g., the quasi-harmonic approximation and fully anharmonic molecular dynamics. For this purpose, anharmonic properties such as the thermal expansion and the Grüneisen parameters are computed for a set of materials with increasing degree of anharmonicity (Si, Mg_2Si, CuCl, and ZrO_2). This reveals that a third order expansion can still lead to quantitative and even qualitative errors at elevated temperatures and/or in highly anharmonic systems. Eventually, we discuss the impact of the chosen exchange-correlation functionals on these calculations and the implications of these findings for the computation of thermal conductivities [2].

[1] D. A. Broido, *et al.*, *Appl. Phys. Lett.* 91, 231922 (2007).
[2] C. Carbogno, R. Ramprasad, and M. Scheffler, *ArXiv:* 1608.06917.

HL 62.3 Wed 15:30 GER 38

Anharmonic and Quantum Fluctuations in Molecular Crystals from Ab Initio Simulations — •Mariana Rossi[1] and Michele Ceriotti[2] — [1]Fritz Haber Institute of the Max Planck Society, Berlin — [2]École Polytechnique Fédérale de Lausanne, Switzerland

Molecular crystals often exist in multiple competing polymorphs which are challenging to be predicted computationally, but show significantly different physicochemical properties. This challenge is not due only to the combinatorial search space, but also to the complex interplay of subtle effects determine the relative stability of different structures. Here we estimate all contributions to the free energies of these systems with density-functional theory, including the oft-neglected anharmonic contributions and nuclear quantum effects, by using a series of different flavors of thermodynamic integration. As an example, for the two most stable forms of paracetamol we find that anharmonic contributions, different descriptions of van der Waals interactions, and nuclear quantum effects **all** matter to quantitatively determine the stability of different phases [1]. Our studies indicate that anharmonic free energies could play an important role for molecular crystals composed by large molecules and opens the way for a systematic inclusion of these effects in order to obtain a predictive screening of structures.

[1] Rossi, Gasparotto, Ceriotti, *PRL* **117**, 115702 (2016).

HL 62.4 Wed 15:45 GER 38

Exact solutions and approximations in the exact factorization of the electron-nuclear wavefunction — •Graeme Gossel and Neepa Maitra — Department of Physics and Astronomy, Hunter College of the City University of New York, 695 Park Avenue, New York, NY 10065.

"Recently it was shown how a molecular wavefunction may be written exactly as a single product of a nuclear and an electronic wavefunction, with a pair of corresponding equations of motion [1]. This exact factorization provides a new and rigorous starting point for developing intuitive and physical approximations to the exact coupled system. Strikingly, in this factorized picture the electronic Hamiltonian is not strictly Hermitian. Nevertheless, the norm is conserved so long as certain terms persist. This, and other constraints, inform the approximations we apply to make the process numerically feasible. In parallel we present numerical self-consistent solutions of the exact factorization equations devoid of approximations to assess accuracy and behaviour of different terms. Finally, we discuss how a well characterized and robust single-product-picture such as this may be used in TDDFT calculations.

[1] A Abedi, NT Maitra, and EKU Gross, PRL 105 (12), 123002, 2010

HL 62.5 Wed 16:00 GER 38

Insight into time-propagation TDDFT excitations via Kohn–Sham decomposition — •Tuomas P. Rossi[1], Mikael Kuisma[2,3], Martti J. Puska[1], Risto M. Nieminen[1], and Paul Erhart[2] — [1]Aalto University, Espoo, Finland — [2]Chalmers University of Technology, Gothenburg, Sweden — [3]University of Jyväskylä, Jyväskylä, Finland

The real-time-propagation formulation of time-dependent density-functional theory (RT-TDDFT) is an efficient method for calculating optical excitations of large molecules and nanoparticles. However, within RT-TDDFT, the analysis of the response is often limited to photoabsorption spectra and induced densities, in contrast to linear-response formulations of TDDFT, such as the Casida method, in which one can obtain further understanding on the basis of the Kohn–Sham electron-hole decomposition of the excitations.

In this work, we show that the Kohn–Sham decomposition can be equivalently obtained from RT-TDDFT calculations. We demonstrate the approach for the optical response of organic molecules and large metallic nanoparticles. The focus is especially on plasmonic applications, for which the method enables the analysis in terms of transition contribution maps [1]. By using the decomposition, we can shed light on the microscopic origin of plasmon resonances and their damping via plasmon–single-electron coupling, while retaining the favorable scaling of RT-TDDFT compared to linear-response formulations.

[1] S. Malola *et al.*, ACS Nano **7**, 10263 (2013).

HL 62.6 Wed 16:15 GER 38

Gauge-invariant Magnetic Properties from Time-Dependent Current-Density-Functional Theory — •Nathaniel Raimbault[1], Paul de Boeij[3], Pina Romaniello[2], and Arjan Berger[1] — [1]Laboratoire de Chimie et Physique Quantiques, IRSAMC, Université Toulouse III - Paul Sabatier — [2]Laboratoire de Physique Théorique, CNRS, IRSAMC, Université Toulouse III - Paul Sabatier — [3]University of Twente, Faculty of Science and Technology, Physics of Interfaces and Nanomaterials

Standard formulations of magnetic response properties are often plagued by gauge dependencies, which can lead to unphysical results, and to a slow convergence with basis-set size. In this talk we present a novel method for obtaining magnetic properties from the current density [1]. This alternative scheme is fully gauge-invariant, numerically efficient, and can be applied to any method from which the current density can be obtained. To illustrate our method, we applied it to time-dependent current-density-functional theory (TDCDFT). While different types of magnetic properties can be calculated in this way, we here emphasize the calculation of circular dichroism spectra, which are notably important in order to characterize secondary structures in biomolecules. The circular dichroism spectra we thus obtain for methyloxirane, dimethyloxirane and α-pinene are in good agreement with experiment [2]. [1] N. Raimbault, P.L. de Boeij, P. Romaniello, and J.A. Berger, PRL 114, 066404 (2015); [2] N. Raimbault, P.L. de Boeij, P. Romaniello, and J.A. Berger, JCTC 12, 3278 (2016)

HL 62.7 Wed 16:30 GER 38

Calculation of charge transfer integrals using constrained-DFT — •Tobias Lettmann and Nikos Doltsinis — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Straße 10, 48149 Münster, Deutschland

For the investigation of charge transport properties of organic semiconductor materials, the fast and accurate calculation of charge transfer integrals (or transition matrix elements) is desirable. It has been suggested that the transfer integrals depend on a universal linear function of the corresponding wavefunction overlap, which can then be used to approximate the integral at a reduced computational cost[1].

We have calculated transfer integrals for dimers of poly(3-hexylthiophene) (P3HT) and diperylene bisimide (DiPBI), which are used in organic solar cells, in a large variety of intra- and intermolecular conformations and polymer lengths using a constrained-DFT approach[2]. Our results show, that there is indeed a universal relation between transfer integral and wavefunction overlap. However this relation is (i) nonlinear for large overlaps and (ii) only holds true if the transfer integral is rescaled by the number of electrons of the respective system.

[1] F. Gajdos et al.: *J. Chem. Theory Comput.*, 2014, **10**, 4653
[2] H. Oberhofer, J. Blumberger: *J. Chem. Phys.*, 2010, **133**, 244105

HL 62.8 Wed 16:45 GER 38

Towards ultra long-range ab-initio calculations — •Tristan Müller[1], Sangeeta Sharma[1,2], Eberhard K.U. Gross[1], and John K. Dewhurst[1] — [1]Max-Planck-Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany — [2]Department of physics, Indian Institute for Technology-Roorkee, 247997 Uttarkhand, India

We propose a generalization of the Bloch state which involves an additional sum over a finer grid in reciprocal space around each k-point. This allows for ab-initio calculations of ultra long-range modulations in the density which may involve millions of unit cells but with an efficiency rivaling that of a single unit cell. This is due to a new algorithm developed specifically for solving the particular eigenvalue problem that this ansatz requires. Thus physical effects on the micron length scale, which nevertheless depend on details of the electronic structure on nanometer length scales, can be computed exactly within density functional theory.

HL 62.9 Wed 17:00 GER 38

Local density fitting within a Gaussian and plane waves scheme for large-scale density functional theory calculations — •Dorothea Golze[1,2], Marcella Iannuzzi[1], and Jürg Hutter[1] — [1]Aalto University, Otakaari 1, 02150 Espoo, Finland — [2]University of Zurich, Winterthurerstrasse 190, CH-8057 Zurich, Switzerland

A local resolution-of-identity (LRI) approach is introduced in the Gaussian and plane waves (GPW) scheme to enable large-scale Kohn-Sham (KS) density functional theory calculations. The construction of the KS matrix in GPW scales already linearly with respect to system size by using a plane wave expansion of the density for the evaluation of the Coulomb term in combination with a local basis. The intention is to retain the linear scaling of the GPW approach, while reducing the prefactor for computing the KS matrix. The locality of the density fitting ensures an $O(N)$ scaling and is implemented by approximating the atomic pair density by an expansion in one-center fit functions. The prefactor is smaller with LRI since the computational demands for the grid-based operations become negligible, while they are dominant in GPW. We observe a speed-up of the self-consistent field (SCF) procedure by a factor of up to 30 for periodic systems dependent on the symmetry of the simulation cell and the grid cutoff. The accuracy of LRIGPW is assessed for different systems and properties. Generally, total energies, reaction energies, intramolecular and intermolecular structure parameters are well reproduced. LRIGPW yields also high quality results for extended condensed phase systems such as liquid water, ice XV and molecular crystals.

HL 62.10 Wed 17:15 GER 38

From the Electron Localization Function to a Coalescent-Pair Locator — •Stefano Pittalis[1], Daniele Varsano[1], Alain Delgado[2,3], and Carlo Andrea Rozzi[1] — [1]Istituto Nanoscienze, Consiglio Nazionale dellle Ricerche, Via Campi 213a, 41125 Modena, Italy — [2]Department of Physics, University of Ottawa, Ottawa, ON K1N 6N5, Canada — [3]Centro de Aplicaciones Tecnológicas y Desarrollo Nuclear, Calle 30 # 502, 11300 La Habana, Cuba

The Electron Localization Function (ELF), as proposed originally by Becke and Edgecombe, uses the information on the distribution of pairs of electrons with parallel spins. The ELF has been widely adopted as a descriptor of atomic shells and covalent bonds, but it is not useful to visualize the bond in H_2 – the simplest neutral molecule in the universe. Here we propose a complementary descriptor which also works for H_2 by exploiting the information on pairs of electrons with opposite spins. Remarkably, only quantities derived from occupied single-particle orbitals are required in the calculations. If time allows, implications for developing improved approximate density functionals will also be discussed.

HL 62.11 Wed 17:30 GER 38

Band structure interpolation via maximally localized Wannier functions implemented in LAPW+lo basis — •Sebastian Tillack, Andris Gulans, and Claudia Draxl — Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin

The band structure is one of the most fundamental quantities of any solid that carries a lot of information about the material's properties. Obtaining a smooth dispersion from density-functional theory (DFT) and especially from the *GW* approximation of many-body perturbation theory may be very expensive. To this extent, we have implemented a method for generating maximally localized Wannier functions (WF) [1] from Kohn-Sham wavefunctions in the full-potential all-electron code `exciting` [2] using a (linearized) augmented plane-waves plus local-orbitals basis. These WF are used for interpolating wavefunctions and corresponding eigenenergies for arbitrary **k**-points in a computationally cheap post-processing step. The interpolated Kohn-Sham and *GW* bands of conventional and two-dimensional semiconductors and insulators are also used as an input to calculations of optical-excitation spectra.

[1] N. Marzari and D. Vanderbilt, *Phys. Rev. B* ***56***, 12847 (1997)
[2] A. Gulans, et al. *J. Phys.: Condens. Matter* ***26***, 363202 (2014)

HL 62.12 Wed 17:45 GER 38

Chemical insight from Fermi-Löwdin orbitals — •Torsten Hahn[1], Sebastian Schwalbe[1], Simon Liebing[1], Jens Kortus[1], and Mark Pederson[2] — [1]Institute for Theoretical Physics, TU Freiberg, Germany — [2]Department of Chemistry, Johns Hopkins University, Baltimore Maryland (MD), US

The recently developed Fermi-Löwdin orbital based method for correcting the self-interaction error in Density Functional Theory (FLO-SIC DFT) [1,2,3] is briefly introduced. Contrary to standard DFT approaches, where only auxiliary Kohn-Sham orbitals are available, FLO-SIC DFT delivers a set of well-defined, localised Fermi-Löwdin orbitals. These localised orbitals together with their optimised reference positions yield an inherently 'chemical' representation of bonding details in molecules that resembles remarkably well Lewis concept of

lone and binding electron pairs. For complex examples, the method provides detailed insights into the bonding situation in terms of multicenter many-electron bonds in a natural, chemically-intuitive fashion.

[1] M. R. Pederson et al., JCP 140, 121103 (2014).
[2] M. R. Pederson, JCP 142, 064112 (2015).
[3] T. Hahn et al., JCP 143, 224104 (2015).

HL 62.13 Wed 18:00 GER 38

Conditions for describing triplet states in reduced density matrix functional theory — Iris Theophilou[1], Nektarios N. Lathiotakis[2], and •Nicole Helbig[3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany — [2]Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Vass. Constantinou 48, GR-11635 Athens, Greece — [3]Peter-Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany

We consider necessary conditions for the one body-reduced density matrix (1RDM) to correspond to a triplet wave-function of a two electron system. The conditions concern the occupation numbers and are different for the high spin projections, $S_z = \pm 1$, and the $S_z = 0$ projection. Hence, they can be used to test if an approximate 1RDM functional yields the same energies for both projections. We employ these conditions in reduced density matrix functional theory calculations for the triplet excitations of two electron systems. In addition, we propose that these conditions can be used in the calculation of triplet states of systems with more than two electrons by restricting the active space. We assess this procedure in calculations for a few atomic and molecular systems. We show that the quality of the optimal 1RDMs improves by applying the conditions in all the cases we studied.

HL 63: Poster: Quantum Dots and Optics

Time: Wednesday 15:00–19:00 Location: P1A

HL 63.1 Wed 15:00 P1A

Time-resolved optical spectroscopy of guiding modes a in CdZnTe/CdMgTe structure — •Jonas Vondran[1], Felix Spitzer[1], Nils Weber[2], Régis Andre[3], Henri Mariette[3], Cedrik Meier[2], Torsten Meier[2], Ilya Akimov[1], and Manfred Bayer[1] — [1]Technische Universität Dortmund, Dortmund, Germany — [2]Universität Paderborn, Paderborn, Germany — [3]Université Grenoble-Alpes, Grenoble, France

We report on pump-probe reflectivity measurements with 30 fs temporal resolution in a 170 nm thick CdZnTe waveguiding layer cladded between 100 nm width CdMgTe cap and 400 nm thick buffer layer. In order to excite and detect guiding modes gold gratings with periods from 230 to 310 nm are patterned at the top of the sample. Steady state measurements show distinct polarization, angle and wavelength-dependent features indicating the dispersion of waveguiding modes and their interaction with the excitonic resonance at 760 nm wavelength. The transient optical response is strongly influenced by the polarization of pump and probe beams as well as the grating period. The largest modulation depth is observed when the modes are resonantly excited in TM-polarization. We observe clear signatures of free induction decay at negative delay times when the probe reaches the sample earlier than the pump pulse with coherence times of 80-120 fs at T=10K.

HL 63.2 Wed 15:00 P1A

Creation of long-living exciton polariton like states: The impact of pulsed excitation to a steady-state condensate — •Daniel Schmidt[1], Bernd Berger[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-44227 Dortmund, Germany — [2]Technische Physik, Physikalisches Institut, Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, D-97074 Würzburg, Germany

High quality GaAs microcavities offer the possibility to investigate long-living and therefore far traveling exciton polariton condensates. Although much research has been performed using continuous-wave (CW) and pulsed excitation to drive the condensation, few studies investigated the differences in the build-up of the exciton polariton condensation process. We present the impact of pulsed excitation near the threshold power on a steady-state exciton polariton condensate that is confined by a CW pumped ring potential. After the initial decay of the pulsed excited condensate, a surprisingly long-living polariton-like state arises that exceeds the polariton lifetime by an order of magnitude.

HL 63.3 Wed 15:00 P1A

On the phonon assisted absorption in Cu_2O — •Florian Schöne and Heinrich Stolz — Universität Rostock, Institut für Physik

A common approach to describe the shape of the excitonic absorption close to the band gap is based on the formalisms introduced by Elliott[1] 60 years ago utilising the transition probabilities between electronic bands. We follow his ansatz for indirect transitions via second order perturbation theory which can be visualised as an excitation into a virtual intermediate state and the subsequent relaxation to the final state through the emission of a phonon. However, instead of assuming the intermediate states to be pure band states, for materials with large exciton binding energies it is necessary to use the corresponding exciton states. This leads to the invalidity of the commonly assumed square root dependence of the absorption[2]. Applying our theory to the indirect absorption of the yellow exciton states in Cu_2O we find the 1S blue exciton states to be the dominant intermediate states. To describe the experimental observed line shape[3] it is furthermore necessary to assume a momentum dependent deformation potential for the Γ_3^- phonon.

[1] Elliott R.J., Phys. Rev. **108**, 1384 (1957)
[2] Kuper C. G., Whitfield G. D., "Polarons and Excitons." Oliver and Boyd, London (1963)
[3] Naka N., Satoshi H., Teruya I., Jpn. J. Appl. Phys. **44** 5096 (2005)

HL 63.4 Wed 15:00 P1A

Exceptional points in optically anisotropic microcavities — •Steffen Richter[1], Tom Michalsky[1], Chris Sturm[1], Bernd Rosenow[2], Marius Grundmann[1], and Rüdiger Schmidt-Grund[1] — [1]Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig, Germany — [2]Universität Leipzig, Institut für Theoretische Physik, Brüderstr. 16, 04103 Leipzig, Germany

Optical microcavities incorporating anisotropic media can yield effectively biaxial symmetries. They furthermore have dissipative character due to finite broadening of photonic modes. Generally, each mode with a given mode number N is split up into two modes with different polarization. We show that the optical biaxility can lead to the occurrence of exceptional points (EPs) in momentum space. At such points, not only mode energies and broadenings but also their polarization states degenerate, allowing only propagation of circularly polarized photons. Hence, the phenomenon of EPs is similar to singular optic axes in absorptive biaxial media. Here, we show how to realize EPs even in a fully transparent structure and how to tune their position in momentum space through the structure's geometry.

HL 63.5 Wed 15:00 P1A

Determining the band offset of Ga(NAsP)/GaP heterostructures on Si — Sebastian Gies, •Sarah Karrenberg, Wolfgang Stolz, and Wolfram Heimbrodt — Department of Physics and Materials Science Center, Philipps-Universität Marburg, Renthof 5, 35032 Marburg, Germany

The quaternary direct band-gap semiconductor Ga(N,As,P) is a promising candidate for optoelectronic integration on silicon. It can be grown lattice matched to Si and first lasing operation has been demonstrated. To optimize the laser design, it is necessary to have exact knowledge about the electronic structure of the material, especially the band-offset. In this study, we present a thorough investigation of photoluminescence properties of Ga(N,As,P)/Si heterostructures. Using temperature dependent PL we will reveal the disorder of the material and determine optizimed growth parameters. Furthermore, the conjunction of PL excitation spectroscopy and a QW model al-

lows us to reveal the nature of the underlying transitions. In addition, we are able to determine the hitherto unknown band offset between Ga(N,As,P) and GaP with very high precision.

HL 63.6 Wed 15:00 P1A

Optical properties of Tin(IV) oxide prepared by different growth techniques — •Nils Mengel[1], Nils W. Rosemann[1,2], Martin Becker[2], Yinmei Lu[2], Angelika Polity[2], Peter J. Klar[2], and Sangam Chatterjee[2] — [1]Faculty of Physics and Materials Science Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]Institute of Experimental Physics I, Justus-Liebig-University Giessen, Heinrich-Buff-Ring 16, D-35392 Giessen, Germany

Transparent conducting oxides (TCOs) are currently receiving broad attention for device applications in displays or photovoltaics. An emerging TCO with promising properties is Tin(IV) oxide - SnO2. This material is cheap, very transparent and very thermally and chemically stable while it is at the same time virtually non-toxic [1]. Furthermore, SnO2 shows pronounced infrared reflection which is desirable for heat-managing window-applications. Here, we compare the optical properties of Tin(IV) oxide thin films by absorption and time-resolved photoluminescence spectroscopy. The thin films were deposited by either chemical vapor deposition (CVD) or ion-beam sputter deposition (IBSD) on c-plane and r-plane cut sapphire as well as quartz substrates. The CVD-grown layers are of higher structural quality than the IBSD-grown ones. Regardless, all samples are microcrystalline and the photoluminescence properties are hence dominated by impurity emission. [1] R. G. Gordon, Criteria for Choosing Transparent Conductors, MRS Bulletin 25, 52-57 (2000)

HL 63.7 Wed 15:00 P1A

Towards deterministic fabrication of circular Bragg gratings for enhanced quantum-dot based light sources — •Sascha Kolatschek, Stefan Hepp, Marc Sartison, Simone L. Portalupi, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

Highly efficient single photon sources are a crucial component for quantum information processes. Semiconductor quantum dots (QDs) have been proven to be excellent candidates due to their outstanding optical properties. Among different stratergies to increase light extraction, the use of photonic nanostructures enables, together with increased brightness, also an improved indistinguishability and reduced lifetime using linear optics and cavity quantum electrodynamic effects. Here we show a novel deterministic fabrication method for the integration of preselected QDs into a circular Bragg grating cavity. Besides their significant Purcell enhancement these cavities show due to the asymmetric design a more probable emission in the upside direction (i.e. upwards with respect to the substrate located underneath) with a highly directional far-field pattern.

HL 63.8 Wed 15:00 P1A

Exciton-light binding and lifetime of polaritons — •Hannes Lagemann[1] and Klaus Morawetz[2,3,4] — [1]University of Münster, — [2]Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [3]International Institute of Physics (IIP) Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — [4]Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Polaritons are investigated as quasiparticles formed when light and matter are strongly interacting. The exciton-photon interaction is modeled with the help of a separable potential. The dipole matrix element and the dipole transition rates are calculated and various lifetimes are discussed. Two modes are found whose lifetimes differ quantitatively and qualitatively as a function of the photon frequency. The regime where the exciton decays faster respectively slower than the polariton is determined.

HL 63.9 Wed 15:00 P1A

Fermi edge singularity and the functional renormalization group — •Fabian Kugler[1,2] and Jan von Delft[1] — [1]Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, D-80333 München — [2]Max-Planck-Institut für Quantenoptik, D-85748 Garching

We study the Fermi edge singularity, describing the response of a degenerate electron system to optical excitation, in the framework of the functional renormalization group (fRG). Results for the (interband) particle-hole susceptibility from various implementations of fRG are tested against the summation of all leading log. diagrams, achieved by a solution of parquet equations. For the (zero-dimensional) special case of the X-ray edge singularity, we analytically reproduce the (first-order) parquet formula in a consistent way from a truncated fRG flow. Reviewing the underlying diagrammatic structure, we show that this derivation relies on partial cancellations special to the form of and accuracy applied to the X-ray problem and does not generalize. In fact, we show that the truncated fRG flow can only generate a fraction of the parquet graphs.

HL 63.10 Wed 15:00 P1A

Electron transport in small CdSe Quantum Dots coupled with Methyl Viologen — •Mona Rafipoor[1,2], Jan-Philip Merkl[1], Zhi Wang[1], Gabriel Bester[1,2], and Holger Lange[1,2] — [1]Physikalische chemie, Uni Hamburg, Germany — [2]center of ultrfas imaging, Hamburg, Germany

Semiconductor nanocrystals have drawn significant interest due to their light absorption and electron transport properties which are mostly used for solar cells materials. Electron transfer and light absorption in very small CdSe quantum rods (QRs) (diameter of 1.8 nm) coupled with electron acceptors Methyl Viologen (MV+2) were investigated by Transient Absorption spectroscopy.

HL 63.11 Wed 15:00 P1A

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

PbTe is a leading thermoelectric material, notable for its low thermal conductivity and large carrier mobility at low doping levels. Using time-resolved differential reflectivity measurements, we shed light on the ultrafast relaxation of highly excited carriers, probing the dynamics of electron-phonon interactions on the femtosecond and picosecond time-scales. Our results suggest that phonon-mediated intervalley scattering involving the Σ-point band gap plays a significant role in the carrier cooling process due to its unique energy dispersion. In addition, anomalous temperature dependencies in the carrier relaxation rates support recent observations of giant anharmonic interactions between LA and TO phonons in this material.

HL 63.12 Wed 15:00 P1A

Source Development for Ultrafast Transmission Electron Microscopy — •Nora Bach, Armin Feist, Katharina E. Priebe, Nara Rubiano da Silva, Thomas Danz, Marcel Möller, Jan Gregor Gatzmann, Stefan Rost, Jakob Schauss, Stefanie Strauch, Reiner Bormann, Murat Sivis, Sascha Schäfer, and Claus Ropers — 4th Physical Institute - Solids and Nanostructures, University of Göttingen, Germany

Ultrafast transmission electron microscopy (UTEM) is a novel experimental technique that combines nanoscale spatial with femtosecond temporal resolution [1]. However, the achievable performance for imaging and diffraction is limited by the brightness of current laser-driven electron sources.

Here, we present the design and implementation of an advanced UTEM instrument based on the modification of a commercial Schottky field emission TEM [2,3]. Single-photon photoemission from a tip-shaped ZrO/W(100) emitter is employed, yielding electron pulses with a spectral bandwidth of 0.6eV, a low beam emittance of about 1-10nm mrad, and an electron probe size down to 0.9nm. We characterize the temporal structure of the electron pulses by electron-photon cross-correlation and obtain pulse widths down to 200fs (full-width-at-half-maximum). The high beam quality demonstrated will enable new applications in the study of nanoscale ultrafast dynamics, including ultrafast electron holography and phase-contrast imaging.

[1] A. H. Zewail, Science 328, 187 (2010) [2] A. Feist et al., Nature 521, 200 (2015) [3] A. Feist et al., arXiv:1611.05022 (2016)

HL 63.13 Wed 15:00 P1A

Time evolution of the non-thermal phonon gas after laser excitation in antimony — •Sergej Krylow, Bernd Bauerhenne, Tobias Zier, Eeuwe S. Zijlstra, and Martin E. Garcia — Universität Kassel, Theoretische Physik II, Heinrich-Plett-Straße 40, 34132 Kassel,Germany

We study the decay of the femtosecond-laser excited coherent A_{1g} phonon mode in antimony using electronic temperature dependent density-functional-theory molecular-dynamics simulations for supercells with 576 atoms, in which a decay time due to phonon-phonon interactions of about 3 ps can be seen. By utilizing a second type of MD simulations where the A_{1g} phonon is de-occuppied after laser excitation we are able to unravel the decay channels without relying on the usual perturbative approaches. In particular, we can see two decay channels which depend on the applied laser fluence and which we account to a third and a fourth order scattering process.

HL 63.14 Wed 15:00 P1A

An ultrafast electron diffraction setup for molecules in aqueous solution — •Arne Ungeheuer, Arne Senftleben, Marlene Adrian, Silvio Morgenstern, and Thomas Baumert — Institut für Physik, Universität Kassel, 34132 Kassel, Germany

Here we present a scheme for an ultrafast electron diffraction setup for electron diffraction on liquids and molecules in aqueous solution. We adapt the idea to use two obliquely colliding single laminar jets for the creation of a leaf-shaped flatjet with submicrometer thickness required for electron diffraction in transmission mode. The issue of multiple scattering in these relatively thick samples is addressed by the use of a Wien energy-filter to increase the signal-to-noise ratio. Preliminary results of field-simulations for a suitable filter-geometry are shown.

HL 63.15 Wed 15:00 P1A

CO2 activation on ZnO surface studied by ultrafast photoelectron spectroscopy — •Sesha Vempati, Lukas Gierster, and Julia Stähler — Fritz-Haber-Institute, Berlin, Germany

We investigate the electron injection dynamics from ZnO(10-10) into an adsorbed layer of CO_2 molecules via time-resolved two-photon photoelectron spectroscopy (TR-2PPE). ZnO is known to be a catalyst for the hydrogenation of the CO_2 producing methanol like fuels in heterogeneous catalysis. CO_2 adsorbs on ZnO in a bent geometry to form a tridentate configuration possibly due to partial reduction. Despite of various studies, the energies of the frontier molecular orbitals of CO_2 on ZnO are unknown. Using TR-2PPE we unveil the energies of the frontier molecular orbitals of CO_2 on ZnO. We find that CO_2 adsorption causes a significant increase in the work function ($\approx$ 1.2 eV for 0.5 ML) consistent with a partial reduction ($CO_2^{-\delta}$) and/or the dipole moment associated with the bent molecules. Furthermore, TR-2PPE measurements suggest that above gap excitation in fact injects electrons from ZnO into the lowest unoccupied molecular orbital (LUMO) of $CO_2^{-\delta}$ molecule. After this electron capture, the LUMO shifts below the Fermi energy within 2 ps and forms a metastable state. This down shift is presumably accompanied by the changes of the nuclear coordinates of CO_2 due to the additional charge. This is probably the stage where the CO_2 molecule is completely activated for hydrogenation.

HL 63.16 Wed 15:00 P1A

Biomimetic imitation of strongly scattering beetle scales — •Marie-Christin Angermann[1] and Georg von Freymann[1,2] — [1]Physics Department and Research Center OPTIMAS, University of Kaiserslautern, Kaiserslautern, Germany — [2]Fraunhofer Institute for Physical Measurement Techniques IPM, Kaiserslautern, Germany

The white beetle Chyphochilus is covered with 5 μm thick scales consisting of a chitin network. These scales reflect 80% of the light [1] and are strong scatterers. The composition of the scattering network is not yet understood.

To mimic the beetle, we therefore simplify this network with a tailored disordered model. The model bases on a periodic grid. All intersection points of the grid lines are shifted in up to 8 different directions. The shifting is determined by an aperiodic series, an approach similar to [2]. The optical response is theoretically calculated by a finite difference time domain method. Corresponding structures are fabricated via direct laser writing.

First results show a total reflectance of about 32% to 42% over the whole visible spectrum. The backscattered intensity is evenly distributed over the half space. The most important parameter for high reflectance is the number of layers. Furthermore, the distribution of the backscattered light depends on the disorder in a single layer. Further optimization might pave the way towards highly efficient scattering materials.

[1] Burresi, M., et al. Scientific reports 4, 6075 (2014)
[2] Renner, M., et al. Scientific reports 5, 13129 (2015)

HL 63.17 Wed 15:00 P1A

Single photons slowed down by cesium-vapour — •Lucas Bremer[1], Alexander Thoma[1], Max Strauss[1], Sarah Fischbach[1], Sven Rodt[1], Tobias Heindel[1], Jin-Dong Song[2], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, TU Berlin, Berlin, Germany — [2]Center for Opto-Electronic Materials and Devices, KIST, Seoul, Korea

Semiconductor quantum dots (QDs) proved to be close to ideal emitters of single and indistinguishable photons, which can be further combined with deterministic device fabrication technology [1]. Atomic vapours in contrast can be used to slow down photons spectrally in resonance with their absorption lines [2]. Thus, hybrid systems interfacing single photons from a quantum dot with atoms show promise for the storage of quantum information [3]. In this work we investigate the temporal delay introduced by the high dispersion of the excited state hyperfine resonances of cesium-vapour, which is a crucial step towards the realization of quantum memories. Tuning the QD emission into the atomic resonance we are able to study the amount of photons delayed by the atoms. Increasing the temperature of the cesium-vapour enables us to observe a maximum delay of $\tau = (11.4 \pm 0.5)$ ns.

[1] Gschrey et al., Nat. Commun. 7662, 6 (2016)
[2] Akopian et al., Nat. Photonics 5, 230 (2010)
[3] Chanelière et al., Nature 438, 833 (2005)

HL 63.18 Wed 15:00 P1A

Quantum dots interfaced with cesium atoms for photonic delay: study on the photon linewidth dependence — Hüseyin Vural[1], Jonas Weber[1], Markus Müller[1], •Simon Kern[1], Julian Maisch[1], Matthias Widmann[2], Robert Löw[3], Jörg Wrachtrup[2], Ilja Gerhardt[2], Simone Portalupi[1], Michael Jetter[1], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]3. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart — [3]5. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart

Hybrid quantum systems, based on semiconductor quantum dots (QDs) and alkali vapors, constitute a recent research field which is attracting a growing attention. An important step for future applications is constituted by the possibility to slow down single photons coming from a QD. This effect has been investigated with photons coming from QDs under different pumping conditions, but always focusing on the absolute achievable delay and not investigating the effect of the photon linewidth. Here we report on a study on the photonic delay for photons with different linewidths. An atomic cell filled with Cs atoms is used as a variable delay line (via vapor temperature variation). Different QDs, which emit photons spectrally on resonance with the atomic transitions, are resonantly pumped and the emitted photons are transmitted through the vapor. QDs with different linewidths bring a different ratio between delayed and non-delayed photons.

HL 63.19 Wed 15:00 P1A

Interfacing single QD photons with Cesium Vapor — •Janik Wolters[1], Tim Kroh[2], Alexander Thoma[3], Stephan Reitzenstein[3], Rinaldo Trotta[4], Eugenio Zallo[5], Armando Rastelli[4], Oliver G. Schmidt[6], and Oliver Benson[2] — [1]Universität Basel — [2]Humboldt-Universität zu Berlin — [3]Technische Universität Berlin — [4]Johannes Kepler Universität Linz — [5]Paul-Drude-Institut für Festkörperelektronik, Berlin — [6]IFW Dresden

Hybrid quantum dot-atom systems might become a key ingredient for future heterogeneous quantum networks. In such a heterogenous quantum network quantum dots may serve as fast and efficient deterministic single photon sources, while atomic ensembles can be used to store quantum information with sufficiently long storage time, fidelity and efficiency to realize e.g. long distance quantum repeater links. A first step towards this vision is to interface single photons emitted by a semiconductor quantum dot with one single atomic hyperfine transition.

We have performed this step using a strain tunable InGaAs quantum dot emitting at 894 nm, corresponding to the Cs D1 line. The QD is excited non-resonantly by 50 ps laser pulses and precisely tuned the absorption minimum between two hyperfine transitions of the Cs D1 line. Under these conditions, strong dispersion occurs and already at moderate optical densities photons are slowed down to $\sim c/20$, where c is the speed of light in vacuum. This result is an important first step towards storage of the photons in a quantum memory with on-demand storage and retrieval.

HL 63.20 Wed 15:00 P1A

Currents in a chain of quantum dots — •Klaus Morawetz — Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics (IIP)Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Using the quantum kinetic equation analytical expressions for the currents in chains of quantum dots are derived. During the transient behaviour non-dissipative quantum correlations lead to a decay of the initial correlations. After this short time behaviour the total current for homogeneous electric fields is ballistic. For wavelength-modulated electric fields, an effective capacitance, inductance and Ohmic resistance can be realized given in terms of quantum parameter.

HL 63.21 Wed 15:00 P1A

Persistent Spin Textures and Quantum Interference in Arbitrary Oriented 2DEGs with Spin-Orbit Coupling — •Michael Kammermeier, Paul Wenk, and John Schliemann — Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

We discover general conditions for the realization of spin-preserving symmetries for 2DEGs with Rashba and Dresselhaus spin-orbit coupling [1]. In particular, such scenarios can be found for semiconductor heterostructures of zinc-blende type if and only if at least two Miller indices of the growth direction are equal in modulus. We determine the appropriate requirements on the leading Rashba and Dresselhaus contributions and discuss the impact of cubic Dresselhaus terms corresponding to third angular harmonics. Also, we identify the orientation of the homogeneous conserved spin state and the momentum shift which allows for a controlled spin rotation giving rise to a persistent spin helix. To support experimental probing, we provide analytical expressions for the weak (anti)localization correction and the characteristic shift of the magnetoconductivity minima which show an imprint of the peculiar symmetry. The latter enables a fitting-free determination of the system's transport parameters and is consistent with recent experimental observations [2].

[1] M. Kammermeier *et al.*, Phys. Rev. Lett. **117**, 236801 (2016).
[2] K. Yoshizumi *et al.*, Appl. Phys. Lett. **108**, 132402 (2016).

HL 63.22 Wed 15:00 P1A

High precision microscopic setup for optical analysis of TMD Monolayers — •Magnus Neumann, Jens Hübner, and Michael Oestreich — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, D-30167 Hannover

Transition metal dichalcogenides (TMDCs) are promising candidates for establishing valleytronic devices as their valley degree of freedom becomes both optically accessible and tunable for single layer structures [1]. The high binding energies of the resulting excitons make TMDCs favorable for room temperature applications. However, the investigation of micrometer-sized monolayers requires high spatial resolution and mechanical stability of the employed optical set-ups. Here, we design and characterize a confocal microscope applicable for transmission Faraday-rotation spectroscopy. By photoluminescence measurements on a quantum dot sample with moderate QD density we determined the spatial resolution and absolute repeatability. The high precision microscopic setup provides us with high resolution photoluminescence maps of TMDC monolayers. We will further examine the rich spin physics of TMDC monolayers by all-optical spin-noise-spectroscopy [2], as our setup is both suitable for reflection and transmission measurements. SNS does not rely on the high absorption coefficient of TMD Monolayers, leaving the sample in thermal equilibrium and thus revealing the intrinsic spin dynamics.

[1] G. Wang et al., PRL **117**, 187401 (2016).
[2] J. Hübner, F. Berski, R. Dahbashi and M. Oestreich, phys. stat. sol. (b) **251**, 1824 (2014).

HL 63.23 Wed 15:00 P1A

Proximity induced exchange interaction in graphene-YIG devices — •Alexey Kaverzin, Johannes C. Leutenantsmeyer, Magdalena Wojtaszek, and Bart J. van Wees — Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747AG, The Netherlands

Graphene is one of the promising platforms for the realisation of various spintronics devices. Large spin relaxation length and long spin relaxation time insure a reliable transport of the spin signal over a relatively large distances. Moreover, graphene is extremely sensitive to the environment and, therefore, can potentially adopt the properties of the underlying substrate via proximity effect.

In this work we study the effect of the ferrimagnetic electrically insulating substrate on the spin transport in exfoliated monolayer graphene. As a substrate we use yttrium iron garnet which preserves the magnetic ordering even at room temperature and induces a finite exchange interaction in the nearby graphene [1,2]. The change in the band structure results in a modified behavior of spins in graphene. We extend the standard Bloch diffusion equation with an additional exchange field and employ the solutions to fit the results. The extracted exchange field is found to be around 0.2 T. With these findings we show the robust method for producing ferromagnetic graphene and demonstrate a most direct method to probe the presence of an exchange interaction.

[1] Z. Wang et.al., Phys Rev Letters 114, 016603, (2015)
[2] J.C. Leutenantsmeyer et.al., 2D Materials 4, 1 (2017)

HL 63.24 Wed 15:00 P1A

Spin noise spectroscopy on a single InAs quantum dot — •André P. Frauendorf[1], Julia Wiegand[1], Dmitry S. Smirnov[2], Mikhail M. Glazov[2], Jens Hübner[1], and Michael Oestreich[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstraße 2, D-30167 Hannover — [2]Ioffe Institute, Polytechnicheskaya 26, 194021 St. Petersburg, Russia

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) in order to access the intrinsic spin dynamics of confined carriers in individualy selected single 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]. We show by high precision measurements a deviation from the spin dynamics which would be expected from the usual two level system. Particularly, accurate measurements in dependence of the probe laser detuning reveal the existence of an additional spin noise contribution that arises from the intriguing interaction with the solid state environment.

[1] J. Hübner, F. Berski, R. Dahbashi, and M. Oestreich, phys. stat. sol. (b) **251**, 1824 (2014).
[2] R. Dahbashi, J. Hübner, F. Berski, K. Pierz, and M. Oestreich, Phys. Rev. Lett. **112**, 156601 (2014).

HL 63.25 Wed 15:00 P1A

A stable laser for interferometric spin noise and high precision absorption spectroscopy — •Selina Volkert, Michael Beck, Jens Hübner, and Michael Oestreich — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, D-30167 Hannover

The inherent fluctuations of external cavity diode lasers impede the next generation interferometrically enhanced homodyne detection of spin noise at low frequencies [1]. To reduce its phase and frequency fluctuations by means of the Pound-Drever-Hall technique we will stabilize an external cavity diode laser onto a self-built and characterized high finesse Fabry-Perot reference cavity made from ultra low expansion glass. We will show the indispensability of this kind of stabilized laser for amplified detection of spin noise in the kHz frequency domain [2]. Furthermore, we will demonstrate the capabilities of the complete system by high resolution absorption spectroscopy of defect bound excitons in isotopically enriched silicon which inherently exhibits an ultra narrow homogeneous linewidth below $1MHz$ [3].

[1] S. Cronenberger *et al.*, Rev. Sci. Instr. **87**, 093111, (2016).
[2] R. Dahbashi *et al.*, Phys. Rev. Lett. **112**, 156601 (2014).
[3] A. Yang *et al.*, Appl. Phys. Lett. *95*, 122113 (2009).

HL 63.26 Wed 15:00 P1A

Nuclear Spin Relaxation in n-type GaAs — •lida abaspour, jan gerrit lonnemann, eddy patrick rugeramigabo, jens hübner, and michael oestreich — Institute for Solid States Physics, Leibniz University of Hannover, Germany

The intriguing mutual interaction of nuclear and electron spins in semiconductors [1] has been identified as a major source of nuclear as well as electron spin relaxation. Their relative impact significantly depends on the doping density which determines the degree of localization and the density of free electrons. The nuclear spin diffusion is governed

by the interaction with electron spins of localized impurities [2] and delocalized conduction band electrons [3], respectively. Here, we investigate the detailed impact of doping density on the nuclear spin relaxation by all optical Hanle depolarization. The n-type MBE-grown GaAs samples cover two orders of magnitude around the metal to insulator transition. Consequently, we are able to precisely determine the effects of dipole-dipole type and carrier mediated nuclear spin diffusion. Moreover, the technique allowed us to investigate the complex interaction with the spin of electrons either localized to impurities or constrained to a confining impurity band.

[1] F. Berski et al., Phys. Rev. Lett. 115, 176601, (2015).
[2] M. Kotur et al., Phys. Rev. B 94, 081201(R) (2016).
[3] M. Kotur et al., JETP Lett. 99, 37 (2014).

HL 63.27 Wed 15:00 P1A

Dependences of the spin-flip Raman scattering efficiency of Mn^{2+} ions in (Zn,Mn)Se/(Zn,Be)Se quantum wells — •Katja Barthelmi[1], Henning Moldenhauer[1], Carolin Lüders[1], Dennis Kudlacik[1], Victor Sapega[2], Jörg Debus[1], and Manfred Bayer[1,2] — [1]Experimentelle Physik 2, Technische Universität Dortmund, Dortmund, Germany — [2]Ioffe Institute, Russian Academy of Sciences, St. Petersburg, Russia

Due to the possibility of controlled manipulation of the spin properties of carriers, diluted magnetic semiconductors (DMS) are promising materials for spintronic applications. Extensive studies on DMS containing Mn^{2+} ions have investigated the carrier-Mn interactions, but still many questions remain unanswered.
In that context, we have studied the dependences of the spin-flip Raman scattering (SFRS) efficiency of Mn^{2+} ions in (Zn,Mn)Se/(Zn,Be)Se quantum wells with Mn concentrations of about 1.5%. We have shown that the Mn spin-flip scattering efficiency is strongly amplified by resonant excitation of the exciton in close-to-Faraday geometries and at certain magnetic field strengths. We could attribute this amplification to an interaction of single Mn^{2+} spins with clusters of several Mn^{2+} spins. Furthermore, we have observed that the Mn^{2+} SFRS exhibits a strong dependence on temperature and excitation density. In addition to that, we have detected a significant difference between the Mn^{2+} SFRS shift on the Stokes and anti-Stokes side, which may result from the nonlinear dispersion of the exciton magnetic polaron involved in the SFRS process.

HL 63.28 Wed 15:00 P1A

Optical orientation of hole magnetic polarons in (Cd,Mg)Te/(Cd,Mn,Mg)Te quantum wells — •Erik Kirstein[1], Evgeny A. Zhukov[1], Yuri G. Kusrayev[2], Kirill. V. Kavokin[2,3], Dmitri R. Yakovlev[1,2], Jörg Debus[1], Alexander Schwan[1], Ilya A. Akimov[1,2], Grzegorz Karczewski[4], Tomasz J. Wojtowicz[4], Jacek Kossut[4], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universit\"at Dortmund, 44221 Dortmund, Germany — [2]Ioffe Physical-Technical Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia — [3]Spin Optics Laboratory, St. Petersburg State University, 198504 St. Petersburg, Russia — [4]Institute of Physics, Polish Academy of Sciences, 02668 Warsaw, Poland

The hole magnetic polaron (HMP) formation was investigated in a CdMnTe diluted magnetic semiconductor quantum well structure. The HMP is formed by the anisotropic exchange field of holes along the sample growth axis acting on free Mn Spins. The HMP occurs as a long living non oscillating contribution to the Kerr rotation Pump Probe signal, with observed dephasing times up to 60 ns. The HMP polaron is analyzed in dependence of the magnetic field, the lattice temperature and different carrier concentrations. Moreover, the full picture of the investigated QW structures show clear dynamics of hole, Mn and high effective g-factor electron spins. One obtains a detailed view on the theory of the HMP formation and relaxation. With the heavy hole as the dominant factor of HMP complex, a potential barrier is introduced to explain the HMP relaxation.

HL 63.29 Wed 15:00 P1A

Spin dynamics and magneto-optical effects in YAG:Ce — •Kai Hühn, Jan Gerrit Lonnemann, Jens Hübner, and Michael Oestreich — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, D-30167 Hannover

The peculiar spin dynamics of carriers localized at Ce sites in YAG has recently drawn considerable attention [1]. Here we present the magneto-optical investigation on the $^2F_{5/2} \rightarrow {}^2D_{3/2}$ transition in a highly doped YAG:Ce^{3+} crystal at low temperatures. The photoluminescence spectrum reveals the zero-phonon-line position at 2.53346(16) eV. We resolve the complex system of phonon replicas which are explained with an idealized theoretical model. Furthermore, we measure the magneto-optical Voigt-Effect on a linear polarized probe laser beam for transversal magnetic fields showing a strong temperature and strain dependence.
The information of spin dynamics is generally contained within its equilibrium noise spectrum. A spin noise spectrum is obtained by mapping the spin fluctuations onto the linear polarization of a transmitted probe laser beam [2]. By using this technique we determine a spin decoherence time T_2 of 10.6(13) ns which coincide well with previously reported values [3].

[1] P. Siyushev *et al.*, Nature Com. **5**, 3895 (2014)
[2] J. Hübner *et al.*, phys. stat. sol. b **251**, 1521-3951 (2014)
[3] R. Kolesov *et al.*, Phys. Rev. Lett. **111**, 120502 (2013)

HL 63.30 Wed 15:00 P1A

Spin and charge transport in epitaxial graphene nanoribbons — •Talieh Ghiasi[1], Alexey Kaverzin[1], Jantje Schommartz[1,2], Johannes Aprojanz[2], Christoph Tegenkamp[2], and Bart van Wees[1] — [1]Physics of Nanodevices, Zernike Institute for Advanced Materials, University of Groningen, the Netherlands — [2]Institut für Festkörperphysik, Leibniz Universität Hannover, Germany

Graphene Nanoribbon (GNR) is the essential component of the future graphene-based Spintronics. Investigation of charge and spin transport in these quasi-one dimensional carbon based channels is the main focus of this experimental research. Evidence of ballistic transport in epitaxially grown GNR and the controlled well-defined spin-selective edges of the channel [1], show promises for ballistic fully spin-polarized transport in GNR-based devices. In this study, epitaxially grown GNRs on templated sidewalls and natural steps of SiC substrate are probed by ferromagnetic Cobalt electrodes made by electron-beam lithography technique. The use of the combination of local and non-local measurement geometries allows us to address charge and spin transport properties of studied GNRs independently. The finite conductance of the underlying SiC substrate is eliminated via using liquid Helium temperatures where the substrate becomes an order of magnitude more resistive than the studied nanoribbon. Various multi-terminal measurement configurations are used to separate the contact contribution and study directly the properties of the charge transport in GNR at different channel lengths and temperatures.

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

HL 63.31 Wed 15:00 P1A

Probe laser induced spin polarization of donor bound electrons in ^{28}Si:P — •Michael Beck[1], Nikolay Abrosimov[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

The decoupling of donor atoms from the nuclear spin bath of the host lattice in isotopically enriched silicon leads to very long coherence times of donor electron spins [1]. The exceptional purity of this system also entails an ultra narrow optical linewidth and well resolvable hyperfine splitting of the donor bound exciton transition [2] which is commonly used to probe spin properties of the localized electron ensemble [3]. We employ Faraday rotation spectroscopy and observe a strong spin polarization caused by the linearly polarized probe laser only [4]. The findings are explained by supplemental phase modulation absorption spectroscopy which reveals the evolution of the hyperfine coupled states in small magnetic fields.

[1] A.M. Tyryshkin *et al.*, Nature Matter. **11**, 143, (2012).
[2] M. L. W. Thewalt *et al.* J. Appl. Phys. **101**, 081724 (2007).
[3] J. Hübner *et al.*, Phys. Stat. Solidi (B), **251**, 1824 (2014).
[4] A. Yang *et al.*, Phys. Rev. Lett. **102**, 257401 (2009).

HL 63.32 Wed 15:00 P1A

Interferometrically Enhanced Spin Noise Spectroscopy of Rubidium — •Pavel Sterin, Jens Hübner, and Michael Oestreich — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany

Spin noise spectroscopy is a powerful method for detecting the unaltered spin dynamics in atomic gases and semiconductors [1] since the spin fluctuations in these systems implicitly contain information about

the intrinsic spin correlation which can be extracted from the spin noise power spectrum. Transparent samples allow to use the Faraday effect to map these spin fluctuations onto small rotations of a linearly polarized probe laser light. Here, the probe photon energy should be in the vicinity of an optical transition in order to ease the detection of the Faraday rotation. Hence, low probe laser intensities are necessary in order to reduce residual absorption and keep the system at thermal equilibrium [2], however, at the cost of the difficulties connected with low light detection. Recent advancement on high frequency measurements were achieved using a heterodyne setup [3]. Here, we employ a homodyne approach to concentrate on low frequencies, that are not accessible in the heterodyne setup. Conversely, the homodyne setup will allow to amplify the polarization signal, thereby making very low probe laser intensities accessible. A ^{87}Rb vapor reference cell will be used as a test system during the development of this experiment.

[1] Hübner et al., phys. stat. sol. B **251**, 1824, (2014).
[2] Dahbashi et al., Appl. Phys. Lett. **100**, 031906, (2012).
[3] Cronenberger et al., Rev. Sci. Instrum., **87**, 093111 (2016).

HL 63.33 Wed 15:00 P1A

Quantitative analysis of the hole-g-tensor in low-symmetry two dimensional hole systems — Christian Gradl[1], Michael Kempf[1], •Johannes Holler[1], Roland Winkler[2], Dieter Schuh[1], Dominique Bougeard[1], Alberto Hernández-Mínguez[3], Klaus Biermann[3], Paulo Santos[3], Christian Schüller[1], and Tobias Korn[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D-93040 Regensburg, Germany — [2]Department of Physics, Northern Illinois University, DeKalb, Illinois 60115, USA — [3]Paul-Drude-Institut für Festkörperelektronik, D-10117 Berlin, Germany

The complex structure of the valence band in most semiconductors leads to varied and in some cases unusual properties for spin-3/2 hole systems compared to typical spin-1/2 electron systems. In particular, two-dimensional hole systems show a highly anisotropic Zeeman spin splitting. We have investigated this anisotropy in GaAs/AlAs double quantum well structures both experimentally and theoretically. By performing time-resolved Kerr rotation measurements, we found a non-diagonal hole g-tensor, manifesting itself in unusual signal shapes as well as distinct dependencies on the magnetic field direction. We quantify the individual tensor components for [110]-, [113]- and [111]-grown samples and find very good agreement with our theoretical calculations.

HL 63.34 Wed 15:00 P1A

Electronic Raman scattering from spin-density excitations in a (001)-grown GaAs-AlGaAs quantum well — •Sven Gelfert[1], Alexander Glötzl[1], Christian Reichl[2], Dieter Schuh[1], Werner Wegscheider[2], Dominique Bougeard[1], Tobias Korn[1], and Christian Schüller[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany — [2]Laboratory for Solid State Physics, ETH Zürich, 8093 Zürich, Schweiz

We performed inelastic light scattering experiments on a 12-nm-wide (001)-oriented GaAs-AlGaAs single quantum well. The investigated system is asymmetrically Si doped to obtain a balanced Rashba and Dresselhaus SOI contribution (α=β). The resulting effective spin-orbit field is either parallel or antiparallel to the [110] in-plane direction.

Measurements on intrasubband transitions of the conduction band in backscattering geometry feature a double peak structure for the [110] direction due to spin splitting, while the [1$\bar{1}$0] direction only shows a single peak. By rotating the sample we could demonstrate a cosine behavior of the spin splitting for intermediate angles between these crystal directions.

HL 63.35 Wed 15:00 P1A

Optical characterization of polycrystalline YMnO3 films — •Daniela Täuber[1], Mirko Goldmann[1,2], Venkata Rao Rayapati[3], Danilo Bürger[3], Ilona Skorupa[3], Ivan G. Scheblykin[1], and Heidemarie Schmidt[3] — [1]Single molecule spectroscopy group, Lund University, Sweden — [2]TU Ilmenau, Germany — [3]Nanospintronics group, TU Chemnitz, Germany

Due to its electro-optical properties multiferroic $YMnO_3$ is a promising candidate for a new generation of multifunctional materials. Depending on the chemical composition and underlying substrate $YMnO_3$ thin films may exhibit orthorhombic or hexagonal crystal structure. Here we present the room-temperature spectral ellipsometry and photoluminescence data recorded on polycrystalline $YMnO_3$ and compare the Stokes shift in dependence on chemical composition. The Stokes shift of stochiometric $YMnO_3$ is larger than 300 meV. Smaller Stokes shifts of 130 meV, 110 meV, and 60 meV have been observed for off-stochiometric $Y_1Mn_{0.99}O_3$+1.0$at\%Ti$, $Y_{0.94}Mn_{1.05}O_3$+1.0$at\%Ti$, and $Y_{0.95}Mn_{1.05}O_3$, respectively. Measured PL lifetimes are independent of chemical composition and are shorter than 200 ps.

HL 63.36 Wed 15:00 P1A

Sensing Weak Microwave Signals by Quantum Control — •Timo Joas, Andreas M. Waeber, Georg Braunbeck, and Friedemann Reinhard — Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4, 85748 Garching

Solid state qubits, such as the Nitrogen-Vacancy (NV) center in diamond, are attractive sensors for nanoscale magnetic and electric fields, owing to their atomically small size [1]. A major key to their success have been dynamical decoupling protocols (DD), which enhance sensitivity to weak AC signals such as the field of nuclear spins from a single protein [2]. However, those methods are currently limited to signal frequencies up to several MHz.

Here, we present a novel DD protocol specifically designed to detect weak fields close to the NV's transition frequency ($\approx$ 2 GHz). Our scheme is a pulsed version of Autler-Townes spectroscopy [3] with improved spectral resolution. As a result, we demonstrate slow Rabi oscillations with a period up to $\Omega_{Rabi}^{-1} \sim T_2$ driven by a weak signal field. The corresponding sensitivity could enable various applications. Specifically, we consider detectors for radio-astronomy and ultrasound, as well as fundamental research on spin-phonon coupling.

[1] Taylor et al., Nature Physics 4 (2008) [2] Lovchinsky et al., Science 351 (2016) [3] Gordon et al., Appl. Phys. Lett. 105 (2015)

HL 63.37 Wed 15:00 P1A

Broadband Electrically Detected Magnetic Resonance using Optimal Control — •Lukas Stelzer[1], Florian M. Hrubesch[1], Wolfgang Kallies[2], Steffen J. Glaser[2], and Martin S. Brandt[1] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München — [2]Chemie-Department, Technische Universität München

We present a broad-band spin resonance setup with the ability to apply shaped pulses for electrically detected magnetic resonance (EDMR). The setup uses non-resonant stripline structures for on-chip radiofrequency and microwave delivery and was tested to work in the frequency range from 4 MHz to 18 GHz. In combination with a broadband microwave amplifier with a saturated power of 10 W the stripline structures allow for B_1 fields of 0.3 mT and higher. We first demonstrate the functionality of this EDMR spectrometer using adiabatic BIR4 pulses for arbitrary rotations of both electron spins as well as nuclear spins in ENDOR experiments using adiabatic pulses only [1]. We then extend this approach to optimal control pulses and systematically explore the applicability of optimal control point-to-point, universal rotation and cooperative pulses to the various types of EDMR experiments.

[1] F. M. Hrubesch, G. Braunbeck, A. Voss, M. Stutzmann and M. S. Brandt, JMR 254, 62 (2015)

HL 63.38 Wed 15:00 P1A

Meeting the Technical Requirements for High-Power Spin Pumping in Silicon Carbide — •Moritz Fischer[1], Andreas Sperlich[1], Georgy Astakhov[1], 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

Silicon vacancies in silicon carbide (SiC) have recently been put into the focus of research due to their spin-dependent optical properties being similar to NV centers in diamond [1]. Due to spin-dependent relaxation, optical excitation results in a population inversion at room temperature. As the electron spin resonance associated with the silicon vacancy S=3/2 states can be shifted in an external magnetic field, one can preciseley tune the stimulated microwave emission to the microwave cavity resonance modes. In this study, we concentrate on strongly pumped SiC with the goal to achieve positive MASER gain. A box cavity was designed for the X-Band microwave regime (10 GHz) to be filled with stacked SiC wafers. The gain material is excited with a 15 W diode laser, operating at 810 nm. We investigate the power dependence of the electron spin resonance. The microwave resonator characteristics are analyzed in terms of the cavity Q factor and how it depends on heating due to laser light absorption.

[1] H. Kraus et al., Nature Physics **10**, 157 (2014)

HL 63.39 Wed 15:00 P1A

Commercial Silicon Carbide Diodes for Quantum Sensing Applications — •Dimitrij Poprygin[1], Christian Kasper[1], Hannes Kraus[1], Dmitrij Simin[1], Takeshi Ohshima[2], Andreas Sperlich[1], Georgy V. Astakhov[1], and Vladimir Dyakonov[1,3] — [1]Exp. Physics VI, Julius Maximilian University of Würzburg — [2]National Institutes for Radiological Science and Technology (QST, formerly Japan Atomic Energy Agency), Takasaki, Japan — [3]ZAE Bayern, Würzburg

Silicon carbide (SiC) is a technologically advanced semiconductor for high-power and high-temperature electronics and is also a viable candiate for solid-state quantum applications in sensing, rf-devices and quantum computing. This is due to the properties of atomic-scale defects, which rest in stable and cost-effective SiC crystals.
In this study, commercial SiC diodes with varying spatial distribution of Si-vacancies (V_{Si}), produced by electron irradiation, are analyzed in respect of their electrical properties. The work contains current-voltage characteristic measurements and detection of optically-active V_{Si} centers in the intrinsic layer of the diodes. The determination of an irradiation threshold to develop operative diodes with sufficient amount of V_{Si} for nanotesla magnetic field sensing is the main goal in this research. Silicon vacancies in SiC reveal a rf-free and room temperature alternative to nitrogen vacancies (NV) in diamond for sensing applications [1], which is the standard solid state system for quantum-sensing so far.

[1] D. Simin et al., Phys. Rev. X **6**, 031014 (2016).

HL 63.40 Wed 15:00 P1A

Self assembled InAs islands growth on high-index GaAs substrate by Stranski-Krastanov mode — Patrick Krawiec, Johann Peter Reithmaier, and •Mohamed Benyoucef — Institute of Nanostructure Technologies and Analytic (INA), CINSaT, University of Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

Quantum dots (QDs) grown on high-index substrates are promising candidates for generating polarization-entangled photons due to their low excitonic fine structure splitting. However, QDs grown on such substrates using conventional Stranski-Krastanov (SK) mode are difficult to realize. The failure of SK-growth on e.g., (111) surfaces has driven the development of alternative growth techniques. In our work, we revisit the challenging SK growth on high-index GaAs substrates using molecular beam epitaxy. By careful control of the growth parameters it was possible to produce a low density of InAs islands, which was confirmed by atomic force microscopy (AFM) measurements. Angle measurements of the island side walls using data derived from AFM reveal clear facets. Optical properties of the grown structure such as emission wavelengths and polarization are determined by microphotoluminescence (μ-PL) measurements. The low temperature μ-PL measurements prove the formation of 3D nanostructures.

HL 63.41 Wed 15:00 P1A

InP-based photonic crystal microcavities embedded with InAs quantum dots for telecom wavelengths — Andrei Kors, Kerstin Fuchs, Johann Peter Reithmaier, and •Mohamed Benyoucef — Institute of Nanostructure Technologies and Analytic (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 optimized InP-based QDs. Medium InP-based 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. L3-photonic crystal air-bridge cavities are fabricated by electron beam lithography, inductively coupled plasma reactive ion etching and wet etching technique. The sacrificial layer is removed by selective wet etching, forming a suspended PhC membrane. Optical properties of microcavities such as polarization, emission wavelengths and quality factors are determined by microphotoluminescence measurements. Results reveal enhanced quantum dot emission, sharp cavity modes and measured quality factors in excess of 8500 at telecom C-band wavelengths.

HL 63.42 Wed 15:00 P1A

Effect of Gold/Silicon implantation for catalyst assisted growth of III/V-Core-Shell-Nanowires — •Marcel Schmidt, Rüdiger Schott, Sven Scholz, Arne Ludwig, and Andreas D. Wieck — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum

Semiconductor nanowires (NWs) have a huge potential in the aim of further miniaturization of nanoscale devices due to there large surface to volume ratio as well as there strong light and carrier confinement. A prerequisite for the fabrication of nanowire devices is their doping. With the tempting prospect to achieve doping of the NWs by just using Si-doped Au metal seeds as NW catalysts, we investigate catalyst assisted molecular beam epitaxy (MBE) grown GaAs-AlGaAs-core-shell NWs. A focused ion beam system equipped with an ExB filter and a liquid metal alloy ion source (LMAIS) is used to implant the metals seeds. We will present our results on structure, morphology and optical properties, comparing Au and AuSi catalysed GaAs-AlGaAs-core-shell NWs.

HL 63.43 Wed 15:00 P1A

Optical enhancement of quantum dot emission by surface nanowires — •Sven Scholz, Rüdiger Schott, Carlo Sgroi, Yannick Raffel, Andreas D. Wieck, and Arne Ludwig — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Germany

Molecular beam epitaxy (MBE) quantum dot (QD) structures are used as fundamental research structures to investigate quantum optical phenomena. To further enhance their optical properties we use nanowires as a subwavelength waveguide. While common photonic crystal structures work with holes or micro pillars, we use focused ion beam (FIB) to catalyze nanowire growth on QD structures. The LED-QD structure is optimized regarding the optical emission. Therefore we use a methode to remove the wetting layers (WL) PL signal. To access a wide emission spectrum we use rapid-thermal annealing (RTA) and a flushing technique coupled with the WL suppression. This results in tunable and good separated QD emission peaks. The NW growth is characterized and optimized with regards to crystalline quality and morphology. The samples are characterized by photoluminescence/electroluminescence, scanning electron microscope imaging and capacitance-voltage spectroscopy.

HL 63.44 Wed 15:00 P1A

Multi-excitonic structure of type-II quantum dots — •Petr Steindl[1,2] and Petr Klenovsky[1,2] — [1]Central European Institute of Technology, Masaryk University, Czech Republic — [2]Department of Condensed Matter Physics, Faculty of Science, Masaryk University, Czech Republic

We study the multi-particle structure of quantum dots with spatially separated electrons and holes, usually termed type II. Our calculations based on customarily developed full-configuration interaction approach reveal that exciton complexes consisting of more electrons than holes are enormously antibinding in type II making those the hallmark of that kind of confinement. By an extension of our model we obtain approximate self-consistent solution of the multi-exciton problem and we explain the elusive blue-shift of the emission with pumping as well as the reason for the large inhomogeneous spectral broadening seen for type-II systems as an effect of trap filling. The results are confirmed by detailed intensity and polarization resolved photoluminescence measurements on large number of samples.

HL 63.45 Wed 15:00 P1A

Challenges of low density indium-flushed self-assembled quantum dots growth — •Rüdiger Schott, Julian Ritzmann, Sven Scholz, Sascha R. Valentin, Andreas D. Wieck, and Arne Ludwig — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Germany

Self-assembled InAs quantum dots (QDs) have been widely investigated due to their prospect applications in futuristic optoelectronic devices like single-photon sources.

For single optically addressable QDs, growth is usually performed with a rotation stop to obtain an indium flux gradient on the sample with reasonable low QD-density (10^8 cm^{-2}) at a transition point. Starting from such a gradient sample, we report on our attempts to achieve homogeneous high quality MBE growth of low density indium-flushed QDs. We identify the main challenges to be related to substrate temperature inhomogeneity and slight indium flux variations. Detailed photoluminescence spectroscopy maps of the grown structures are presented and correlated with the profile of the heater and the indium cell

geometry.

HL 63.46 Wed 15:00 P1A

Optical and Electronic Characterization of Coupled Quantum Dots — •Clara Junggebauer[1], Shovon Pal[2], Sascha R. Valentin[1], Sven Scholz[1], Andreas D. Wieck[1], and Arne Ludwig[1] — [1]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Germany — [2]NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, Pisa, Italy

Self-assembled quantum dots are promising candidates for the development of quantum information processing units like quantum bits, single photon sources or quantum memories. Coupled quantum dots, also called quantum dot molecules (QDM) in a semiconductor solid state matrix allow for controlled charging and tuning of the electronic energy level's coupling. The research so far is mostly done in other works by optical spectroscopy on single QDMs. Here, we present capacitance-voltage spectroscopy with and without illumination to access electronically the energy level structure of a QDM ensemble coupled to an electron reservoir. This is possible due to a high size homogeneity of the prepared QDM ensembles.

HL 63.47 Wed 15:00 P1A

Resonance Fluorescence of Plasmon-Quantum Dot Hybrids — •Chiara Bauer, Gerhard Schäfer, and Markus Lippitz — Experimental Physics III, University of Bayreuth, Germany

Many groups have used resonance fluorescence spectroscopy as a powerful tool to investigate single quantum dots. We present first steps towards resonance fluorescence spectroscopy of plasmon-quantum dot hybrids using a crossed-polarizer setup. We investigate which optical elements have limiting effects on the suppression of the incident light in benefit of detecting the scattered photons. We also discuss how a Fano resonance reveals the coupling of quantum dots and plasmonic structures.

HL 63.48 Wed 15:00 P1A

Speeding up a single quantum dot pump-probe experiment — •Gerhard Johannes Schäfer[1], Christian Dicken[1,2,3], Christian Wolpert[2,3], Armando Rastelli[4,5], and Markus Lippitz[1,2,3] — [1]Experimentalphysik III, Universität Bayreuth, Bayreuth, Germany — [2]4th Physics Institute and Research Center SCOPE, University of Stuttgart, Stuttgart, Germany — [3]Max Planck Institute for Solid State Research, Stuttgart, Germany — [4]Institute for Integrative Nanosciences, IWF Dresden, Dresden, Germany — [5]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, Linz, Austria

We recently showed [1], that it is possible to measure transient reflection on single semiconductor quantum dots in the far field. Here we discuss how to improve those measurements.

The lifetime of an excited quantum dot is around of 300 ps. The time delay between two laser pulses in the old setup (repetition rate 78 MHz) is 12 ns. By changing the laser system to another one with a higher repetition rate (1 GHz) we reduce this time delay to 1 ns.

We are interested in the characterization of a single quantum dot two-level system and its interaction with environment through transient absorption spectroscopy. We will add plasmonic structures to do antenna enhanced single quantum dot spectroscopy.

[1] C. Wolpert, C. Dicken, P. Atkinson, L. Wang, A. Rastelli, O. G. Schmidt, H. Giessen, and M. Lippitz, Nano Lett. 12, 453 (2012).

HL 63.49 Wed 15:00 P1A

Resonantly excited quantum dots embedded in GaAs rib waveguides — •Jonas Binz, Thomas Herzog, Mario Schwartz, Ulrich Rengstl, Matthias Paul, Simone Portalupi, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Allmandring 3, D-70569 Stuttgart

One of the major goals to realize linear optic quantum computation circuits is the fully on-chip integration of single-photon sources, single-photon detectors and waveguide (WG) structures. The circuit itself needs bended WG structures for building elements like a beamsplitter. However the bend radius cannot be chosen arbitrary small since the losses are increasing. In our approach, we investigate InGaAs quantum dots (QDs) embedded in GaAs/AlGaAs single-mode WG structures with varying curvature radii. By improving our design from a cosine shaped WG to a round shaped one, we could reduce the curvature radius to 10 μm from previously 20.6 μm while maintaining losses of 2.8 dB/mm.

For experiments on the single-photon level, the laser background under resonant excitation has to be as low as possible. Our measurements via pulsed resonant excitation with the polarization parallel to the WG allow us to efficiently excite a QD having almost no unwanted laser background contribution ($\sim 1\%$). This results in observation of Rabi-oscillations with more than two periods of QD emission as a function of the laser excitation power.

HL 63.50 Wed 15:00 P1A

Two-color two-photon biexciton generation in single quantum dots — •Björn Jonas, Amlan Mukherjee, Alexander Leier, Alex Widhalm, Nand Lal Sharma, Dirk Reuter, and Artur Zrenner — Center for Optoelectronics and Photonics Paderborn (CeOPP), Universität Paderborn, Paderborn, Germany

Quantum dots are among the best controlled solid state emitters at the single photon level. One particular area of interest is the generation of single photons at emission wavelength different from the excitation wavelength using nonlinear two-photon transitions between the biexciton state and the ground state of quantum dots. A promising approach to gain even more control over the emission wavelength and polarization is to generate single photons by a stimulated downconversion process from the biexciton state. [1] As preliminary work, we performed degenerate (one-color) and nondegenerate (two-color) resonant two-photon biexciton generation in InGaAs-quantum dots embedded in a n-i-Schottky-photodiode. This allows for the detection of the resulting excitations in the photocurrent with good accuracy. We demonstrate two-color two-photon excitation of the biexciton state and compare it to the degenerate process. Furthermore, we measure the biexciton peak amplitude as function of the energy separation between the two excitation lasers.

[1] D. Heinze et al., Nature Communications 6, 8473 (2015).

HL 63.51 Wed 15:00 P1A

Towards coherent optical coupling of two single quantum dots in a microdisk photonic molecule — •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 coherent control of the interaction of two quantum dots in a coupled quantum system promises e.g. the implementation of parallel qubit operation for quantum information processing applications. To grant individual addressability and selective tunability of each quantum dot, attempts are undertaken to realize coherent coupling between two dots each in a different GaInP-based microdisk resonator.

We apply optical spectroscopy and mode selective real space imaging as well as photoluminescence mapping to discern single quantum dots possibly coupled to a microdisk supermode. These means provide evidence of mode coupling across the inter-disk gap as well as dots in resonance with such coupled modes. Second-order correlation measurements performed on a quantum dot located in the non-excited disk reveal an antibunching, thus indicating that its excitation is mediated via the coupled disk mode.

HL 63.52 Wed 15:00 P1A

Hole spin mixing due to biaxial strain on GaAs/AlGaAs quantum dots — •Fritz Weyhausen-Brinkmann[1] 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 GaAs/AlGaAs 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 biaxial strain for different types of QDs [1]. We find a heavy-hole spin mixing when LH-HH mixing is strong. The degree of linear polarization (DLP) is related to the heavy-hole weight of the wave function. This allows the determination of the latter by measuring the in-plane polarization, but the results are different in comparison to the model. We also find a universal relation between DLP and the polarization in

z-direction for lens shaped QDs.

[1] Y. Huo et al., Nature Physics 10, 46-51 (2014).

HL 63.53 Wed 15:00 P1A

Analyzing quantum-light sources via a photon-number-resolving transition edge sensor — •Martin von Helversen[1], Alexander Thoma[1], Marco Schmidt[1,2], Manuel Gschrey[1], Peter Schnauber[1], Jan-Hindrik Schulze[1], André Strittmatter[1], Jörn Beyer[2], Sven Rodt[1], Tobias Heindel[1], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany — [2]Physikalisch-Technische Bundesanstalt, Abbestraße 1, 10587 Berlin, Germany

Solid-state quantum-light sources based on single semiconductor quantum dots (QDs) are promising candidates for a variety of applications in the research fields of quantum communication and quantum metrology. In order to better understand and directly access the photon statistics emitted by such sources, we employ a state of the art photon-number-resolving detection system consisting of a transition edge sensor (TES). Using the TES-detectors, we investigate two different types of sources, namely a single-photon source [1] and a twin-photon source [2], both based on deterministic QD devices. The obtained results enable us to reconstruct the photon number distribution emitted by the respective quantum emitter.

[1] M. Gschrey, A. Thoma et al., Nature Commun. 6, 7662 (2015)
[2] A. Thoma, T. Heindel et al., A bright triggered twin-photon source in the solid state, arXiv:1608.02768 (2016)

HL 63.54 Wed 15:00 P1A

Optical Spectroscopy of Single Elongated CdSe/CdS Core/Shell Nanoparticles — •Alexandra Hinsch, Sven-Hendrik Lohmann, Christian Strelow, Tobias Kipp, and Alf Mews — Institut für Physikalische Chemie, Universität Hamburg, Grindelallee 117, 20146 Hamburg, Deutschland

Semiconductor nanoparticles show great potential for a multitude of opto-electronic applications such as LEDs or photovoltaic cells. Core/shell nanoparticles allow the tailoring of the emission wavelength via composition and size of the system. In elongated nanoparticles with a dot-like core and a rod-like shell, the length of the system is a further parameter for the control of optical properties. Here we present elongated CdSe/CdS core/shell nanoparticles with varying rod- and core-size. We show that green-fluorescent dot/rods are strongly polarized emitters at room temperature. Orange-fluorescent dot/rods with larger dots, however, exhibit a decreased degree of polarization at room temperature. At cryogenic temperatures the typical blinking of single dot/rod particles rarely occurs and an increase in polarization can be observed. We further show that it is possible to directly correlate TEM and PL measurements to visualize single measured particles.

HL 63.55 Wed 15:00 P1A

Quasi-resonant pulsed excitation of quantum dots emitting in the telecom O-band — •Jonatan Höschele, Fabian Olbrich, Jan Kettler, Matthias Paul, Simone L. Portalupi, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

Efficient quantum computing and quantum information require high quality single photons. In particular for long distance quantum communication one may want to benefit from low losses in standard fibers at telecom wavelength. QDs have demonstrated to fulfill both requirements: they are sources of high performance single photons and can be grown to reach telecom emission. In our case, we showed efficient emission up to the telecom O-band. This gives the possibility to profit from low absorption and zero dispersion at this wavelength.

While In(Ga)As QDs grown on a GaAs substrate already serve as high quality single-photon sources at 900 nm, sticking to this material system at higher wavelengths gives perspective to equally high performances. The MOVPE-process used to grow the QDs makes our single-photon sources even more industrially relevant.

In order to improve the source performance, we implement a pulsed quasi-resonant excitation scheme, which helps in reducing phonon contribution to pure dephasing and minimizes the time jitter. This yields triggered single-photon emission in the telecom O-Band with high coherence time and small linewidth.

HL 63.56 Wed 15:00 P1A

Capacitance calculations for charge detection in indium arsenide nanowires — •Felix Jekat[1], Moritz Sallermann[1], Sebastian Heedt[2], Patrick Zellekens[3], Stefan Trellenkamp[4], Werner Prost[5], Marcus Liebmann[1], and Markus Morgenstern[1] — [1]II. Institute of Physics B, RWTH Aachen — [2]Qutech, Kouwenhoven Lab, TU Delft — [3]PGI-9, Forschungszentrum Jülich, Germany — [4]PGI-8, Forschungszentrum Jülich, Germany — [5]Center for Semiconductor Technology and Optoelectronics, University of Duisburg-Essen

Indium arsenide (InAs) nanowires have been shown to be suitable as tips for scanning tunneling microscopy (STM) with similar quality compared to tungsten tips [1]. We present a device with the goal to enable time-resolved counting of single electrons directly at these InAs nanowire STM tips. To realize electron counting in the nanowire tip we place a second nanowire in close proximity and couple the two wires with a floating gate [2]. In order to determine the sensitivity of this setup we preformed capacitance calculation using Comsol Multiphysics. The results show that the sensitivity is high enough to detect individual electrons in the Quantum Dot of the nanowire STM tip.

[1] K. Flöhr et al. "Scanning tunneling microscopy with InAs nanowire tips", Appl. Phys. Lett. 101, 243101 (2012)
[2] Y. Hu et al. "A Ge/Si heterostructure nanowire-based double quantum dot with integrated charge sensor", Nature Nanotechnol. 2, 622 (2007)

HL 63.57 Wed 15:00 P1A

Design and Fabrication of a Double Quantum Dot System with Two Independent Charge Detectors — •Friso Ohlschläger, Johannes C. Bayer, Timo Wagner, Eddy P. Rugeramigabo, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover

We designed a tunable system of two tunnel-coupled quantum dots in series. The fabrication procedure includes optical lithography as well as electron beam lithography on an MBE-grown GaAs/AlGaAs heterostructure forming a 2DEG 110 nm beneath the surface. High tunability should be achieved using standard split gate technique. The quantum dots are then electrostatically defined by applying negative potentials to each gate. We designed a specific double quantum dot system (DQD) with two separate quantum point contacts enabling independent and simultaneous real-time detection of single electron tunneling events in the DQD. This allows the investigation of many different phenomena including feedback experiments [1].

[1] T. Wagner, et al., Nature Nanotechnology (2016)

HL 63.58 Wed 15:00 P1A

Internal wavelength stabilization of a quantum dot photon source — •Amran Al-Ashouri[1], Annika Kurzmann[1], Benjamin Merkel[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, Germany — [2]Chair for Applied Solid State Physics, Ruhr-Universität Bochum, Germany

Single-photon sources are desirable for many quantum optical experiments and are essential for a practicable implementation of quantum networks. Being able to emit antibunched, indistinguishable photons with a high flux, epitaxially grown quantum dots (QDs) are a realistic choice for building such sources. Furthermore, QD systems are conveniently integrable into existing semiconductor technologies, however, charge and spin noise are ubiquitous in common host materials, introducing random wavelength fluctuations of the emitted photons.

In this work, single self-assembled InAs QDs are used to demonstrate a noise-suppressing, internal feedback loop [1]. This feedback loop leads to a stabilization scheme that relies solely on charge carrier dynamics inside a Schottky diode heterostructure, in which a QD layer is embedded. Key to the observed effect is micropillar patterning, leading to charge storage near the QDs. First measurements show a noise filtering bandwidth of 10 Hz and model calculations are in good agreement with our data. With optimized material parameters, our model predicts bandwidths of several 100 kHz, enough for eliminating most noise and enabling wavelength-stabilized photon emission.

[1] B. Merkel et al., arXiv:1606.03215 [cond-mat.mes-hall] (2016).

HL 63.59 Wed 15:00 P1A

Fock states, annihilation and creation operators, and quantum statistical applications of quasinormal modes — •Sebastian Franke, Andreas Knorr, and Marten Richter — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, EW 7-1, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany

A quantum description of an open optical cavity, e.g. a metal nanoparticle or a micropillar cavity, is of high interest in the field of quantum optics of nanostructures. The open and dissipative character of these systems prevents the use of a canonical quantization scheme with photon modes for such cavities.

Our objective is to develop a quantization scheme via a Green's function approach[1] for an inhomogeneous and dispersive medium for the open cavity. Therefore, we use quasinormal modes[2] (QNM) with complex eigenfrequencies ω_μ and complex eigenfunctions $\mathbf{f}_\mu$ as a basis for the quantization. We construct suitable non-bosonic annihilation and creation operators $\hat{\boldsymbol{\alpha}}_\mu, \hat{\boldsymbol{\alpha}}_\mu^\dagger$ for every quasinormal mode ω_μ in the cavity. Furthermore the calculation of commutation relations and Heisenberg equations of motion for these operators coupled to quantum emitters (like quantum dots) will be shown together with a construction of the analogue of Fock states.

[1]T. Gruner and D.-G. Welsch, Phys. Rev. A 53, 1818, 1996

[2]P. T. Leung, S. Y. Liu, and K. Young, Phys. Rev. A 49, 3057, 1994

HL 63.60 Wed 15:00 P1A

Energy scales in quantum dots for single electron pumps — •Tobias Wenz[1], Friederike Stein[1], Frank Hohls[1], Hans Werner Schumacher[1], and Vyacheslavs Kashcheyevs[2] — [1]Physikalisch-Technische Bundesanstalt (PTB), 38116 Braunschweig, Germany — [2]Faculty of Physics and Mathematics, University of Latvia, LV 1002 Riga, Latvia

Quantum dots with tunable barriers can be used as single electron pumps. By capturing a well-defined number of electrons n from source and emitting them to drain with a high frequency f a quantized current $I = nef$ is produced, where e is the electron charge [1]. This concept is useful for on-demand electron sources for electron quantum optics and for the redefinition of the ampere by fixing the value of e. Several theoretical models, like the decay cascade model [2], describe the performance of tunable-barrier pumps in different regimes of operation. While they yield good fits, the respective energy scales cannot be easily obtained. This work aims at putting a number to these energy scales. One approach is to investigate the performance of single electron pumps at different temperatures and observe the broadening of transition lines in different pumping regimes. Another method is to use custom-tailored waveforms to extract tunneling rates during the loading phase of the quantum dot. Furthermore, this method can be used to study excited states in the quantum dot and reveal two-electron effects.

[1] B. Kaestner & V. Kashcheyevs, Rep. Prog. Phys. 78, 103901 (2015)

[2] V. Kashcheyevs & B. Kaestner, Phys. Rev. Lett. 104, 186805 (2010)

HL 63.61 Wed 15:00 P1A

Spectral tuning of GaAs-based photonic crystal cavities for the deterministic coupling of individual quantum dots — •Stephanie Bauer, Stefan Hepp, Simone L. Portalupi, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology IQ^{ST} and Research Center SCoPE, University of Stuttgart

Quantum dots (QDs) have been proven to be ideal candidates as single-photon sources especially when they are placed inside a cavity to benefit from cavity quantum electrodynamic effects. For sufficient enhancement it is important to spatially position the QD inside the field maximum of the cavity mode and to reduce the spectral mismatch between the cavity and the emitter. Recently, a lot of efforts have been made in terms of quality factor optimization and the deterministic positioning of individual QDs in nanostructures. However, the high Q-factor results in narrow cavity linewidth and the sensitivity of the spectral position due to unavoidable fabrication imperfections makes the deterministic coupling to preselected QDs complicated. Therefore, a postprocessing tuning mechanism is required to reduce the spectral detuning between the cavity and the embedded emitter. Here we show that we can tune the resonant wavelength of L3-photonic crystal cavities via several digital etching steps independently from individual QD lines to the wavelength of interest. This process can be repeated several times whereby the typical tuning is in the range of 3 nm. Furthermore, an improvement of the Q-factor could be observed for a large number of cavities depending on the initial design parameters of the cavity.

HL 63.62 Wed 15:00 P1A

Epitaxial growth and characterization of InP-based coupled quantum well - quantum dot structures — •Sven Bauer[1], Vitalii Sichkovskyi[1], Wojciech Rudno-Rudziński[2], Grzegorz Sek[2], and Johann Peter Reithmaier[1] — [1]Technische Physik, Institute of Nanostructure Technologies and Analytics (INA), CINSaT, University of Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany — [2]Institute of Physics, Wrocław University of Technology, Wybrzeze Wyspiańskiego 27, 50-370 Wrocław, Poland

InP-based directly modulated quantum dot (QD) lasers are promising candidates for usage in telecommunication at 1.55 μm. In order to improve the performance of these lasers, limited by the intraband carrier relaxation time, one might use a so called tunnel injection scheme. Carriers are captured and relax in a quantum well (QW) and tunnel through a thin barrier for recombination into the QDs. In order to get better understanding of the mechanisms involved in this scheme, coupled QW-QD structures have been grown on Fe-doped InP substrates. These consist of a compressively strained $In_{0.66}Ga_{0.34}As$ QW and InAs QDs separated by a thin InAlGaAs barrier. High density QD growth was optimized beforehand. A set of samples with different QW (2.4 nm, 4 nm, 5.6 nm) and barrier thickness (2 nm, 4 nm, 10 nm) combinations was grown and investigated with photoluminescence and photoreflectance spectroscopy. The working principle with respect to coupling strength as well as the importance of a favourable band alignment for performance and dominating recombination channel could be shown.

HL 63.63 Wed 15:00 P1A

All-optical tailoring of single-photon spectra in quantum-dot microcavity systems — •Dominik Breddermann[1], Dirk Heinze[1], Rolf Binder[2], Artur Zrenner[1], and Stefan Schumacher[1,2] — [1]Department of Physics and Center for Optoelectronics and Photonics Paderborn (CeOPP), Paderborn University, Warburger Strasse 100, 33098 Paderborn, Germany — [2]College of Optical Sciences, University of Arizona, Tucson, Arizona 85721, USA

Quantum-dot microcavity systems are promising nanostructures for solid-state based on-demand generation of single photons. Commonly, the spectral properties, such as frequency and linewidth, of the emitted single photon are pre-determined by the characteristics of the system, such as electronic transition energies and spectral properties of the resonator. Here, we theoretically analyze the spectral properties of a single photon generated from partly stimulated non-degenerate two-photon transitions [1] in quantum-dot-based multilevel systems in different configurations. We demonstrate that frequency and linewidth of the single photon are determined by the external control beam [2], and thus can be all-optically controlled during the photon-creation process.

[1] D. Heinze, D. Breddermann, et al., Nature Commun. 6, 8473 (2015) [2] D. Breddermann, D. Heinze, et al., Phys. Rev. B 94, 165310 (2016)

HL 63.64 Wed 15:00 P1A

Build-up of electron spin precession modes upon pulsed optical excitation in (In,Ga)As/GaAs quantum dots — •Eiko Evers[1], Vasilii Belykh[1], Alex Greilich[1], Dmitri Yakovlev[1,2], Dirk Reuter[3], Andreas Wieck[4], and Manfred Bayer[1,2] — [1]Experimentelle Physik 2, TU Dortmund University, 44221 Dortmund, Germany — [2]Ioffe Physical-Technical Institute, Russian Academy of Sciences, 194021 Saint Petersburg, Russia — [3]Optoelectronic Materials and Devices, Paderborn University, 33098 Paderborn, Germany — [4]Angewandte Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany

The electron-spin orientation of an ensemble of singly charged quantum dots with a periodic train of laser pulses in an external magnetic field leads to spin precession mode-locking. The recently developed extended pump-probe technique enables to tailor the number of polarizing pump pulses as well as to vary the delay of the probe pulse with a resolution limited only by the pulse duration over a time of several laser repetition periods. It is used to measure the electron-spin polarization build-up in the time domain as well as to monitor the decay of spin polarization after a given number of polarizing pulses which gives the mode structure of the electron-spin precession. Subsequently, we applied a continuous radio-frequency electromagnetic field decoupling the nuclear spin bath from the electron-spin polarization. This gives us the opportunity to study the build-up without nuclear effects such as frequency focusing and allows to determine their influence on the precession modes build-up.

HL 63.65 Wed 15:00 P1A

Magneto-optical study to reveal the exciton fine structure

in InP/ZnSe core/shell quantum dots. — •Annalisa Brodu[1], Mariana Ballottin[2], Dorian Dupont[3], Zeger Hens[3], Peter C. M. Christianen[2], Celso de Mello Donega[1], and Daniel Vanmaekelbergh[1] — [1]Debye Institute for Nanomaterials Science, Utrecht University, The Netherlands — [2]High Field Magnet Laboratory, IMM, Radboud University, The Netherlands — [3]Physics and Chemistry of Nanostructures, Ghent University, Belgium

Colloidal quantum dots (QDs) are of significant interest in nanoscience and opto-electronic applications due to their size-tunable emission spectrum in combination with broad absorption and excitation spectra. For decades, Cd-chalcogenide QDs have been the workhorse in this field. However, application in devices requires toxicologically harmless materials. As a result, the demand for Cd-free colloidal QDs is rising rapidly and therefore the knowledge of the electronic structure of InP-based core/shell QDs is of large interest.

In this work we studied the exciton fine-structure of InP/ZnSe QDs with various core diameters using different techniques: fluorescence line-narrowing spectroscopy, polarized photoluminescence (PL) spectroscopy and time-resolved PL spectroscopy, in high magnetic fields up to 30 T at temperatures down to 4 K. The high magnetic field allowed us to obtain a considerable Zeeman splitting of spin degenerate states and to induce significant mixing of exciton levels with different angular momentum. Combined with detection of the polarization of the emitted photons, the nature of the states has been resolved unambiguously.

HL 63.66 Wed 15:00 P1A

Investigation of quantum-well and defect luminescence of PAMBE-grown AlGaN/GaN nanowires for single-photon applications — •Johannes Dühn[1], Pascal Hille[2], Jörg Schörmann[2], Martin Eickhoff[1,2], 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. Due to confinement, these excitons also possess large binding energies, even exceeding 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 nanowires with GaN nanodiscs embedded in AlGaN barriers. We identify emission from single nanowires centered at 3.47eV and 3.45eV belonging to donor-bound excitons and inversion domain boundaries, respectivly. Furthermore, two emission bands from the nanodiscs centered at 3.55eV and 3.66eV are investigated, belonging to the quantum well emission and inversion domain boundaries. The emission from single excitons bound to defects is investigated with respect to their single-photon emission properties by using an HBT interferometer.

HL 63.67 Wed 15:00 P1A

Numerical Investigation of the Nonlinear Optical Properties of Quantum Dot Molecules (QDM) — •Peter Kölling and Jens Förstner — Universität Paderborn, Germany

We theoretically study the optical properties of epitaxially grown InAs quantum dot molecules which are integrated in Schottky diode structures. From optical experiments one knows that the electronic states inside the single quantum dots are coupled [1]. Applying gate voltages at these diode structures allows manipulation of the relative energies inside the single quantum dots as well as manipulation of carrier tunneling between the dots [2,3]. This in turn can be used to achieve switching between electronic states at nano- or picosecond time scales. Nonlinearities arise due to the excitation of exciton complexes with variable numbers of electrons and holes.

We investigate single particle eigenenergies and eigenstates under the influence of an external electric field by means of k.p-theory with the nextnano3 software package [4]. From the resulting single particle eigenstates we calculate Coulomb matrix elements and optical matrix elements required for Heisenberg equations of motion for a reduced density operator of the underlying system. The Heisenberg equations of motion are then solved to calculate theoretical nonlinear absorption spectra.

[1] G. Ordner et al., Phys. Rev. Lett. **94**, 157401 (2006)
[2] E. A. Stinaff et al., Science **311**, 636-639 (2006)
[3] M. Schreibner et al., Solid State Comm. **149**, 1427-1435 (2009)
[4] http://www.nextnano.de/nextnano3/

HL 63.68 Wed 15:00 P1A

Microsecond two-electron spin relaxation 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 — [2]Chair for Applied Solid State Physics, Ruhr-Universität Bochum, Universitätsstr. 150, 44780 Bochum, Germany

Self-assembled quantum dots (QDs) are promising candidates for quantum computation devices that require a two level system. One possibility is the two-electron excited spin triplet and its singlet ground state. The self-assembled 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 temporal decay of the triplet states by time-resolved transconductance spectroscopy [1]. This allows us to determine - by electrical means - the spin relaxation time after the injection of the second electron into the p- or d-shell. We find spin relaxation times of 25 μs (p-shell) and 23 μs (d-shell), orders of magnitude longer compared to optical experiments where an additional hole is present [2]. Future measurements in presence of a magnetic field are expected to demonstrate even longer spin-relaxation times in such an electrical device. [1] B. Marquardt. et al., Nature Commun. 2, 209 (2011) [2] F. Sotier et al., Nature Physics 5, 352 - 356 (2009)

HL 63.69 Wed 15:00 P1A

Angle-dependent magnetotransport measurements on single GaN nanowires — •Patrick Uredat, Matthias T. Elm, Pascal Hille, Martin Eickhoff, and Peter J. Klar — I. Physikalisches Institut, Justus Liebig University, Heinrich-Buff-Ring 16, D-35392 Giessen, Germany

III-V nanowires increasingly attract attention as building blocks for nanotechnological devices, in particular for optoelectronic devices such as light-emitting diodes or sensors. Thus, it is essential to study the influence of dopants on the transport properties. Angle-dependent magnetotransport measurements yield detailed information about electron transport in nanowires.

Here, we present investigations of the transport properties of GaN nanowires grown by molecular beam epitaxy. Single nanowires have been electrically contacted in four-point geometry using photo- and electron-beam lithography. Temperture-dependent measurements show semiconducting behavior for slightly doped nanowires, whereas nanowires with high doping concentration exhibit a metallic behavior. Magnetotransport measurements reveal a negative magnetoresistance due to weak localization reagardless of the doping concentration. In addition, universal conductance fluctuations (UCFs) have been observed for highly doped wires. Angle-dependent magnetotransport measurements have been performed by varying the angle between magnetic field and nanowire axis. From the angle-dependence of the UCFs one can deduce the distribution of elastic scattering centers and thus reveal the motion of electrons within a single nanowire.

HL 63.70 Wed 15:00 P1A

Computer-aided cluster expansion: An efficient algebraic approach for open quantum many-particle systems — •Alexander Foerster[1], Alexander Leymann[2], and Jan Wiersig[1] — [1]Otto-von-Guericke University Magdeburg, D-39016 Magdeburg, Germany — [2]Max Planck Institute for the Physics of Complex Systems, D-01187 Dresden, Germany

We introduce a computer-aided algebraic approach for a microscopic description of open quantum systems that we made available as open-source software[1]. The presentation combines the conceptual ideas of the computer-aided cluster expansion with the application to a current research topic - superradiance of semiconductor quantum dots. We exploit a configuration formulation that allows for an exact treatment of a subsystem e.g. a multilevel quantum dot [2,3]. The fundamental object of the system is described exactly while correlations between objects can be treated on different levels of approximation. Our program provides an efficient algebraic approach to derive equations of motion, while the user can focus on the physical modeling and conceptional questions. The procedures offer a variety of approximations applicable for finite systems with strong coupling as well as large systems where augmented mean-field theories apply.

[1] A. Foerster, H.A.M. Leymann, and J. Wiersig , Comput. Phys. Commun., http://dx.doi.org/10.1016/j.cpc.2016.10.010, (2016)
[2] H.A.M. Leymann, A. Foerster, et al., Phys. Rev. Applied **4**, 044018 (2015)
[3] F. Jahnke, ..., A. Foerster, et al., Nat. Comm. **7**, 11540 (2016)

HL 63.71 Wed 15:00 P1A

Spatial and temporal evolution of coherent polariton modes in ZnO microwire cavities — Tom Michalsky, Marcel Wille, •Evgeny Krüger, Stefan Lange, Marius Grundmann, and Rüdiger Schmidt-Grund — Institut für Experimentelle Physik II, Universität Leipzig, Linnéstraße 5, D-04103 Leipzig, Germany

We present experimental results for the spatial and ps-temporal evolution of coherent polariton states in ZnO based hexagonal microwires at room temperature. The estimation of the carrier density at the threshold excitation power reveals that the gain process is connected to the recombination out of an electron-hole plasma. The small spatial region of the cavity which is optically highly excited ensures together with a large intrinsic coupling constant of $V \approx 300$ meV that the cavities remain in the strong coupling regime as the highly excited region acts only as a small perturbation and source for the polariton population. We furthermore show that the model developed for the real- and k-space evolution of Bose-Einstein condensates based on the Gross-Pitaevskii equation [1] applies to our observations and gives similar results as obtained from nonlinear ray optics using a spatially varying particle density dependent refractive index for the cavity material.

[1] M. Wouters, I. Carusotto and C. Ciuti, Phys. Rev. B **77**, 115340 (2008)

HL 63.72 Wed 15:00 P1A

Numerical modeling of InP/AlGaInP quantum dots semiconductor optical amplifier — •Thomas Breier, Zhihua Huang, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen and Research Center ScoPE and IQST, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

Semiconductor Optical Amplifiers (SOAs) show great promises in many applications (e.g. optical communication networks, laser amplifications). Nowadays, the active regions of most SOAs are still mainly focused on the bulk materials and quantum wells. However, quantum dots (QDs) as active region have shown remarkable advantages in SOAs due to its higher material gain, larger gain bandwidth, faster gain recovery and lower threshold current density. This research work is aimed on numerically modeling of a tapered InP/AlGaInP quantum dots SOA emitting at around 660nm. The material gain of the QD layers was obtained by measuring the net model gain in combination with T-Matrix calculations of the confinement-factor of the QDs embedded in waveguides. Based on the measured gain value, the small signal gain, the output saturation power, and the amplified spontaneous emission (ASE) power were estimated. Furthermore, the output electrical field of the tapered waveguide was simulated by using traveling-wave equations (TWE), in order to evaluate the fundamental mode output. Additionally, the field distribution for different taper angles and taper shapes were compared. The simulation results provide a guideline to find the trade-off between high amplification and high beam quality.

HL 63.73 Wed 15:00 P1A

Optical gain and laser characteristics of InP/AlGaInP quantum dots red-emitting laser — •Zhihua Huang, Thomas Breier, Stefan Hepp, Roman Bek, 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

Quantum dots (QDs) as an active layer in laser sources are attractive for many applications due to their excellent properties resulting from their zero-dimensional density of states, e.g. higher optical gain, larger gain bandwidth, lower threshold current density, and temperature insensitivity. In this contribution, we experimentally investigate the properties of the single- and double-layers of InP quantum dots assembled in AlGaInP barrier emitting in the wavelength range around 660 nm, as well as the characteristics of edge emitting lasers with the above mentioned QDs as active region. The self-assembled InP quantum dots layers were grown in the Stranski-Krastanow growth mode by MOVPE at 710 degree with an estimated density of 1e10 cm-2. The optical gain and internal optical loses were measured at room temperature by utilizing segmented contact method at different injected current density, to analyze the amplified spontaneous emission (ASE) as a function of contact stripe length. For a 1-mm long laser with uncoated facets, the experimental results indicated that the single-layer QDs laser has lower threshold current density of 550 A/cm-2 at the heatsink temperature of 278 K. Furthermore, an output power of more than 100 mW per fact was achieved.

HL 63.74 Wed 15:00 P1A

Absorptive lasing mode suppression in highly excited ZnO nano- and microcavities — •Marcel Wille, Tom Michalsky, Chris Sturm, Evgeny Krüger, Marius Grundmann, and Rüdiger Schmidt-Grund — Institut für Experimentelle Physik II, Universität Leipzig, Germany

A variety of lasing experiments in nano- and microstructures reveal different lasing mode energies as well as linewidths for various excitation conditions. However, a conclusive explanation of the resonator mode properties is missing so far. Here, we explain the spectral position and linewidth of lasing modes of three ZnO nano- and microstructures, tetrapod-like nanoparticles, nanowires and microwires. We found that the structure size strongly influences the emission properties. The limited penetration depth of usually used excitation lasers and carrier diffusion lead to an inhomogeneous carrier distribution [1]. Hence, weakly or even nonexcited areas remain present after excitation and lead to strong absorption. This effect is most pronounced for whispering-gallery modes in microwires due to their larger dimensionality. Furthermore, the absorptive lasing mode suppression will be demonstrated for a single nanowire by varying the spot size of the excitation laser. In time-resolved PL measurements we found an ultrafast energy loss of the resonant modes, leading to a linewidth broadening in time-integrated spectra [2]. A model of the time dependent dielectric function fits the experimental observations quite well.

[1] M. Wille et al., Appl. Phys. Lett. 109, 061102 (2016)
[2] M. Wille et al., Nanotechnology 27, 225702 (2016)

HL 63.75 Wed 15:00 P1A

Magnetotransport in narrow-gap semiconductor nanostructures — •Johannes Boy[1], Olivio Chiatti[1], Christian Heyn[2], Wolfgang Hansen[2], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Institut für Angewandte Physik, Universität Hamburg, 20355 Hamburg, Germany

The Shubnikov de-Haas effect is a powerful tool to determine the electric transport parameters of a two-dimensional electrongas (2DEG). Our experimental work has been directed at the magnetotransport under the influence of in-plane gates. We have combined quantum point contacts (QPCs) with in-plane gates and Hall-bars (HB) in a narrow-gap semiconductor heterostructure with strong spin-orbit interaction. The investigated structures were fabricated by micro-laser photolithography and wet-chemical etching from an InGaAs/InAlAs/InAs quantum well [1]. The 2DEG has carrier densities of about $6.7 \cdot 10^{11}$ cm^{-2}, mobilities of $0.8 - 1.8 \cdot 10^5$ cm^2/Vs and an effective mass of $0.042 \cdot m_e$ after illumination. We have performed magnetotransport measurements at temperatures down to 250 mK. Hall-bar structures were investigated in tilted magnetic fields up to 10 T. Combined QPC and HB structures were studied using various gate voltages in perpendicular magnetic fields up to 10 T. We determined the effective Lande-factor $g^* = 16$ and the Landau-level broadening $\Gamma = 2.2$ meV. We observed the transition of reflection of the quantum Hall edge channels at the QPC to transmission by changing the gate voltage.

[1] Chiatti *et al.*, Appl. Phys. Lett. **106**, 052102 (2015).

HL 63.76 Wed 15:00 P1A

Impact of rotational twin boundaries of GaP/Si(111) substrates on III-V nanowire growth — •Matthias Steidl[1], Christian Koppka[1], Lars Winterfeld[2], Katharina Peh[1], Peter Kleinschmidt[1], and Thomas Hannappel[1] — [1]Photovoltaics Group, Institute of Physics, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Theoretical Physics I, Institute of Physics, Technische Universität Ilmenau, 98693 Ilmenau, Germany

The epitaxial integration of III-V nanowires (NWs) with silicon has attracted considerable interest as one of the most promising ways of combining the tuneable, high-performance properties of III-V materials with the well-established Si technology. The Au-mediated vapor-liquid-solid (VLS) growth represents a common, powerful technique for the fabrication of III-V NWs. As direct growth of NWs on Si(111)

entails several difficulties, a widespread approach is to grow a III-V-transition layer prior to NW growth. However, this is generally accompanied by the formation of rotational twins. In the present study we thoroughly investigate the impact of rotational twin boundaries (RTBs) in GaP/Si on the NW growth both for GaP and GaAs NWs. RTBs can either suppress NW growth at all or lead to different undesired growth directions, such as horizontal and diagonal growth. It was found that homoepitaxial NW growth (GaP) and hetereoepitaxial NW growth (GaAs) differs in many aspects. To explain these experimental findings, we developed a model based on classical nucleation theory.

HL 63.77 Wed 15:00 P1A

Growth and characteristics of lateral $In_{1-x}Ga_xAs$ nanowires on silicon substrates — •Thorsten Wierzkowski[1,2], Martin Mikulics[1,2], Hilde Hardtdegen[1,2], and Detlev Grützmacher[1,2] — [1]Peter Grünberg-Institut 9, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA - Fundamentals of Future Information Technology

The integration of low direct band gap and high electron mobility III/V-nanostructures, such as $In_{1-x}Ga_xAs$ nanowires, into conventional silicon circuits is a promising approach to overcome limits in future Si-CMOS technology. Our approach is to realize $In_{1-x}Ga_xAs$ nanowire structures horizontally on Si (110) and Si (100) substrates by using low pressure selective area (SA) MOVPE instead of the employment of gold to induce growth since it is detrimental for silicon technology. Another advantage over the catalyst-induced growth method is the position-controlled deposition, which simplifies further processing. Conventionally, $In_{1-x}Ga_xAs$ nanowires grown vertically in [111] direction exhibit stacking faults in growth direction i.e. the current direction of the future device, which can be detrimental to the carrier mobility. By growing the nanostructures laterally on the Si (110) and Si (100) surface the direction of the stacking faults may have less influence on electron mobility. In this contribution, we will present the effect of trench orientation on lateral nanowire growth on Si (110) substrates and a growth study of lateral nanowires with different $In_{1-x}Ga_xAs$ compounds on technological important Si (100) substrates.

HL 63.78 Wed 15:00 P1A

InAs quantum dots without wetting layer photoluminescence — Sven Scholz, •Yannick Raffel, Sascha René Valentin, Carlo Alberto Sgroi Penagos, Andreas D. Wieck, and Arne Ludwig — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Universitätsstrasse 150, D-44780 Bochum, Germany

InAs quantum dots (QDs) are promising hosts for various applications and can be used as a model system for zero dimensional quantum physics. During strain driven growth of QDs by the Stranski-Krastanow (SK) mechanism, also a monolayer of InAs is formed. This so called wetting layer (WL) acts as a two dimensional quantum well. While SK-QDs usually come along with such a WL, it is an interesting question whether we can purify our QD photoluminescence (PL) from the influence of this. We found a reliable growth mechanism described and analyzed in this contribution. With this mechanism we are indeed able to grow QD samples with all dominant PL peaks stemming from the QDs and not from the wetting layer. Capacitance voltage measurements to monitor the QD loading with single electrons allow deeper insights in the conduction band energy structure.

HL 63.79 Wed 15:00 P1A

Investigation of spatial variation in molecular beam flux - gradients — •Vivienne Bippus, Rüdiger Schott, Pia Eickelmann, Julian Ritzmann, Andreas D. Wieck, and Arne Ludwig — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Universitätsstrasse 150, D-44780 Bochum, Germany

Semiconductor quantum wells (QWs) are essential tools for many research fields and devices such as LEDs, laser diodes or tunnel structures. To precisely control the emission wavelength, QWs are typically grown by molecular beam epitaxy (MBE) which offers monolayer precision. Due to the cell geometry of the MBE-setup, flux gradients can lead to spatial variations in the layer thickness on the wafer. A typical mitigation measure is to rotate the wafer during the epitaxy.

However, alloy composition and thickness variations of the QWs still appear. Therefore, we perform a systematic investigation to study the inhomogenities of the Ga, In and Al content via photoluminescence mapping of full three inch wafers. This will also be compared to MBE-growth without rotation, i.e. intentional flux gradients.

HL 63.80 Wed 15:00 P1A

Spin-flip Raman scattering in colloidal CdSe nanoplatelets — •Dennis Kudlacik[1], Victor Sapega[2], Jörg Debus[1], Benoit Dubertret[3], Dmitri Yakovlev[1], 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]Laboratoire de Physique et d'Etude des Matériaux, UMR8213 du CNRS, ESPCI, 75231 Paris, France

Colloidal CdSe nanoplatelets (NPLs) are highly efficient light emitting materials exhibiting unique optical properties that are very promising for many applications in nanotechnology. Even though there has been a continuous study on these colloidal nanostructures investigating their optical properties, a comprehensive and unified picture of electronic spin-based interactions is still missing up to now. Therefore, we have studied the resonant spin-flip Raman scattering (SFRS) in self-assembled colloidal CdSe nanoplatelets in Faraday and tilted geometries at external magnetic fields of up to 10 T. We have observed an intense first and second order Raman signal, which can be attributed to a spin-flip of a resident electron induced by a photocreated exciton inside of this colloidal quantum well. From a magnetic field dependence of the electron spin-flip energy, measured in Faraday and Voigt geometry, isotropic g-factors of $g_e = 1.623$ and 3.242 have been determined. Furthermore, we have observed that the SFRS exhibits a strong dependence on temperature. With increasing temperature, the electron spin dephasing time is considerably reduced.

HL 64: Poster: Photovoltaics and Optics

Time: Wednesday 15:00–19:00 Location: P1C

HL 64.1 Wed 15:00 P1C

Chemical and electronic properties of Pt/In_2O_3 interfaces — •Jonas Michel[1], Theresa Berthold[1], Stefan Krischok[1], Marcel Himmerlich[1], Julius Rombach[2], Oliver Bierwagen[2], Holger von Wenckstern[3], and Marius Grundmann[3] — [1]Institut für Physik & Institut für Mikro- und Nanotechnologien MacroNano, Technische Universität Ilmenau, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [3]Universität Leipzig, Institut für Experimentelle Physik II, Leipzig, Germany

Indium oxide (In_2O_3), a transparent semiconduting oxide, is known to exhibit tunable electron transport characteristics, from semi-insulating to highly n-doped characteristics [1]. One important property of In_2O_3 is the existence of a surface electron accumulation layer which allows generation of ohmic contacts for devices, but hinders production of rectifying contacts. Recently it has been shown that sputtering from metal targets in a reactive oxygen atmosphere allows formation of Schottky contacts [2]. We have studied metallic Pt contacts deposited by different thin film methods as well as the influence of an In_2O_3 surface pretreatment by oxygen plasma in order to determine the relevant changes that influence the electron transport characteristics of the Pt/In_2O_3 interface and to identify the origin of Schottky barrier formation. For this purpose, photoelectron spectroscopy was applied to characterize the chemical composition of the semiconductor surface and the metal contacts as well as to determine the electronic barriers at the heterointerface. [1] O. Bierwagen, Semicond. Sci. Technol. 30 (2015), 024001; [2] H. v. Wenckstern et al., APL Mater. 2 (2014), 046104.

HL 64.2 Wed 15:00 P1C

Charge storage in β-$FeSi_2$ nanoparticles — •Fangfei Li[1], Martin Geller[1], Hans Orthner[2], Jens Theis[1], Hartmut Wiggers[2], and Axel Lorke[1] — [1]Experimental Physics and CENIDE, University of Duisburg-Essen, Germany — [2]Institute for Combustion and Gas Dynamics and CENIDE, University of Duisburg-Essen, Germany

Especially, for mobile electronics, rechargeable batteries or supercapacitors with high capacities and energy density are needed. Nanomaterials can fulfill this demand because of their large specific surface

area, providing space for electrochemical reactions.

In our research, a capacitor with non-toxic, semiconducting β-$FeSi_2$ nanoparticles shows a relatively high capacity, which points towards a yet unexplored potential of β-$FeSi_2$ nanoparticles in energy storage technologies. The β-$FeSi_2$ capacitor does not require an electrolyte and operates under ambient conditions. However, its capacitance is quite sensitive to solvents in the gaseous atmosphere (i.e. water, acetone) and humidity. With increasing relative humidity, the capacitance increases exponentially. Compared to the bare electrodes without β-$FeSi_2$ nanoparticles, the β-$FeSi_2$ nanoparticles-coated samples exhibit an up to 3−4 orders of magnitude increased capacitance. Time-resolved current-voltage measurements show that for a short time after the charging pulse (seconds to minutes), the capacitance on average reaches 2.5 As/g at a charging voltage of 3V. Moreover, the devices are robust, show almost no degradation under ambient conditions, and can still be used after months of storage and repeated measurements.

HL 64.3 Wed 15:00 P1C

Optimizing Vertical Organic Field Effect Transistors — •Marco Höppner, Alrun Günther, Michael Sawatzki, and Karl Leo — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Dresden, Germany

Organic switchable resistors such as field effect transistors (OFETs) are important to realize future flexible electronic devices. In order to reach the needed switching speeds (e.g. for logic applications) and current densities (e.g. for display pixel driving) it is most important to overcome the low charge carrier mobilities and large channel lengths. In this sense, optimizing the geometry is a key element which is done by the novel approach of vertical organic field effect transistors (VOFETs). Here, the vertical channel length where the electric field driven charge carrier drift takes place can easily be scaled down into the sub 100 nm regime. However, a lateral charge diffusion component limits scooping the full potential of the short vertical channel length which is accessible in this device geometry. Here several approaches to surmount this difficulty are presented.

HL 64.4 Wed 15:00 P1C

Template-directed Nanoengineering for Promoted Solar Water Splitting — •Min Zhou, Yang Xu, Liying Liang, Benrong Hai, and Yong Lei — Ilmenau University of Technology, Ilmenau 98693, Germany

Highly ordered nanostructures have attracted intensive attention in the field of solar water splitting due to their ordered nanoscale features, such as huge surface area, favorable transport properties and extended light absorption range from UV to visible light, etc. Template-directed fabrication is a facile and controllable approach to realize such nanoarchitectures. Having inherited the geometrical characteristics of the templates, the resulting water splitting cells demonstrate that the as-obtained nanoarchitectures benefit the photoelectrochemical reactions. For example, based on anodic aluminium oxide (AAO) templates, well-ordered CdTe/TiO2 core/shell nanowire arrays show promoted photocurrent response to visible light. Au particle array together with ferroelectric materials was realized by a cost-effective nonlithographic route, resulting in enhanced water splitting performance through surface plasmon resonance and controllable charge transfer/transport. Overall, template-directed nanoengineering shows excellent promising to make progress in solar energy-related applications.

HL 64.5 Wed 15:00 P1C

Solution-producible solar cells with CuInS2- and ZnO nanoparticles — •Harald Reinhold, Dorothea Scheunemann, Jürgen Parisi, and Holger Borchert — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, 26111 Oldenburg

Solar cells with CuInS2 nanocrystals are a nontoxic alternative to solar cells with Pb chalcogenides. On the other hand, CuInS2 solar cells show a considerably lower power conversion efficiency. A main reason for this are insufficient transport properties originating from long organic ligands which are essential in the synthesis of CuInS2 nanocrystals [1]. In order to raise the efficiency of our CuInS2 solar cells, we exchanged the long organic ligands by short ionic ligands. After the exchange reaction, the nanoparticles were examined by FTIR spectroscopy and thermogravimetric analysis (TGA), which shows an exchange rate around 90%. Results on the ligand exchange and the impact on the performance of corresponding solar cells will be presented.

[1] D. Scheunemann et. al., Towards depleted heterojunction solar cells with CuInS2 and ZnO nanocrystals, Appl. Phys. Lett.,2013, 103, 133902.

HL 64.6 Wed 15:00 P1C

Empirical electronic structure correction for DFT-based calculations — •Hanh Bui[1,2], Jens Hühnert[1], Anastasia Karpulevich[1,2], Peng Han[1], and Gabriel Bester[1,2] — [1]Institut fur Physikalische Chemie, Universität Hamburg, Grindelallee 117, D-20146 Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, D-22761 Hamburg, Germany

While DFT is extremely successful in the prediction of ground state properties and is already used as a *data mining* tool to design materials with certain target properties it suffers from significant deficiencies in the prediction of the electronic structure. The hope to interpret Kohn-Sham eigenvalues as quasiparticle levels to predict, e.g., optical band gaps is far from fulfilled in most semiconductors. We offer a simple correction scheme based on a modification of the non-local part of norm-conserving pseudopotentials that allows for a quantitative use of the electronic structure in nanostructures. The method is implemented with the AEP [1,2] framework and demonstrated for various semiconductor nanostructures.

HL 64.7 Wed 15:00 P1C

Influence of long chain carboxylates as precursor on the performance of ZnO TFTs — •Cristian Telescu, Jonas Köhling, and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

To produce ZnO TFTs with good morphological and electrical properties the need for very high deposition temperatures is the bottle neck for using bendable substrates like polyimides. Long chain carboxylates are known as ZnO precursors with low decomposition temperature. In this study ZnO films with thicknesses below 30 nm were deposited by spray pyrolysis at various temperatures and varying the chain length of the carboxylates. In addition UV/ozone treatment was used to decompose remaining organic ligands and residues. The deposited ZnO films were systematically characterized by XPS, AFM, UV-VIS, FTIR and Raman measurements. Finally TFTs were fabricated and exhibit mobilities beyond 10 cm^2/Vs for proper deposition conditions.

HL 64.8 Wed 15:00 P1C

Influence of long chain carboxylates as precursor on the performance of ZnO TFTs — •Jonas Köhling and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

To produce ZnO TFTs with good morphological and electrical properties the need for very high deposition temperatures is the bottle neck for using bendable substrates like polyimides. Long chain carboxylates are known as ZnO precursors with low decomposition temperature. In this study ZnO films with thicknesses below 30 nm were deposited by spray pyrolysis at various temperatures and varying the chain length of the carboxylates. In addition UV/ozone treatment was used to decompose remaining organic ligands and residues. The deposited ZnO films were systematically characterized by XPS, AFM, UV-VIS, and Raman measurements. Finally TFTs were fabricated and exhibit mobilities beyond 10 cm^2/Vs for proper deposition conditions.

HL 64.9 Wed 15:00 P1C

MgZnO/ZnO quantum wells with distinct quantum-confined stark effect grown on a highly conductive ZnO:Al back contact layer — •Max Kneiss, Gabriele Benndorf, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Leipzig, Germany

Since stable p-type doping in ZnO has not been achieved until now [1], methods beyond traditional doping strategies have to be employed to realize high hole densities. One approach is the separation of photo-excited electrons and holes in the internal electric field of polar MgZnO/ZnO quantum wells (QWs) [2]. The effectiveness of the separation can be estimated by the gound state recombination energy and decay time of the QW emission and the internal field. To directly determine the latter, external field-dependent photoluminescence (PL) measurements can be used where a highly conductive back contact layer is needed. We have grown MgZnO/ZnO QWs on a degenerately doped ZnO:Al layer via pulsed laser deposition. Low temperature PL spectra showed a blue-shift of the QW emission with increasing excitation density indicating a quantum-confined stark effect resulting from the internal field. We modeled the temporal dynamics of the QW emission and determined ground state recombination energies and decay times of the QW excitons in dependence on the well width for sym-

metric QWs as well as the Mg-content in the upper MgZnO layer for QWs with asymmetric barriers. We further verified the internal field by field-dependent cw-PL spectroscopy. [1] Fan *et al.*, Prog. Mater. Sci. **58**, 874 (2013) , [2] Stölzel *et al.*, Phys. Rev. B **88**, 045315 (2013)

HL 64.10 Wed 15:00 P1C

H_2S-sensing with ZnO NWs and the role of oxygen in the sensing mechanism — •Angelika Kaiser, Florian Huber, Sören Riegert, Manfred Madel, and Klaus Thonke — Institute of Quantum Matter / Semiconductor Physics Group, Ulm University

ZnO nanostructures are a promising candidate in the realization of a fast and portable H_2S-sensing device. However the lack of a reliable detection mechanism has hindered the development and manufacture of an effective sensor yet. General detection properties like selectivity, sensitivity and sensing recovery are still in need of further enhancement.

In our work we demonstrate the H_2S-sensing performance of two sets of differently grown ZnO nanowires. Besides conventionally grown ZnO nanowires, using gold as catalyst material on silicon, catalyst-free ZnO nanowires grown on sapphire are equally fabricated. We investigate oxygen as the crucial contributor in the H_2S-sensing mechanism. It is found that flushing the sensor device with different concentrations of oxygen reveals an additional increase in the H_2S-sensitivity and primarily a clear enhancement in the recovery property of the ZnO nanowires. Furthermore we characterize the temperature dependency of our sensor structure in regards of an overall optimal operating ambient.

HL 64.11 Wed 15:00 P1C

Is the oxygen vacancy in ZnO connected to the E3 deep level defect? — •R. Pickenhain[1], M. Schmidt[2], H. von Wenckstern[1], A. Pöppl[1], G. Benndorf[1], and M. Grundmann[1] — [1]Universität Leipzig, Fakultät für Physikund Geowissenschaften, Inst. für Exp Physik II,Linnéstr. 5, 04103, Leipzig, Germany — [2]Helmholtz-Centre for Environmental Research, Permoserstr. 15, 04318 Leipzig, Germany

The E3 defect is typically incorporated in bulk crystals and thin films of ZnO. We examined this defect in ZnO single crystals with deep level transient spectroscopy (DLTS), optical DLTS (ODLTS), electron paramagnetic resonance (EPR) and photoluminescence(PL). With DLTS- and ODLTS we demonstrate experimentally that the E3 level in ZnO can bind two electrons and exhibits negative U-property. The thermal activation energy of the defect is about 280 meV and corresponds to the emission of two electrons into the conduction band. The effective correlation energy of the negative U-defect was determined from the measured photo cross section $\sigma^o(h\nu)$ to be $U_{cor} \sim -1\,eV$. Temperature dependent EPR experiments suggest that the oxygen vacancy V_O is the microscopic origin of the E3 defect. Further we find with temperature dependent PL that the E3 defect has a radiative recombination for the transition $V_O^0 \Rightarrow V_O^+$ with a peak maximum energy of 2.09 eV. The comparatively low experimental value of 280 meV of the thermally activated $V_O^0 \Rightarrow V_O^{2+}$ transition should re-stimulate discussions on the contribution of the oxygen vacancy to the free electron density and on its role in the difficulty to obtain *p*-type ZnO.

HL 64.12 Wed 15:00 P1C

Optical Characterization of iron doped ZnO — •Sebastian Bauer[1], Florian Huber[1], Benjamin Neuschl[1], Matthias Schreck[2], and Klaus Thonke[1] — [1]Institute of Quantum Matter, Semiconductor Physics Group, University Ulm, Germany — [2]Institute of Physics, University Augsburg, Germany

Typically Fe is deliberately incorporated into III-V- and II-VI-semiconductor materials for the realization of semi-insulating substrates which are needed for optoelectronic and electronic devices. However in ZnO iron on a Zn lattice site acts as a deep donor. Also the realization of ferromagnetic semiconductors for spintronics is a subject of interest.

In ZnO the influence of transition metals on magnetic, optical and electronic properties of the material are still subject to research. In this study we present results on the preparation of iron containing ZnO layers grown by chemical vapour deposition technique. Iron has been incorporated both during the growth of the sample itself and by ion implantation. Further optical and magneto-optical investigations on the photoluminescence band at 1.78 eV are presented. This band emerges for Fe^{3+} from the spin-forbidden electric-dipole transition from the excited state ${}^4T_1(G)$ to the ground state ${}^6A_1(S)$ transition. Additionally isotope and other effects leading to fine splittings are discussed.

HL 64.13 Wed 15:00 P1C

Nonlinear Optical Properties of SnS based Cluster Molecules — •Vanessa Dahmen[1], Nils W. Rosemann[2], Jens P. Eussner[3], Andreas Beyer[1], Kerstin Volz[1], Stephan W. Koch[1], Stefanie Dehnen[3], and Sangam Chatterjee[2] — [1]Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, Renthof 5, 35032 Marburg, Germany — [2]Institute of Experimental Physics I, Justus-Liebig-University Giessen, 35392 Gießen, Germany — [3]Faculty of Chemistry and Materials Sciences Center, Philipps-Universität Marburg, Hans-Meerwein-Straße, 35043 Marburg, Germany

Supercontinuum sources are used in various scientific experiments and technical applications. Such sources provide broad spectra with well-defined beam parameters. The most common method of generation such supercontinua is by using tapered or photonic-crystal fibers. In this approach, self-phase modulation of the propagating light in the fiber leads to the generation of the supercontinuum. To achieve the field strength required for this process one has to use pulsed pump sources.

Here, we present a powder compound, composed of organyl-protected [Sn4S6] cluster molecules, which shows extreme nonlinear properties. This material enables the generation of a supercontinuum by pumping with a medium-power, commercial, continuous-wave laser diode. The distinct geometry and frustrated mesoscopic order of the tinsulfide-based cluster molecules is responsible for the nonlinear response. By studying the nonlinear properties we are getting closer to characterize and understand the material system.

HL 64.14 Wed 15:00 P1C

Determination of electronic trap states in polymer based diodes and their impact on the charge carrier mobility — •Michael Bretschneider, Alexander Wagenpfahl, and Carsten Deibel — Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

Aiming for more efficient organic electronic devices, one has to understand the limiting factors in terms of charge transport and recombination, which are often related to trap states. We characterise and quantify the energetic distribution of charge carrier traps of a PCDTBT diode by fractional thermally stimulated current measurements. We find that the density of occupied states shows an approximately Gaussian shape, which is often expected for disordered organic semiconductors. Time of flight measurements are used to determine the electron and hole mobility, respectively. We investigate the correlation of the charge carrier mobility with the trap distribution and discuss the impact on the device performance.

HL 64.15 Wed 15:00 P1C

Hole Transport in Low Donor Content Organic Solar Cells — •Donato Spoltore, Andreas Hofacker, Johannes Benduhn, Sascha Ullbrich, Olaf Zeika, Sebastian Schellhammer, Frank Ortmann, and Koen Vandewal — Dresden Integrated Center for Applied Physics and Photonic Materials, George-Bähr Str. 1, 01069 Dresden

Organic solar cells for which a small molecule electron donor is diluted in a fullerene matrix have a reduced density of donor-fullerene contacts, resulting in reduced free carrier recombination and increased open-circuit voltages. In such devices, the low donor concentration prevents the formation of pathways of directly adjacent hole transporting molecules. Despite this, high external quantum efficiencies in the strongly absorbing region of the fullerene can still be reached, suggesting an interesting hole transport mechanism. Here we perform a systematic study of the hole mobilities of 18 donor:C60 blends, where the donors are diluted at ~6 mol% and have varying frontier energy level offsets and relaxation energies. We find that hole mobilities are dominantly rendered by the relaxation energy of the donor allowing the formulation of an empirical law to estimate hole mobilities in low donor content organic solar cells. Surprisingly, the energy offset between the C60 matrix and the donor material shows no contribution indicating the formation of an effective hole transport level. The C60 matrix only adds by a constant contribution to the activation energy of the transport process.

HL 64.16 Wed 15:00 P1C

Solution processing of vertical organic field-effect transistors with TIPS-Pentacene — •David Kneppe — Dresden Integrated Center for Applied Physics and Photonic Materials, Dresden, Germany

The interest in organic transistors has been growing rapidly in the past

years due to their importance for the realization of future organic electronic devices such as flexible displays or logic applications. By using a novel device architecture with a short channel length and a high mobility organic semiconductor, key parameters like the maximum drain current as well as the switching frequency can be improved further. Therefore, vertical organic field-effect transistors (VOFETs) with vertical channel lengths in a regime of several nanometers are promising devices. Here, organic semiconductors with a high charge carrier mobility especially in the vertical direction are needed. However, vacuum deposition of several layers to produce these devices is rather expensive for later massive industrial fabrication. Here, first approaches in solution processing of VOFETs with the promising polycrystalline organic semiconductor TIPS-Pentacene are presented.

HL 64.17 Wed 15:00 P1C

Voltage dependent photoluminescence spectroscopy of dye-sensitized solar cells — •Nico Hofeditz[1], Ingo Meyenburg[1], Jane Falgenhauer[2], Melanie Rudolph[2], Nils Rosemann[1], Sangam Chatterjee[3], Derck Schlettwein[2], and Wolfram Heimbrodt[1] — [1]Department of Physics, Philipps-University Marburg, Renthof 5, 35032 Marburg — [2]Institute of Applied Physics, Justus-Liebig-University Giessen, Heinrich-Buff-Ring 16, 35392 Gießen — [3]Institute of Experimental Physics I, Justus-Liebig-University Giessen, Heinrich-Buff-Ring 16, 35392 Gießen

Dye-sensitized solar cells with indoline dyes D149 and D131 and the squaraine dye SQ2 on mesoporous TiO_2 or ZnO have been prepared. The energy level alignment at the organic inorganic interface is important for an optimized electron transfer. We present a new method to determine the band offset. Photoluminescence spectra were recorded with varying applied voltages. Systematical analysis of the spectra shows a significant dependence of the photoluminescence intensity on the applied voltage as well as a small energy shift. The observed characteristics are discussed as interface effects of the dye-semiconductor interface. Time resolved photoluminescence spectroscopy gives further insight into these processes.

HL 64.18 Wed 15:00 P1C

Reorganization and disorder effects of the charge transfer state in organic solar cells — •Clemens Göhler and Carsten Deibel — Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

The efficiency of organic solar cells is directly linked to their ability to dissociate light-induced excitons into separate charge carriers. By using a bulk-heterojunction (BHJ) with a mixture of donor and acceptor semiconductors, a charge-transfer (CT) state between the acceptor LUMO and donor HOMO is created. Due to its lower binding energy, the exciton dissociation increases via the CT state.

This found state is believed to be affected by both its reorganization energy and ensemble disorder effects. Therefore, we expect a complex temperature dependence of both the CT states' energy and line-broadening.

We use electrooptical spectroscopy with respect to absorption and emission of the CT state. By measuring the ensemble CT energy and linewidth while varying the cell-temperature over a broad range, we are able to unravel whether molecular reorganization energy or disorder have a stronger influence on the CT state of common polymer-fullerene BHJs.

HL 64.19 Wed 15:00 P1C

Diffuse Transmission and Reflection of Light Scattering Polymer Substrates for Organic Light-emitting Diodes — •Pen Yiao Ang, Georg Marks, Abdalla Mahmoud, Axel Fischer, Simone Lenk, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, TU Dresden

Organic light-emitting diodes (OLEDs) are gaining more attention as the next generation of light sources. Still, the cost-performance ratio is not comparable to inorganic LEDs. One solution is to further enhance the performance of OLEDs by improving the outcoupling efficiency. Light trapped in waveguided modes of the substrate can be outcoupled if scattering particles are added to the OLED structure. The property of a scattering film to redirect light correlates with the haze factor, depending on the wavelength. Ideally, light is scattered into a direction which does not suffer from total internal reflection in the substrate. However, light having the right direction might be scattered in a way that it is coupled into waveguided modes or even reflected. Hence, it cannot be generalized that a higher haze factor automatically leads to a better performance of the scattering film. Here, we compare different self-made scattering films based on thin polymer substrates with incorporated nano-particles. By measuring the scattering of an incident light ray into all directions (360°), we identify the amount of direct transmission, diffuse transmission as well as diffuse reflection. The gained insights are related to the efficiencies of OLEDs using our substrates in order to specify optimal scattering properties.

HL 64.20 Wed 15:00 P1C

Nongeminate Recombination in Organic Solar Cells — •Christopher Wöpke, Christoph Baumbach, and Carsten Deibel — Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

Despite ongoing efforts to improving the overall efficiency of organic solar cells, nongeminate recombination - the dominant performance limiting mechanism - is still not fully understood. Nongeminate recombination depends strongly on the solar cell morphology.

The aim of this study is to explore the relationship between recombination and the morphology of P3HT:PCBM bulk-heterojunction organic solar cells. In a first step the charge carrier concentrations and recombination rates of devices with systematically varied morphologies will be studied with the method of time-delayed collection field (TDCF). Analysing the TDCF transients an approximated mean charge carrier mobility will be extracted. We will present our progress in finding the relationship between the devices morphology and the parameters recombination rate, charge-carrier mobility and concentration.

HL 64.21 Wed 15:00 P1C

Charge carrier mobility in fullerene-blended squaraine thin films and the impact of correct layer thickness determination — •Majvor Mack[1], Matthias Schulz[2], Arne Lützen[2], and Manuela Schiek[1] — [1]Energy and Semiconductor Research Laboratory, Institute of Physics, University of Oldenburg, D-26111 Oldenburg, Germany — [2]Kekulé Institute for Organic Chemistry and Biochemistry, University of Bonn, Gerhard-Domagk-Str. 1, D-53121 Bonn, Germany

Squaraine-based solar cells suffer from a low fill factor which leads to a small efficiency. A possible reason for this could be the built up of space charges due to imbalanced hole and electron mobility. To address this issue, the mobility is determined from I-V-measurements of single carrier devices, which follow the Mott-Gurney law for space-charge-limited current (SCLC). Under these circumstances the current has a quadratic dependence of the voltage and an inversely cubic dependence of the organic layer thickness. Thus, the determination of the layer thickness is important. Two methods for the thickness measurement are opposed: atomic force microscopy (AFM) as a tactile method and spectroscopic ellipsometry (SE) as contactless, optical method. Topographic AFM images across scratches in the organic film are evaluated with the software Gwyddion and compared to the result obtained by modeling and fitting of ellipsometric data with the software WVASE32.

HL 64.22 Wed 15:00 P1C

Influence of white light and voltage bias on EQE measurements for squaraine based solar cells with varying active layer parameters — •Oliver Kolloge[1], Matthias Schulz[2], Arne Lützen[2], and Manuela Schiek[1] — [1]Energy and Semiconductor Research Laboratory, Institute of Physics, University of Oldenburg, D-26111 Oldenburg, Germany — [2]Kekulé Institute for Organic Chemistry and Biochemistry, University of Bonn, Gerhard-Domagk-Str.1, D-53121 Bonn, Germany

Anilino-Squaraines are stable dyes and are readily available via environmentally friendly condensation reactions. Organic solar cells whose active layer consists of a model squaraine donor blended with a fullerene acceptor are particularly interesting because they show absorption within the deep-red combined with a high Voc. However, these devices suffer from a low fill factor around 40%.

The purpose of this study is a deeper understanding of the performance of these organic solar cells via advanced EQE measurements. J-V-measurements show a linear dependence of Jsc and illumination intensity independent of the active layer thickness. However, white light biased EQE measurements suggest a sublinear intensity response which becomes more obvious for increasing active layer thickness. Furthermore, voltage-dependent EQE measurements hints to a saturation of photocurrent at higher reverse bias voltages.

HL 64.23 Wed 15:00 P1C

Optical Spectroscopy on Organic DNTT Crystals — •Benjamin Heidelmeier[1], Marleen Axt[2], Andrea Karthäuser[2], Gregor Witte[2], and Wolfram Heimbrodt[1] — [1]Experimental Semiconductor Physics, Department of Physics, Philipps-Universität Marburg, Germany — [2]Molecular Solid State Physics, Department of Physics, Philipps-Universität Marburg, Germany

DNTT (dinaphtho[2,3-*b*:2',3'-*f*]thieno[3,2-*b*]thiophene) is a promising organic semiconductor for application in organic field effect transistors (OFET). It shows a higher charge carrier mobility in comparison to the common OFET material Pentacene while it is stable under ambient conditions. To improve the performance of OFETs it is important to study and understand the optoelectronic processes in such organic solids.

Here we report an optical characterization of DNTT single crystals that were grown by molecular beam deposition onto glass substrates coated with thin oil films. This yields platelet shaped single crystals with a typical diameter of 50μm. Using photoluminescence, absorption and time resolved spectroscopy we investigated the optical properties of such crystals. In particular we measured the polarization dependence of absorption and photoluminescence with respect to the crystallographic axes. The transition dipole moment is oriented along the short molecular axis. We were able to reveal both Davydov components. Even the excitonic luminescence exhibits a strong linear polarization.

HL 64.24 Wed 15:00 P1C

Optical Spectroscopy on Organic Molecules and Organic-Inorganic Hybrid Structures for Photodynamic Therapy and Organic Solar Cells — •Luise Rost[1], Ingo Meyenburg[1], Martin Liebold[2], Jan Tinz[3], Derck Schlettwein[3], Jörg Sundermeyer[2], and Wolfram Heimbrodt[1] — [1]Philipps-Universität Marburg department of physics and material siences center, Marburg — [2]Philipps-Universität Marburg department of chemistry,Marburg — [3]Justus-Liebig-Universität, institute of applied physics, Gießen

In the last two decades organic dyes and organic semiconductors get increasing attention due to the high molecular variability and the resulting wide applicability. For example in promising light-activated cancer therapy (Photodynamic Therapy PDT), where near-infrared light absorbing molecules produce reactive oxygen species by energy transfer which leads to cell death. Another application are dye sensitized solar cells (Grätzel cells). Naphthalocyanine-variations were synthesized and tested for their suitability as photosensitizer in Photodynamic Therapy with optical spectroscopy. The newly synthesized four different metal-naphthalo-derivates differ in axial and peripheral anchoring groups. The influence of different amount of nitrogen and tert-butyl or mesityl groups was tested. Different newly sensitized organic molecules (derivatives of Phthalocyanine) were characterized optically and tested for application in Grätzel cells. The impact of different substrates like titanium dioxide (TiO2) and zinc oxide (ZnO) will be discussed. Time Resolved Photoluminescence was performed on this newly processed solarcells.

HL 64.25 Wed 15:00 P1C

Electric field controlled dopant distribution in P3HT Films — •Marc-Michael Barf[1,2], Christian Willig[1,2,3], Lars Müller[1,2,3], Robert Lovrincic[1,2], and Wolfgang Kowalsky[1,2,3] — [1]IHF, TU Braunschweig — [2]InnovationLab, Heidelberg — [3]KIP, Heidelberg University

Doping of organic semiconductors has become a common method to improve the efficiency of devices like organic light emitting diodes, organic solar cells and more recently also organic field effect transistors. So far in most devices doping is used statically to increase the conductivity of certain regions and to create space charge layers at interfaces in order to enhance charge transport. Here, the drift of p-type dopants like 2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ) in films of Poly(3-hexylthiophene-2,5-diyl) (P3HT) is actively used to operate a device. We control the drift of the dopants in devices such as simple memristors and thereby switch those on and off by shifting highly conductive regions within the device. We explore this mechanism for possible application in an organic field effect transistor.

HL 64.26 Wed 15:00 P1C

Electroreflectance studies of Cu(In,Ga)(S,Se)$_2$ solar cell absorber and buffer layers — •Jasmin Seeger[1], Oliver Kiowski[2], Michael Powalla[2,3], Heinz Kalt[1], and Michael Hetterich[1,3] — [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 (LTI), KIT, 76131 Karlsruhe, Germany

Cu(In,Ga)(S,Se)$_2$ (CIGS) is one of the most promising thin-film solar cell absorber materials with demonstrated conversion efficiencies of up to 22.6% [1]. However, the commonly used CdS buffer still poses a problem due to the absorption losses in this layer. Further research into alternative buffer layers with less parasitic absorption, which enable even higher efficiencies, is therefore required. For that purpose we employ electro-modulated reflectance (ER) spectroscopy to study the CIGS absorber and CIGS/buffer interface for different fabrication conditions as well as absorber compositions and buffer materials.

[1] P. Jackson, R. Wuerz, D. Hariskos, E. Lotter, W. Witte, and M. Powalla. *Effects of heavy alkali elements in Cu(In,Ga)Se$_2$ solar cells with efficiencies up to* 22.6%, Phys. Status Solidi RRL 10(8), 583-586, 2016.

HL 64.27 Wed 15:00 P1C

Co-evaporated CZTSe solar cells: influence of Cu deposition rate during precursor processing on the growth and device performance — Lwitiko Mwakyusa[1,4], •Markus Neuwirth[1], Max Reimer[1], Simon Woska[1], Willi Kogler[2], Thomas Schnabel[2], Erik Ahlswede[2], Bryce Richards[3,4], Heinz Kalt[1], and Michael Hetterich[1,3] — [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, KIT, 76131 Karlsruhe, Germany — [4]Institute of Microstructure Technology, KIT, 76344 Karlsruhe, Germany

The performance of $Cu_2ZnSnSe_4$ (CZTSe) thin film solar cells is still limited by a high open-circuit voltage deficit and low fill factor. To boost device performance it is crucial to improve grain size and quality, control the formation of defects and inhibit the formation of secondary phases. It is often assumed that a Cu–Se eutectic liquid-phase is beneficial for the growth of a high-quality CZTSe absorber layer. However, too much Cu may provoke the formation of $Cu_{2-x}Se$ which can act as a shunt path in the solar cell thus deteriorating overall device performance. In this contribution we investigate solar cells with CZTSe absorbers fabricated using low-temperature co-evaporation and following high-temperature annealing in a Se atmosphere. The Cu concentration in the absorber is varied by changing the Cu deposition rate during precursor deposition. The finished devices are compared with respect to their performance in order to optimize growth conditions.

HL 64.28 Wed 15:00 P1C

Effects of selenium-to-sulphur ratio in $Cu_2ZnSn(S,Se)_4$ absorbers for thin-film solar cells — •Elisabeth Seydel[1], Markus Neuwirth[1], Michael Wolf[1], Lwitiko Mwakyusa[1], Thomas Schnabel[2], Erik Ahlswede[2], Willi Kogler[2], 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

$Cu_2ZnSn(S,Se)_4$ is a promising material system for thin-film solar cells as a substantial supply of all constituents is available. Yet the band gap of the resulting absorber of a pure selenide CZTSe (E_g = 1.0 eV) or pure sulphide CZTS (E_g = 1.5 eV) solar cell is not optimal for AM 1.5 radiation. To achieve an optimal value of approximately E_g = 1.3 eV our wet-chemically fabricated precursors are annealed in both selenium atmosphere and sulphur atmosphere. Hereby the ratio of Se and S and thus the band gap can be optimized to fit the solar spectrum best.

HL 64.29 Wed 15:00 P1C

Approaches for the incorporation of Ge into wet-chemically produced $Cu_2ZnSn(S,Se)_4$ solar cells — •Michael Wolf[1], Markus Neuwirth[1], Elisabeth Seydel[1], Thomas Schnabel[2], Erik Ahlswede[2], Willi Kogler[2], 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

$Cu_2ZnSn(S,Se)_4$ (CZTSSe) is a promising absorber material for thin film solar cells. As has been demonstrated, it can easily be doped with elements like germanium, lithium or sodium, leading to improvements

in energy conversion efficiency. Germanium on the one hand is said to be a catalyst for CZTSSe grain growth when used in small amounts during annealing. On the other hand, its substitution of tin in CZTSSe increases the band gap enabling a better match to the solar spectrum and an enhanced open-circuit voltage. In this contribution we utilize two approaches to incorporate Ge into CZTSSe. First the influence of a thin doctor-bladed germanium oxide (GeOx) layer underneath and on top of the precursor on grain growth and solar cell parameters is studied. Furthermore, germanium sulfide (GeS) is used during the annealing process to tune the band gap.

HL 64.30 Wed 15:00 P1C

Absorber surface treatment and alternative buffer layers for $Cu_2ZnSn(S,Se)_4$ solar cells — •Markus Neuwirth[1], Elisabeth Seydel[1], Michael Wolf[1], Lwitiko Mwakyusa[1], Thomas Schnabel[2], Erik Ahlswede[2], 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

Solar cells based on $Cu_2ZnSn(S,Se)_4$ (CZTSSe) are promising since they only comprise environmentally friendly and earth-abundant elements. However, they still struggle with low efficiencies, mainly related to a high open-circuit voltage deficit that could partially result from the presence of secondary phases in the absorber layer. These phases can be especially problematic at the absorber's surface where they influence the CZTSSe/CdS interface. Surface treatments like chemical etching can remove such parasitic phases and improve the interface quality. Alternative buffer layers like ZnSe may also improve the interface quality and modify the band alignment in the interface region. In this contribution we compare CZTSSe solar cells with alternative buffer layers and previous absorber surface treatments to solar cells with chemical bath deposited CdS buffer layer.

HL 64.31 Wed 15:00 P1C

Open circuit voltage (VOC) in GaAs based quantum well solar cell by using III-V semiconducting materials: A Numerical Simulation Study — •Bhaskar Singh and Daniel Schaadt — Institute for Energy Research and Physical Technologies, Technische Universität Clausthal, Germany

The Sun provides an infinite source of green energy in the form of sun-light which can be directly converted into electricity. GaAs is a direct band-gap (Eg=1.42 eV) semiconducting material which is a very promising material for solar cell fabrication in space applications. To increase the current generation in pn homojunction devices, introducing quantum wells in the intrinsic region is an alternate concept while it allows for easy fabrication and reduces problems with lattice and current matching comparing to stacked solar cells but it triggers a significant reduction in open circuit voltage. InGaAs/GaAs based quantum well solar cell shows this kind of effect in the I-V characteristics.1 To elevate this problem, we introduce here AlGaAs in place of GaAs barrier layers in the intrinsic region. Numerical device simulations show a significant enhancement in the open circuit voltage of quantum well solar cell device.

Reference: 1X.H. Li, P.C. Li, D.Z. Hu, D.M. Schaadt and E.T. Yu, J. Appl. Phys. 115, 044303 (2014)

HL 64.32 Wed 15:00 P1C

Time resolved photoluminescence of $Cu_2ZnSn(S,Se)_4$ solar cell absorbers with varying composition — Mario Lang[1], Tobias Renz[1], Niklas Mathes[1], Markus Neuwirth[1], Thomas Schnabel[2], •André Schendel[1], Heinz Kalt[1], and Michael Hetterich[1,3] — [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, KIT, 76131 Karlsruhe, Germany

$Cu_2ZnSn(S,Se)_4$ absorbers offer a huge potential for future thin-film solar cells. Up to now the low efficiency is predominantly caused by the low open circuit voltage V_{OC} compared to the theoretical possible V_{OC}. The reasons for the low open-circuit voltage are amongst others miscellaneous defects and secondary phases within the material. To suppress their formation absorber layers with off-stoichiometric Cu poor and Zn rich composition are used for highly efficient devices. In our contribution we analyze the effect of the composition on the radiative recombination by means of photoluminescence (PL) and especially time-resolved photoluminescence (TRPL).

HL 64.33 Wed 15:00 P1C

Structural and electronic characterization of crystalline silicon-aluminum oxide interfaces — •Hannah Stolzenburg, Arne Ahrens, and Michael Seibt — IV. Physikalisches Institut, Georg-August-Universität Göttingen, Germany

Aluminum oxide deposited on crystalline silicon is known for its high surface passivation capabilities. This surface passivation is attributed to a high negative fixed charge density of about -4×10^{12} cm^{-2} [1] in the aluminum oxide layer close to the silicon-aluminum oxide interface. This makes aluminum oxide an interesting material to increase the efficiency of solar cells by passivation of surface states. Examples of applications are passivated emitter and rear cells (PERC) [2] and rear-emitter inversion layer solar cell [3], for which efficiencies of 20 % [2] and 18,1 % [3] have been reported, respectively.

In this work, we investigate aluminum oxide layers deposited by atomic layer deposition (ALD) for different processing conditions parameters, as e.g. post-deposition heat treatments, layer thickness, and the effect of UV irradiation. Transmission electron microscopy (TEM) imaging combined with electron energy loss spectroscopy (EELS) is used to study the structure and chemistry of the interface between crystalline silicon and aluminum oxide. Electronic characterization of surface states and oxide charges is done using deep-level-transient-spectroscopy (DLTS) and capacitance-voltage measurements.

[1] F.Werner and J. Schmidt Appl. Phys. Lett. Vol.104, 091604 (2014). [2] J. Schmidt et al., Prog. Photovol: Res. Appl. Vol. 16 461-466 (2008). [3] F. Werner et al., J. Appl. Phy. Vol. 115, 073702 (2014).

HL 64.34 Wed 15:00 P1C

Ultra-Thin Resonant Cavity Enhanced Amorphous Germanium Solar Cells on Zinc Oxide Honeycomb Structures — •Colleen Lattyak, Regina-Elisabeth Ravekes, Volker Steenhoff, Martin Vehse, and Carsten Agert — NEXT ENERGY - EWE Research Centre for Energy Technology at the University of Oldenburg, Carl-von-Ossietzky-Str. 15, 26129 Oldenburg, Germany

Hydrogenated amorphous germanium (a-Ge:H) has a high absorption coefficient and similar band gap to microcrystalline silicon (μc-Si:H). Recently, solar cells with ultra-thin (<25nm) a-Ge:H absorber films based on absorbing resonant cavities were developed in our group. Due to strong broadband absorption and good electrical quality they have the potential to replace thick (>1μm) standard μc-Si:H cells. In order to further enhance their optical properties a-Ge:H solar cells are deposited on 3D 1μm-sized zinc oxide (ZnO) honeycomb structures, fabricated in a combined process of nanosphere lithography and electrochemical deposition. The honeycomb structure increases the volume of the overlying absorber layer making it possible for more light to be absorbed. We present external quantum efficiency (EQE) measurements which demonstrate the beneficial optical effects and the potential for a high short circuit current density. We also deduce an optimal fabrication procedure for the ZnO honeycomb structures with optimal geometry for the a-Ge:H absorber system.

HL 64.35 Wed 15:00 P1C

Cross-section electron beam induced voltage investigations of different p-n junctions — •Tobias Westphal, Patrick Peretzki, and Michael Seibt — Georg-August-Universität Göttingen, IV. Physikalisches Institut, Göttingen

P-n heterojunctions consisting of the p-doped manganite $Pr_{1-x}Ca_xMnO_3$ (PCMO) and the n-doped titanite $SrTi_{1-y}Nb_yO_3$ (STNO), both perovskite-structured, have been investigated with Electron Beam Induced Current (EBIC) [1,2]. To further study the photovoltaic properties of this system, the Electron Beam Induced Voltage (EBIV) technique is used in this work. The standard form for EBIV models [3] predicts a behaviour logarithmic to the EBIC, which is useful for measuring the nanometer scale diffusion length of minority charge carriers in this system.

In this work a well-known silicon sample is used at first to understand the results of the EBIV technique. For this reason, both plan view and cross-section measurements are done by combining SEM-based EBIV with Focused Ion Beam preparation in dual beam instruments and comparing them to finite element based simulations. In a next step, the method is brought to PCMO/STNO interfaces.

[1] B. Ifland, P. Peretzki, B. Kressdorf, P. Saring, A. Kelling, M. Seibt and C. Jooss, Beilstein J. Nanotechnol. 2015, 6, 1467-1484

[2] P. Peretzki, B. Ifland, C. Jooss and M. Seibt, Phys. Status Solidi RRL. 2016

[3] H.-C. W. Huang, C. F. Aliotta, and P. S. Ho, Appl. Phys. Lett. 41, 54 (1982)

HL 64.36 Wed 15:00 P1C

Analysis and preparation of In_2S_3:V intermediate band solar cells — •Tanja Jawinski[1,2], Leonard Wägele[1], Holger von Wenckstern[2], Marius Grundmann[2], and Roland Scheer[1] — [1]Martin-Luther-University Halle-Wittenberg, Institute of Physics, 06120 Halle, Germany — [2]Universität Leipzig, Institut für Experimentelle Physik II, Leipzig, Germany

The maximum efficiency of a standard single junction solar cell is given by the Shockley Queisser limit of around 33%. To overcome this limit an intermediate band, which allows the absorption of photons with energies lower than the band gap E_g can be introduced. In addition, thermalization losses can be reduced since within intermediate band solar cells materials with higher E_g than that of conventional cells are used. According to theoretical calculations In_2S_3 doped with vanadium is a promising candidate for such intermediate band devices.

We grew intrinsic In_2S_3:V on n-TCOs ZnO:Al and SnO:F by physical co-evaporation of the elements. In_2S_3:V p-i-n solar cells are formed with $ZnCo_2O_4$ and NiO which are prepared by pulsed laser deposition. Current-voltage measurements in the dark reveal rectification of up to 4 orders of magnitude. Measurements under illumination as well as external quantum efficiency measurements provide a proof of principle, even though the short circuit current and the open circuit voltage need to be improved by optimizing the deposition parameters. For deeper understanding we compare solar cells with varying V-concentrations.

HL 64.37 Wed 15:00 P1C

Secondary phase investigation on kesterite materials using X-ray absorption spectroscopy — •Konrad Ritter[1], Sergio Giraldo[2], Galina Gurieva[3], Laura Elisa Valle Rios[3], Götz Schuck[3], Edgardo Saucedo[2], Susan Schorr[3,4], and Claudia S. Schnohr[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Catalonia Institute for Energy Research (IREC), Jardins de les Dones de Negre 1 08930, Sant Adrià de Besòs, Barcelona , Spain — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Department Crystallography, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [4]Institut für Geologische Wissenschaften, Freie Universität Berlin, Malteserstr. 74-100, 12249 Berlin, Germany

$Cu_2ZnSnSe_4$ based kesterites offers a wide range of promising absorber materials for photovoltaics, but the record efficiency has only reached 12.6% yet. One of the limiting factors seems to be the formation of secondary phases throughout the preparation process. Therefore we used X-ray absorption near edge structure spectroscopy for an element specific detection of secondary phases via linear combination fitting. Kesterite powder samples created by solid state reaction with varying compositions were studied, to better understand the phase formation depending on the initial material composition. Furthermore, kesterite solar cells with and without small amounts of Ge were studied for different stages of preparation. The presence of Ge greatly improves the device performance and a detailed phase analysis will help to understand the underlying absorber formation mechanisms.

HL 64.38 Wed 15:00 P1C

Composition - dependent atomic - scale structure of $Cu_2(Zn,Fe)SnS_4$ — •Cora Preiss[1], Konrad Ritter[1], Philipp Schöppe[1], Susan Schorr[2], and Claudia S. Schnohr[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin und Institut für Geologische Wissenschaften, Freie Universität Berlin, Malteserstr. 74-100, 12249 Berlin, Germany

The chalcogenides Cu_2ZnSnS_4 (kesterite) and Cu_2FeSnS_4 (stannite) are interesting as potential photovoltaic absorbers and provide a promising alternative to other solar cell materials. They offer advantages like the availability of the elements and their non-toxicity but the record efficiencies are still well below the theoretical prediction. In order to further improve the efficiency, a detailed knowledge of the fundamental material properties is needed. Cu_2ZnSnS_4, Cu_2FeSnS_4, and their solid solutions with different Zn/(Zn+Fe) ratios were investigated with extended X-ray absorption fine structure spectroscopy. The absorption at the K-edge of Cu, Zn, Sn and Fe was measured and is analyzed to reveal the bond length of the Cu, Zn, Sn and Fe atoms to their nearest S neighbors thus directly providing the different anion displacements. These results lead to a detailed understanding of the correlation between crystal structure and local atomic arrangements of this material system and show their impact on important material properties like the band gap energy.

HL 64.39 Wed 15:00 P1C

Absolute distance semiconductor laser self-interferometry towards microscopy object position detection — •Daniel Hartnagel, Christoph Weber, and Stefan Breuer — Institute of Applied Physics, Technische Universität Darmstadt, Schlossgartenstr. 7, 64289 Darmstadt, Germany

The precise knowledge of the location of a microscopic object under investigation in nonlinear confocal imaging microscopy is crucial for allowing a concise series of microscopic images. Non-contact high-precision measurement techniques involving triangulation or mechanical position sensing cannot immediately be employed due to the dimension restrictions in the microscopes sample holder. We study a compact semiconductor laser based concept for absolute distance interferometry that is expected to cope with the stringent requirements. An experiment involving a directly modulated commercial diode laser emitting at 1310 nm is presented where the absolute distance can be retrieved by the measured interference frequency and parameters. The results are then validated by spectro-temporal and time-domain analysis. The obtained results suggest paths towards future development and implementation of semiconductor laser based absolute distance interferometry concepts. Support by the Support Initiative Interdisciplinary Science (FiF) of the Technische Universität Darmstadt and the Adolf-Messer Foundation, Germany, is thankfully acknowledged.

HL 64.40 Wed 15:00 P1C

Optical feedback stabilization of a passively mode-locked multi quantum well semiconductor laser emitting at 1070 nm — •Dominik Auth[1], Christoph Weber[1], Andreas Klehr[2], Andrea Knigge[2], and Stefan Breuer[1] — [1]Institute of Applied Physics, Applied Semiconductor Optics and Photonics, Technische Universität Darmstadt, Schlossgartenstr. 7, 64289 Darmstadt, Germany — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Gustav-Kirchhoff-Straße 4, 12489 Berlin, Germany

Passively mode-locked semiconductor lasers emitting at 1070 nm are compact photonic sources for multi-GHz repetition rates and for high-speed data transmission where excellent pulse train stability in time and amplitude are demanded. Timing and amplitude stability (AJ) investigations were performed recently in C. Weber et al., Internat. Conf. on Transparent Optical Networks 2016, We.P.30. In this contribution we study experimentally the influence of self-feedback by an external optical fiber cavity on the mode-locking dynamics of a multi-section narrow ridge quantum-well (QW) laser with an active InGaAs double QW embedded in GaAsP spacer layers. We focus on the timing and amplitude stability improvement by single optical feedback and quantify this improvement by radio-frequency domain, temporal and optical domain analysis in dependence on the feedback delay and feedback strength. The obtained results are compared to investigations performed on the pulse train stability of an InGaAs quantum dot laser emitting at 1250 nm.

HL 64.41 Wed 15:00 P1C

Pulse train stabilization of a passively mode-locked quantum dot laser emitting at 1250 nm subject to single and dual long fiber optical self-feedback — •Sebastian Stutz[1], Oleg Nikiforov[2], Christoph Weber[1], Thomas Walther[2], and Stefan Breuer[1] — [1]Institute of Applied Physics, Applied Semiconductor Optics and Photonics, Technische Universität Darmstadt, Schlossgartenstr. 7, 64289 Darmstadt, Germany — [2]Institute of Applied Physics, Laser and Quantum Optics, Technische Universität Darmstadt, Schlossgartenstr. 7, 64289 Darmstadt, Germany

Passively mode-locked semiconductor lasers are compact photonic sources delivering a train of picosecond short optical pulses for optical clock distribution, high bit-rate optical time division multiplexing and compact microwave/millimeter-wave signal generation. The pulse train can exhibit considerable timing jitter and concepts to reduce timing and amplitude jitter are demanded. Recently the influence of dual optical feedback with fine-delay control and two short feedback cavities has been studied in Optics Express 24, 14301, 2016. Here, we study experimentally the influence of single cavity fiber feedback as well as dual cavity long fiber feedback on an InGaAs quantum dot semiconductor laser. We focus on the timing and amplitude stability as well as the pulse repetition rate control of an InGaAs quantum dot laser subject to self-feedback by long dual fiber delay cavities with fine-

delay control. Simulation results by a simple time-domain model (L. Drzewietzki et al., Optics Express 21, 16142, 2013) allow to reproduce the experiments with good agreement.

HL 64.42 Wed 15:00 P1C

Passively mode-locked quantum dot laser emitting at 1250 nm operated in a low temperature environment — •Sebastian Stutz, Christoph Weber, and Stefan Breuer Breuer — Institute of Applied Physics, Technische Universität Darmstadt, Schlossgartenstr. 7, 64289 Darmstadt, Germany

The pulse train stability and mode-locking (ML) properties of passively mode-locked InAs/InGaAs quantum dot semiconductor laser are studied experimentally. The laser consists of a multi-section cavity with a total cavity length of 8 mm and a 0.9 mm long absorber section length. Initial experimental investigations of a mode-locked GaAs quantum well laser at cryogenic temperatures have been performed by M. H. Kiang et al., Electron. Lett. 3, 880 in 1995 with a focus on radio-frequency linewidth study. Here, we expand these investigations towards a comprehensive study of the mode-locking dynamics under various operating temperatures. We then discuss the experimentally obtained dependencies of mode-locked pulse train stability and emission properties in the radio-frequency and spectral domain on laser biasing conditions and temperature down to -98 °C. The results suggest future perspectives on investigating the mode-locking at low temperatures.

HL 64.43 Wed 15:00 P1C

Development of AlGaInP-based electrically-pumped VECSELs emitting in the red spectral range — •Mona Stadler, Matthias Paul, Stefan Hepp, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen and Research Center SCoPE, Allmandring 3, 70569 Stuttgart, Germany

The electrically-pumped vertical external-cavity surface-emitting laser (EP-VECSEL) is a promising device to combine the advantages of electrically-pumped semiconductor lasers with them of optically pumped vertical-cavity surface-emitting lasers (VCSELs). Next to high and scalable output powers and good beam qualities of the VECSEL, offers the open cavity the use of intra-cavity elements for different applications, e.g. frequency stabilized emission or frequency-doubling. In electrical driven lasers the pumping scheme is simplified drastically, compared to optical pumped systems. Additionally, electrical pumping facilitates higher integration and further miniaturization and is therefore an important step towards compact laser sources. Regarding the chip design of the EP-VECSEL, it should be as easy as possible, keeping optical losses and Joule heating, which are unavoidable in doped layers, minimal. Therefore, a good thermal management, a suitable carrier distribution and a balance between the optical and electrical requirements have to be found. We present the first steps towards an electrically-pumped AlGaInP-based VECSEL emitting in the red spectral range regarding the chip design and its spectral and luminescence characteristics.

HL 64.44 Wed 15:00 P1C

Injection Locking of Spontaneous Emission Enhanced Microlaser — •Felix Krüger[1], Elisabeth Schlottmann[1], Steffen Holzinger[1], Christian Schneider[2], Sven Höfling[2], Martin Kamp[2], Janik Wolters[3], Xavier Porte[1], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin — [2]Technische Physik, Universität Würzburg — [3]present adress: Universität Basel, Switzerland

Micro- and nanolasers are of broad interest because of their size, modulation speed and low energy consumption. In recent years the nonlinear dynamics of such lasers are spotlighted in an interdisciplinary context at the crossroads of classical and quantum physics.

The experimental studies address the influence of the spontaneous emission factor β on the locking properties and on mode switching in bimodal microlasers. Our studies reveal, that for small mode-volume microlasers emission of thermal light is maintained at the solitary cavity mode while only the coherent part of emission locks to the external master laser [1].

Moreover, in bimodal micropillar lasers the master laser allows for a polarization dependent destabilization or stabilization of switching processes. We also discuss more complex injection schemes involving delayed optical feedback.

[1] E. Schlottmann, S. Holzinger et al., Phys. Rev. Applied **6**, 044023 (2016)

HL 64.45 Wed 15:00 P1C

Emitter and absorber assembly for multiple self-dual operation and directional transparency — •Christian V. Morfonios[1], Panayotis A. Kalozoumis[2], Georgios Kodaxis[2], Fotios K. Diakonos[2], and Peter Schmelcher[1,3] — [1]Zentrum für Optische Quantentechnologien, Universität Hamburg, 22761 Hamburg, Germany — [2]Department of Physics, University of Athens, 15771 Athens, Greece — [3]Centre for Ultrafast Imaging, Universität Hamburg, 22761 Hamburg, Germany

We propose a recursive scheme for the design of scatterers acting simultaneously as emitters and absorbers, such as lasers and coherent perfect absorbers in optics, at multiple prescribed frequencies. The approach is based on the assembly of non-Hermitian emitter and absorber units into self-dual emitter-absorber trimers at different composition levels, exploiting the simple structure of the corresponding transfer matrices. In particular, lifting the restriction to parity-time-symmetric setups enables the realization of emitter and absorber action at distinct frequencies and provides flexibility in the choice of realistic parameters. We further show how the same assembled scatterers can be rearranged to produce unidirectional and bidirectional transparency at the selected frequencies. With the design procedure being generically applicable to wave scattering in single-channel settings, we demonstrate it with concrete examples of photonic multilayer setups.

HL 64.46 Wed 15:00 P1C

Inverted HEMT structure with electric field induced 2DEG — •Ismail Bölükbasi, Julian Ritzmann, Andreas D. Wieck, and Arne Ludwig — Ruhr-Universität Bochum, D-44780 Bochum, Germany

Two-dimensional-electron gases (2DEG) have interesting physical properties and allow studies in reduced dimensions. They can function as a host material for electrostatic qubit systems, like quantum dots. These 2DEGs are mostly created in high-electron-mobility transistors with modulation doping.

However, there are deep donor levels, that hinder compatibility with photonic applications. Approaches like short-period-superlattice doping[1] lead to unwanted gate hysteresis. All structures seem to be plagued by charge noise, probably arising from the dopands in the modulation doped region. To avoid the interference with the impurities, the 2DEG can alternatively be induced with an electric field.

An issue with these structures is to produce reliable ohmic contacts to the 2DEG without short-circuits to the inducing gate. Here we use an approach with alloyed ohmic contacts to a global backgate, inducing the 2DEG. The 2DEG is then contacted with non-alloyed epitaxial contacts.

[1] Umansky, V., et al. "MBE growth of ultra-low disorder 2DEG with mobility exceeding $35*10^6 cm^2/Vs$." *Journal of Crystal Growth* 311.7 (2009): 1658-1661.

HL 65: Quantum Optics on the Nanoscale: From Fundamental Physics to Quantum Technologies (joined session, HL, DS, O, TT, organized by HL)

Time: Thursday 9:30–12:30 Location: HSZ 02

Invited Talk HL 65.1 Thu 9:30 HSZ 02

Quantum dot based quantum technologies — •Pascale Senellart — CNRS - Université Paris-Saclay, 91460 Marcoussis, France

Scaling optical quantum technologies requires efficient single photon sources and two-photon gates. Such devices can be obtained using artificial atoms like semiconductor quantum dots (QDs). Yet, an ideal atom-photon interface is required, where the QD interacts with only one mode of the optical field and is free from decoherence. We have developed a near-optimal QD-photon interface by deterministically coupling a QD to a microcavity [1]. With an electrical control, the QD transition is shown to be almost decoherence free. The QD-cavity devices present a cooperativity of 12 and the QD state can be coherently manipulated with a π-pulse obtained for only 4 incident photons [2]. The devices operate as bright solid-state single-photon sources with single photon purity and indistinguishability above 98% and a brightness exceeding 20 times that of parametric down-conversion sources [3]. We also report on a single-photon filter that converts a coherent pulse into a highly non-classical light wavepacket [4], a first step toward deterministic two photon gates.

[1] A. Dousse, et al., Phys. Rev. Lett. 101, 267404 (2008). [2] V. Giesz, et al., Nature Communications 7, 11986 (2016). [3] N. Somaschi, et al., Nature Photonics 10, 340 (2016). [4] L. De Santis, et al., arXiv:1607.05977.

Invited Talk HL 65.2 Thu 10:00 HSZ 02

Controlled strong coupling of a single quantum dot to a plasmonic nanoresonator at room temperature — Heiko Gross[1], Joachim M. Hamm[2], Tommaso Tufarelli[2], Ortwin Hess[2], and •Bert Hecht[1] — [1]Nano-Optics and Biophotonics Group, Universität Würzburg, 97074 Würzburg, Germany — [2]The Blackett Laboratory, Imperial College London, London SW7 2AZ, United Kingdom

We demonstrate controlled and tunable strong coupling of a mesoscopic plasmonic slit resonator and a single colloidal quantum dot at room temperature. Strong coupling is achieved (i) by placing the quantum dot within the mode field of the nanoresonator with nm precision using scanning probe technology and (ii) by exploiting the collective coupling of the band-edge multiplet of states to the broadband plasmonic resonance. Due to the resulting fast rate of energy exchange the strong coupling regime is reached and besides the exciton also the otherwise quenched trion state couples strongly with the slit resonator resulting in a four-peaked spectrum under strong-coupling conditions.

Invited Talk HL 65.3 Thu 10:30 HSZ 02

High efficiency and directional emission from a nanoscale light source in a planar optical antenna — •Mario Agio — Laboratory of Nano-Optics, University of Siegen, 57072 Siegen, Germany

Light emission and absorption are critical to applications such as lighting, sensing and information technology. Despite fundamental progress in the manipulation of light-matter interaction, coupling electromagnetic modes to nanoscale sources and detectors with a very high efficiency remains a challenge. Here, we introduce a simple planar antenna structure based on thin-film optics that attains more than 90% outcoupling efficiency and, at the same time, directional emission with a semiangle below 10 degrees [1,2]. Our findings are particularly relevant for materials with a high refractive index, like semiconductor-based nanophotonic devices, which typically exhibit a large mismatch to free-space and guided modes. Furthermore, our approach is general and thus applicable to any wavelength, provided that materials with the required optical properties are available. Finally, we discuss some results in the context of solid-state singlephoton sources.

[1] S. Checcucci et al., Light: Science & Applications 6, e16245 (2017). [2] H. Galal, M. Agio, to be submitted.

Coffee Break

Invited Talk HL 65.4 Thu 11:30 HSZ 02

Tailoring quantum states by measurement — •Jörg Wrachtrup — Institute for Quantum Science and Technology, IQST, University of Stuttgart, 70569 Stuttgart, Germany

Measurement induced back action is a unique property of quantum mechanics. It is a central challenge for a variety of applications, like error correction. However, it is also a unique tool in e.g. dissipative generation of entanglement or ground state cooling. In my talk, I will describe ways to control spin quantum states by tailored photonic measurements. I will describe of how to extend those measurement to a general scheme also, e.g. allowing to cool mesoscopic elements like mechanical oscillators.

Invited Talk HL 65.5 Thu 12:00 HSZ 02

Quantum optics and quantum control at the nanoscale with surface plasmon polaritons — •Stéphane Guérin — UMR 6303 CNRS-Université Bourgogne Franche-Comté, 21078 Dijon, France

The quantum control of emitters is a key issue for quantum information processing at the nanoscale. This generally necessitates the strong coupling of emitters to a high Q-cavity for efficient manipulation of the atoms and field dynamics (cavity quantum electrodynamics or cQED). Since almost a decade, strong efforts are put to transpose cQED concepts to plasmonics in order to profit of the strong mode confinement of surface plasmons polaritons [1]. Despite the intrinsic presence of lossy channels leading to strong decoherence in plasmonics systems, it has been experimentally proven that it is possible to reach the strong coupling regim [2]. In this work, we derive an effective Hamiltonian [3,4], which allows us to describe the metallic nanoparticle-emitter interaction in full analogy with cQED formalism using a multimodal lossy cavity. We discuss (i) the concept of dressed states of quantum emitter strongly coupled to a metal nanoparticle [5], leading for instance to efficient/blockade population transfers or superradiance/subradiance effects, and (ii) the multi-emitter adiabatic control via quantum plasmonics, for instance via stimulated Raman adiabatic processes [3].

[1] M.S. Tame, et al., Nature Physics 9, 329 (2013). [2] G. Zengin, et al., Phys. Rev. Lett. 114, 157401 (2015). [3] B. Rousseaux, et al., Phys. Rev. B 93, 045422 (2016). [4] D. Dzsotjan, et al., Phys. Rev. A 94, 023818 (2016). [5] H. Varguet, et al., Opt. Lett. 41, 4480 (2016).

HL 66: Focus Session on 2D Materials: Ballistic Quantum Transport in Graphene (jointly with DY, DS, HL, MA, O)

Ballistic electron waves yielded a plethora of insights already in 2D semiconducting heterostructures. Recent experimental techniques have paved the way to this regime also for graphene. The massless, relativistic, and chiral nature of its charge carriers enriches ballistic transport by qualitatively new physical phenomena, such as ambipolar states near pn-junctions, Klein tunneling, or a zeroth Landau level in a perpendicular magnetic field. This session will review the actual status.

Organisation: Wolfgang Häusler, Universität Augsburg; Reinhold Egger, Universität Düsseldorf; Klaus Richter, Universität Regensburg

Time: Thursday 9:30–13:00 Location: HSZ 03

Invited Talk HL 66.1 Thu 9:30 HSZ 03
Kondo Screening of a Vacancy Magnetic Moment in Graphene — •Eva Y. Andrei — Dept. of Physics, Rutgers University, Piscataway, NJ

Graphene in its pristine form has transformed our understanding of 2D electron systems leading to fundamental discoveries and to the promise of important applications. When the perfect honeycomb lattice of graphene is disrupted by single atom vacancies new phenomena emerge including the buildup of local charge and the appearance of a local moment. Using scanning tunneling microscopy to identify Kondo screening of the vacancy moment by its spectroscopic signature, we demonstrate that the local magnetic moment can be controlled either by doping or through the local curvature. This allows to detect and map the quantum phase transition separating magnetic from nonmagnetic states in this pseudogap system.

Invited Talk HL 66.2 Thu 10:00 HSZ 03
Higher-Than-Ballistic Conduction in Viscous Electron Fluids — •Leonid Levitov — Physics Department, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge MA02139

This talk will argue that in viscous electron flows interactions facilitate transport, allowing conductance to exceed the fundamental Sharvin-Landauer quantum-ballistic limit. The effect is particularly striking for the flow through a viscous point contact, a constriction exhibiting the quantum-mechanical ballistic transport at zero temperature but governed by electron hydrodynamics at elevated temperatures. The crossover between the ballistic and viscous regimes occurs when the mean free path for e-e collisions becomes comparable to the constriction width. Further, we will discuss the negative nonlocal response, a signature effect of viscous transport. This response exhibits an interesting nonmonotonic behavior vs. temperature at the viscous-to-ballistic transition. The response is negative but small in the highly viscous regime at elevated temperatures. The value grows as the temperature is lowered and the system becomes less viscous, reaching the most negative values in the crossover region where the mean free path is comparable to the distance between contacts. Subsequently, it reverses sign at even lower temperatures, becoming positive as the system enters the ballistic regime. This peculiar behavior provides a clear signature of the ballistic-to-viscous transition and enables a direct measurement of the electron-electron collision mean free path.

Invited Talk HL 66.3 Thu 10:30 HSZ 03
Electron Optics in Ballistic Graphene — •Ming-Hao Liu — Department of Physics, National Cheng Kung University

Electrons in clean graphene are known to behave like "charged photons" due to its celebrated energy dispersion linear in momentum, providing an ideal platform for exploring electron optics. Despite the discovery of graphene in 2004, devices of ultraclean samples with micron-scale mean free paths became accessible only recently. Reliable quantum transport simulations in the ballistic limit for understanding and predicting high-quality transport experiments have therefore become increasingly demanded nowadays. In this talk, an overview of our recent progress on simulating a variety of ballistic graphene transport experiments will be given, such as Fabry-Pérot interference, snake states, and gate-defined electron waveguides [1]. Keys to such quantum transport simulations will be briefly introduced [2]. Ongoing works possibly including *pnp* junctions in the presence of 2D Moiré superlattice and Weiss oscillation due to 1D periodic gating will be mentioned at the end of the talk.

[1] P. Rickhaus *et al.*, Nat. Communs. **4**, 2342 (2013); M. Drienovsky *et al.*, Phys. Rev. B **89**, 115421 (2014); A. Varlet *et al.*, Phys. Rev. Lett. **113**, 116601 (2014); P. Rickhaus *et al.*, Nat. Communs. **6**, 6470 (2015); P. Rickhaus *et al.*, Nano Lett. **15**, 5819 (2015).
[2] M.-H. Liu *et al.*, Phys. Rev. Lett. **114**, 036601 (2015).

15 min. break.

Invited Talk HL 66.4 Thu 11:15 HSZ 03
Ballistic Transport in Mesoscopic Graphene Devices — •Christoph Stampfer — JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany

The recent technological advances in encapsulating graphene by hexagonal boron nitride forming artificial van-der-Waals heterostructures allows the fabrication of graphene devices with high electronic quality. Outstanding charge carrier mobilities and mean free paths with more than 10 micrometer are now accessible making this material stack interesting for studying ballistic transport. By further structuring the graphene-hBN based heterostructures mesoscopic devices can be fabricated on which phase coherent ballistic quantum transport can be studied.

Here, I will present low-temperature magneto-transport measurements on both (i) graphene quantum point contacts and (ii) high mobility graphene rings encapsulated in hexagonal boron nitride. Our experiments allow to extract information on quantized conductance, renormalized Fermi velocities close to the charge neutrality point as well as the co-existence of weak localization, Aharonov-Bohm oscillations and universal conductance fluctuations in graphene rings.

Invited Talk HL 66.5 Thu 11:45 HSZ 03
Interaction-Induced Conductance from Zero Modes in a Magnetic Graphene Waveguide — •Alex Zazunov — Heinrich-Heine-Universität Düsseldorf

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 flat 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.

HL 66.6 Thu 12:15 HSZ 03
Ballistic thermophoresis on graphene — •Emanuele Panizon[1], Roberto Guerra[1,2], and Erio Tosatti[1,2,3] — [1]SISSA, Trieste, Italy — [2]CNR-IOM Democritos, Trieste, Italy — [3]ICTP, Trieste, Italy

The textbook thermophoretic force acting on a diffusing body in a fluid is proportional to the local temperature gradient. This is not the case for a diffusing physisorbed body on a submicron sized 2D suspended layer. A Non-Equilibrium Molecular Dynamics study of a test nanosystem - a gold nanocluster adsorbed on a single graphene sheet of length L clamped between two temperatures ΔT apart - reveals a phoretic force that is parallel to, but essentially independent of, the gradient magnitude $\Delta T/L$ up to a substantial L of $150nm$.

This is argued to represent ballistic thermophoresis, where the force is provided by the flux of massively excited flexural phonons, whose flow is in turn known to be ballistic and distance-independent up to relatively long scattering lengths before the eventual onset of the more

standard diffusive regime. The surprising thrust and real momentum provided by the flexural modes are analysed and understood in terms of the large mass non/uniformity involved with these modes. The ensuing surf-riding of adsorbates on the vibrating 2D hard sheet, and the resulting gradient independent thermophoretic force, are not unlikely to possess practical applications.

HL 66.7 Thu 12:30 HSZ 03

Quantum time mirrors in two-band systems with and without broken time-reversal symmetry — •Phillipp Reck[1], Cosimo Gorini[1], Arseni Goussev[2], Viktor Krueckl[1], Mathias Fink[3], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg — [2]Department of Mathematics, Physics and Electrical Engineering, Northumbria University, Newcastle Upon Tyne, UK — [3]Institut Langevin, ESPCI, CNRS, PSL Research University, Paris

Both metaphysical and practical considerations intrigued generations of scientists to devise and implement time-inversion protocols – in particular the Hahn echo [1], different forms of "time mirrors" for classical waves (see e.g. [2]), and recently an instantaneous time mirror for water waves [3]. With our proposal for an instantaneous Quantum Time Mirror [4], we showed the possibility to extend the family of time reversal protocols to *continuous quantum* systems, more precisely to wave packets in Dirac-cone systems, by changing the propagation direction with a short, time-dependent pulse.

In this talk, we discuss the effect on the Quantum Time Mirror of both, a static, out-of-plane magnetic field, which breaks time-reversal symmetry, and band structures other than the Dirac cone, e.g. the valence and conduction bands in direct gap semi-conductors.

[1] E. L. Hahn, Spin echoes. Phys. Rev.. 80, 580 (1950)
[2]M. Fink, IEEE Trans. Ultrason. Ferroelectr. Freq. Control, 39, 555, (1992)
[3]V. Bacot, et al., Nat. Phys. 12, 972–977 (2016)
[4]P. Reck, et al., arXiv:1603.07503 (2016)

HL 66.8 Thu 12:45 HSZ 03

Current flow paths in deformed graphene and carbon nanotubes — Erik Kleinherbers, •Nikodem Szpak, and Ralf Schützhold — Faculty of Physics, University of Duisburg-Essen, Germany

Due to imminent applications in nanoelectronics it is of high interest to understand the precise conductance properties of deformed graphene and bent carbon nanotubes. Since low-energy electronic excitations behave like massless Dirac fermions the current flow can be approximated semiclassically and used as a guide in the design of conducting nanoelectronic elements and nanosenors. Taking into account the curvature effects as well as an emerging inhomogeneous pseudo-magnetic field we calculate the current flow paths theoretically and compare them with numerical simulations of the full electronic transport.

HL 67: Perovskites, Hybrid Photovoltaics and Plasmonics

Time: Thursday 9:30–11:15 Location: POT 81

HL 67.1 Thu 9:30 POT 81

Analytical representation of dynamical quantities in *GW* from a matrix resolvent — •Jan Gesenhues[1], Dmitrii Nabok[2], Michael Rohlfing[1], and Claudia Draxl[2] — [1]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany — [2]Theoretische Festkörperphysik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

A common problem in *GW* calculations is the treatment of the energy dependence of the screened coulomb interaction *W*. While the state of the art approach is the contour deformation technique, plasmon-pole models are often employed to allow for an analytical frequency convolution in calculating *GW*. In this talk we discuss a third alternative, which calculates the frequency dependent screening by determining the resolvent, which is set up from a matrix representation of the dielectric function. On the one hand this poses great educational insight into the topic, because it refrains from a numerical frequency convolution and allows one to actually write down the frequency dependence of *W*. On the other hand, the approach enables the exact description of plasmonic features in the spectral function, since it goes beyond plasmon-pole models. We present results for common materials and discuss some of the issues that appear when dealing with the spectral function (i.e. Im $G(\omega)$).

HL 67.2 Thu 9:45 POT 81

Ultrafast photo-switching of hybrid polaritons in black phosphorus heterostructures — •Fabian Sandner[1], Markus A. Huber[1], Fabian Mooshammer[1], Markus Plankl[1], Leonardo Viti[2], Lukas Z. Kastner[1], Tobias Frank[1], Jaroslav Fabian[1], Miriam S. Vitiello[2], Tyler L. Cocker[1], and Rupert Huber[1] — [1]University of Regensburg, 93040 Regensburg, Germany — [2]NEST CNR, 56127 Pisa, Italy

In recent years, special attention has been paid to surface polaritonics in van der Waals layered materials and their heterostructures. In particular, graphene has been intensely studied, as it exhibits strongly confined and widely tunable mid-infrared Dirac plasmons. However, the absence of an energy gap inhibits high switching contrasts, which are desired for nano-polaritonic devices. Here, we design and fabricate a SiO_2/black phosphorus/SiO_2 heterostructure and demonstrate ultrafast switching of a mid-infrared hybrid polariton by femtosecond near-infrared laser excitation. We trace the mode in energy, time, and space using pump-probe near-field microscopy and spectroscopy, providing us with real-space snapshots of the mode as well as its dispersion. In our heterostructure, surface phonons on the SiO_2 layers couple to transient surface plasmons on the photoexcited black phosphorus layer. The resulting hybrid interface polariton exhibits exceptional coherence properties and features a well-defined frequency and wavevector for the entire lifetime of the mode. Our results, which can be fully reproduced by theoretical calculations, show that the hybrid mode holds significant potential for future ultrafast nano-optical devices.

Coffee Break

HL 67.3 Thu 10:15 POT 81

Hierarchical Anodic Aluminum Oxide Membranes as Promising Platform for Constructing Plasmonic Structure — •Yi Wang[1,2], Shuping Xu[2], Weiqing Xu[2], Huaping Zhao[1], and Yong Lei[1] — [1]Institute for Physics and IMN MacroNano, Ilmenau University of Technology, Ilmenau 98693, Germany — [2]State Key Laboratory of Supramolecular Structure and Materials, Jilin University, Changchun, China

Attributing to the ordered and uniform porous structure, anodic aluminum oxide (AAO) membranes are widely used as templates in preparation of ordered nanostructure arrays of functional materials for various device applications. In particular, different plasmonic structures have been fabricated based on AAO membranes for sensing and energy-related device applications. Here, we demonstrate the fabrication of hierarchical AAO membranes with unique and controllable patterns, which provide a promising platform for constructing plasmonic structures. By precisely controlling the potential during the anodization process, the sophisticated structure of AAO membranes can be regulated into many distinctive patterns. After replicating the hierarchically structural AAO membranes with polymer and noble metal, hierarchical nanostructures with unique surface plasmon resonance (SPR) properties can be obtained, which can be developed as a dynamic plasmonic device or SERS substrate. The elaborate regulation of hierarchical AAO membranes broadens the scope for the functional nanostructure design, as well as applications in the fields of plasmonic switchers, microfluidic engineering, and nanophotonic devices.

HL 67.4 Thu 10:30 POT 81

Investigation of Surface Plasmons on β-Sn Segregations of GeSn-Nanostructures — •Felix Reichmann[1,2], Viktoria Schlykow[1], Subhajit Guha[1], Peter Zaumseil[1], David Stolarek[1], and Thomas Schröder[1,2] — [1]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]BTU Cottbus-Senftenberg, Konrad-Zuse Straße 1, 03046 Cottbus, Germany

GeSn is a promising candidate for future optoelectronic applications compatible with the current Si based technology. The band gap is tuneable by varying the Sn content in the GeSn alloy. However, the

lattice/thermal mismatch of Ge/ α-Sn and Ge/Si leads to defects and the low solubility of Sn in Ge leads to β-Sn segregations during growth and post growth process. High quality growth of GeSn on Si for future high performance devices can be achieved by nanoheteroepitaxy. Furthermore, β-Sn segregations could support surface plasmons (SP) and then be used as antennas for the GeSn nanostructures. SPs on β-Sn are expected for excitation energies in the visible range, in particular for an energy of 2 eV. The dielectric function of β-Sn then fulfils the condition for SPs at a metal-dieletric interface. For very small β-Sn structures, localized SPs should lead to an extraordinary absorbance/scattering of light compared to their size. When cooling down the β-Sn below 13 °C it transforms to α-Sn, resulting in a change of the dielectric function, not supporting the SPs anymore. The goal of our study is to evaluate the SP activity of β-Sn to enhance light emission in GeSn nanostructures for photodetection enhancement.

Invited Talk HL 67.5 Thu 10:45 POT 81

2D Quasicrystals from Semiconducting Perovskite Oxides — •Wolf Widdra[1,2] and Stefan Förster[1] — [1]Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

During the last decade, the fields of interface-driven 2D materials have gained tremendous attention, often due to their promising new structural or advantageous transport properties. One of these are the interface-driven 2D oxide quasicrystals (OQCs) which exhibit perfect, long-range dodecagonal rotational symmetry [1]. Such symmetry is forbidden for periodic structures. However, it can form in systems that are describable by 2D tiling patterns, which follow self-similarity supporting inflation rules. For the class of Perovskite oxides, we show that ultrathin films restructure into 2D quasicrystals on top of a threefold metallic substrate: $BaTiO_3$ as well as $SrTiO_3$ form stable and long-range ordered dodecagonal OQCs on Pt(111) that are characterized by brilliant 12-fold diffraction patterns [1]. Scanning tunneling microscopy resolves the aperiodic structure of surface atoms forming tiling patterns based on triangular, quadratic, and rhombic elements that are self-similar on length scales of $(2+\sqrt{3})^n$ times 0.68 nm. Concept and details of the interface-driven structures will be discussed in context of phason strain and formation of competing approximant structures [2]. First results on the electronic bandstructure will be presented.

[1] S. Förster et al., Nature 502, 215 (2013). [2] S. Förster et al., Phys. Rev. Lett. 117, 095501 (2016).

HL 68: Focus Session: Semiconductor Materials and Nanostructure for Photocatalysis

Time: Thursday 9:30–12:30 Location: POT 51

Invited Talk HL 68.1 Thu 9:30 POT 51

Solar-driven photoelectrochemical water splitting and carbon dioxide reduction — •Joel Ager — Joint Center for Artificial Photosynthesis, Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA USA — Department of Materials Science and Engineering, UC Berkeley

Solar to fuel conversion, if it could be performed in a sustainable manner, could provide an alternative to mankind's currently unsustainable use of fossil fuels. Solar fuel generation by photoelectrochemical (PEC) methods is a potentially promising approach to address this fundamental and important challenge.

While there are number of laboratory-scale solar to hydrogen (STH) conversion devices whose efficiencies exceed 10%, there are very few reports of long term operational stability. In this context, the long term stability of protective coatings for water oxidation photoanodes will be discussed, with an emphasis on the experimental procedures required to predict the operational lifetime.

Electrochemical carbon dioxide reduction is comparatively less mature as a technology and hence the challenges are more basic. Indeed, there are very few report of systems which produce usable fuel products with high selectivity. Recently, building on work performed with Cu nanocubes, we have designed Cu nanostructures which achieve up to 70% conversion of carbon dioxide to C2+ products. When coupled with high efficiency solar cells, overall energy conversion efficiencies exceeding that of natural photosynthesis can be achieved.

HL 68.2 Thu 10:00 POT 51

Tuning the electronic structure of Nb3O7(OH) by titanium doping for enhanced light-induced water splitting — Wilayat Khan[1], •S. Betzler[2], O. Sipr[3], Ch. Scheu[4], and J. Minar[5] — [1]New Technologies-Research Center, University of West Bohemia, Univerzitní 8, 306 14 Plzen, Czech Republic — [2]Department of Chemistry and Center for NanoScience, LMU Munich, Butenandtstraße 11, 81377 Munich, Germany — [3]NTC, University of West Bohemia, Plzen, Czech Republic — [4]Max-Planck-Institut fur Eisenforschung GmbH, Max-Planck-Straße 1, Du*sseldorf, Germany — [5]NTC, University of West Bohemia, Plzen, Czech Republic

Water photolysis is a clean and renewable source for hydrogen fuel and is therefore considered as a potentially important part of the solution of the energy crises. An extensive work has been performed on transition metal oxides semiconductors like TiO2, WO2 and Fe2O3, which can be used as electrode materials. Recently, Nb3O7(OH) has been proposed as a promising material for this propose due to its stability and suitable band gap [1]. Here we report on the modification of the structure and electronic properties of Nb3O7(OH) due to the Ti doping. Our theoretical study is based on the density functional theory using FP-LAPW method. The Ti-doped Nb3O7(OH) showed a direct band gap at the G point in the calculated band structures. In addition, Ti doping modifies the optical properties of the host material in a desirable way. Theoretical study is accompanied by a corresponding detailed experimental EELS study. [1] W. Khan et. al., J. Phys. Chem. C, 2016, 120 (41), 23329-23338

HL 68.3 Thu 10:15 POT 51

Semiconductor surface stabilization under photoelectrochemical conditions — •Waqas Saddique, Klaus Stallberg, Gerhard Lilienkamp, and Winfried Daum — Institute of Energy Research and Physical Technologies, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany

The production of hydrogen by solar energy via water splitting in photoelectrochemical (PEC) cells is a field of current research and challenges in materials research. III-V semiconductors with suitable band gaps are candidates for water splitting but frequently subjected to corrosion during the water splitting process and suffer from corrosion-related decrease in efficiency. GaP has an indirect band gap of 2.26 eV which covers both the hydrogen and oxygen evolution potentials. So GaP can in principle be used as photocathode and photoanode, respectively. We have studied structural and chemical properties and modifications of an n-GaP(100) photoanode after extended photoelectrochemical activity. A 4 nm thin oxide film was produced at the surface of an n-GaP(100) photoanode via oxidizing the surface at specific PEC conditions and subsequently hydrogenating the surface to passivate defects in the oxide film. This specific process results in the formation of a stable Ga surface oxide, which inhibits corrosion while allowing the light and the charge carriers to pass through the thin oxide for the completion of the PEC process. No other prior surface treatments or catalysts were required for this process. An open-circuit potential Voc of 1.2 V vs the reversible hydrogen electrode (RHE) was also determined.

Invited Talk HL 68.4 Thu 10:30 POT 51

Quantum confined colloidal semiconductor nanocrystals for solar fuels — •Frank Jäckel — Stephenson Institute for Renewable Energy and Department of Physics, University of Liverpool, UK

Co-catalyst decorated colloidal semiconductor nanocrystals are currently receiving increasing interest as a potentially cheap and scalable means for the photocatalytic generation of solar fuels such as solar hydrogen. [1,2] At the same time, colloidal semiconductor nanocrystals offer size-tuneable optical and electronic properties which allow the realisation of material properties beyond the bulk. In this talk, I will address how quantum confinement can be used to optimise quantum efficiencies and the use of the solar spectrum for photocatalytic hydrogen generation.[3] I will also present new approaches towards solving the stability-efficiency-dilemma frequently encountered in these systems. [4]

[1] M. Berr, A. Vaneski, A. S. Susha, J. Rodriguez-Fernandez, M. Döblinger, F. Jäckel, A. L. Rogach, and J. Feldmann, Appl. Phys. Lett. 97 093108 (2010).

[2] T. Simon, N. Bouchonville, M. J. Berr, A. Vaneski, A. Adrovic, D. Volbers, R. Wyrwich, M. Döblinger, A. S. Susha, A. L. Rogach, F. Jäckel, J. K. Stolarczyk, J. Feldmann, Nature Materials 13 1013 (2014).

[3] W. Li, G. O*Dowd, T. J. Whittles, D. Hesp, Y. Gründer, V. R. Dhanak, F. Jäckel Nanoscale 7 16606 (2015).

[4] W. Li, J. Lee, F. Jäckel ACS Appl. Mater. & Interf. 8 29434 (2016).

Coffee Break

HL 68.5 Thu 11:30 POT 51

Photo-catalytic carbon dioxide reduction with InGaN photoelectrodes — •Viktoria Kunzelmann, Andreas Zeidler, Andrea Winnerl, and Martin Stutzmann — Walter Schottky Institut, Technische Universität München, Garching, Deutschland

Carbon dioxide (CO_2) has reached a critical level in atmosphere and counts as one of the reasons for global warming. Reducing this greenhouse gas to hydrocarbon fuels would help solving environmental issues and simultaneously address challenges such as energy storage and resource shortage. Using a photo-catalytic reaction to convert CO_2 into fuels is one way to address this issue. Due to the chemical inertness of CO_2 and the instability of suitable catalysts, efficient CO_2 reduction is still challenging. Using gallium nitride (GaN) as a photo-electrode is promising, since GaN is relatively stable under operating conditions and provides electrons with sufficient energy. Tuning the band gap by alloying GaN with indium might additionally enhance desired reduction processes. The current work concerns charge transfer processes on the interface of p- and n-type GaN or indium gallium nitride (InGaN), grown by molecular beam epitaxy, and an electrolyte. The characterization of the photo-electrode material is done by: atomic force and scanning electron microscopy for topography analysis, Kelvin probe force microscopy to analyze the surface potential landscape of the samples, surface photo-voltage measurements to evaluate the change of the electronic band structure due to illumination and Hall effect measurements to clarify the charge charrier density. Additionally, first results of photoelectrochemical measurements will be presented.

HL 68.6 Thu 11:45 POT 51

Omnidirectional Photoelectrochemical Activity of Ultrathin CdS film on Periodic Three-Dimensional Composite Pillar/Truncated-Pyramid Au arrays — •Rui Xu, Liaoyong Wen, Huaping Zhao, Shipu Xu, Max Sommerfeld, Yang Xu, Yan Mi, Yaoguo Fang, and Yong Lei — Institute of Physics & Institute of Micro- and Nanotechnologies (ZIK MacroNano), Ilmenau University of Technology, 98693 Ilmenau, Germany

Photonic mode and surface plasmon resonance show prominent promise in improving light utilization of solar energy-related devices. In order to incorporate both features simultaneously, we designed and manufactured ordered array of three-dimensional metal pillar/truncated-pyramid (PTP) nanostructures. The experiments along with simulation indicate that the Au PTP arrays demonstrate multiple SPR and PM originated from the two structural elements leading to superior and broadband anti-reflection performance. To take these advantages, a conformal 90-nm-thick CdS film was coated on the PTP nanostructures and the resultant photoanode reaches a respectable light absorption over 90% in the overall optical operation regime. More importantly, the efficient light-trapping is omnidirectional and the calculated average absorptivity keeps almost the same in at least 50 degree range. The PTP photoanode demonstrated a dispersive light absorption, which worked in concert with CdS surface extension and strong light absorption to achieve a tremendous current promotion by a factor of 2.8 from the flat counterpart at -0.2 V (vs. Ag/AgCl).

Invited Talk HL 68.7 Thu 12:00 POT 51

Photo-electrochemistry modelling beyond idealised surfaces and the computational hydrogen electrode — •Harald Oberhofer — Technical University Munich Garching, Germany

The role computer modelling plays today in understanding and optimising catalysts for photo-electrochemical reactions is undisputed. Yet, state of the art simulation approaches tend to rely on a number of assumptions and simplifications which—according to newest results—may not be fully justified. For example, simulation of the all-important electro-catalytic water oxidation reaction is mainly based on idealised surfaces and the computational hydrogen electrode (CHE) approach, which evaluates the thermodynamic feasibility of a catalyst looking at pathway where each hydrogen abstraction is coupled to the removal of one electron (PCET). The precise reactive site of the catalyst is thereby viewed as irrelevant, based on the premise of idealised surfaces. Yet, especially on semi-conducting catalysts both the assumption of PCET and of pristine, defect-free catalyst surfaces are not necessarily fulfilled.

The great success of the CHE approach is in part due to its low computational cost allowing a computational screening of suitable catalyst materials. Any other scheme going beyond PCET and pristine surfaces should therefore match this advantage, ideally avoiding costly numerical sampling of solvent degrees of freedom. Yet, recent developments in thermodynamic modelling as well as embedding techniques, both liquid and solid-state, especially considering the interface between catalyst and solvent, point the way towards photo-electrochemistry modelling beyond the computational hydrogen electrode.

HL 69: Quantum Dots: Transport Properties I

Time: Thursday 9:30–12:30 Location: POT 151

HL 69.1 Thu 9:30 POT 151

Transport properties of ferromagnetic-semiconducting hybrid nanowires with well-defined MnAs nanocluster properties — •Matthias T. Elm[1], Ryutaro Kodaira[2], Ryoma Horiguchi[2], Kyohei Kabamoto[2], Shinjiro Hara[2], and Peter J. Klar[1] — [1]I. Physikalisches Institut, Justus Liebig University, Heinrich-Buff-Ring 16, D-35392 Giessen, Germany — [2]Research Center for Integrated Quantum Electronics, Hokkaido University, Sapporo 060-8628, Japan

For the realization of nano-spintronic devices current research focuses on the preparation and characterization of dilute magnetic semiconducting III-V nanowires. An alternative are hybrid nanowires with ferromagnetic nanoclusters, which exhibit well-defined magnetic and structural properties. Here we present the structural and electrical characterization of MnAs/InAs nanowire hybrids, which are prepared by selective-area growth of the nanowires followed by the endotaxy of MnAs nanoclusters. By varying the growth conditions, size, distribution and number of nanoclusters can be accurately controlled. Using SEM, EDX, HR-TEM as well as MFM, the structural and magnetic properties of the nanoclusters were investigated. First magnetotransport measurements reveal the large impact of the clusters on the transport properties in the nanowires. While single InAs nanowires show universal conductance fluctuations as well as a large positive magnetoresistance at low temperatures, a linear negative magnetoresistance is observed for hybrid nanowires with MnAs clusters completely penetrating the nanowires.

HL 69.2 Thu 9:45 POT 151

Influence of Dimensionality on Tunneling into a Quantum Dot — •Jan K. Kühne and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, Deutschland

We study the transport properties of a system of self-assembled InAs quantum dots at low temperatures. Especially, we investigate the influence of the dimensionality of the connected leads on the tunneling into a dot. The transport properties depend on a variety of parameters, such as temperature, size of the dots, magnetic field and the thickness of the tunneling barriers. Measuring shot noise reveals more information about our system than a current or conductance measurement alone. In particular the asymmetry of the tunneling rates can only be observed in the noise signal. Additionally, interaction effects between electrons are known to suppress or enhance shot noise [1].
By changing the current directions of our sample we encounter different behavior of the Fano factor and the shape of the resonance step. This can be explained by a change of dimensionality in the leads and therefore another density of states. By using a Master equation theory we are able to extract the corresponding tunneling rates from our measurements [2]. Further, we are interested in the effect of an applied

magnetic field on the transport and noise behavior of our system.
[1] A. Nauen, et al., Phys. Rev. B 70, 033305 (2004).
[2] G. Kiesslich, et al., Phys. Rev. B 68, 125320 (2003).

HL 69.3 Thu 10:00 POT 151

Development of a new device for CV spectroscopy of InAs quantum dots under internal illumination — •Pia Eickelmann[1,2], Sven Scholz[1], Andreas D. Wieck[1], and Arne Ludwig[1] — [1]Chair for Applied Solid State Physics, Ruhr-Universität Bochum, Universitätsstraße 150, D-44780 Bochum — [2]leaving to Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstraße 1, D-47057 Duisburg

Semiconductor quantum dots are one of the most interesting candidates for the realization of quantum information and communication. Therefore, these materials are investigated by several methods, for example by capacitance-voltage (CV) spectroscopy. The spectra for the conduction band states of InAs quantum dots under illumination by an external LED show additional charging peaks which are assigned to the charging of excitonic states in the quantum dots. [1]

In this talk we present a new device, on which CV spectroscopy can be measured under internal excitation of excitons in InAs quantum dots. In detail a quantum dot LED (QLED) containing five quantum dot layers of similar properties is epitaxially grown on a p-i-n-diode with embedded quantum dots. The CV structure and QLED can be contacted separately. Thus, it is possible to excite optically excitons in the CV-structure, using the QLED within the device. Hence, a purely electrical writing and reading out of the quantum state is possible. In the long term, this could be developed into a quantum memory by slight changes in the sample structure and the experimental setup.

[1] P. A. Labud et al., PRL 112, 046803 (2014)

HL 69.4 Thu 10:15 POT 151

Reflectometry readout of Ge hole spin qubits — •Josip Kukučka, Lada Vukušić, Hannes Watzinger, Elisabeth Lausecker, and Georgios Katsaros — IST Austria

Group IV materials and in particular Si have attracted much interest for the realization of a spin qubit especially since coherence times of almost one second were reported for an electron spin in isotopically purified samples [1]. In our group we are working with hole spin qubits confined in quantum dots formed in Ge hut wires. Due to the recently shown almost purely heavy-hole character of the confined hole states [2], not only long dephasing times but also fast spin manipulation times are expected for this type of hole spin qubit. In order to measure dephasing times, a series of spin-dynamic experiments are going to be performed. Fast qubit state readout is required for these experiments. We have implemented and optimized radio-frequency ohmic reflectometry [3]. The influence of the printed circuit board layout and resonance circuit elements on the sensitivity of the measurements will be addressed. In order to further simplify the sample fabrication and readout protocol, we are currently developing gate reflectometry [4,5], which will use already defined gates that are needed for the electrostatic definition of a double quantum dot system. First results will be presented. [1] Muhonen, J. T et al. Nature Nanotechnology 9, 986 (2014) [2] Watzinger, H. et al. Nano Lett. 16, 6879*6885 (2016) [3] Ares, N. et al. Phys. Rev. Applied 5, 034011 (2016) [4] Colless, J. I. et al. Phys. Rev. Lett. 110, 046805 (2013) [5] Gonzalez-Zalba, M. F. et al. Nature Communications 6, 6084 (2015)

HL 69.5 Thu 10:30 POT 151

Transmon qubits based on InAs/Al core/shell nanowire Josephson junctions — •Patrick Zellekens[1,2], Steffen Schlör[3], Arthur Leis[1,2], Nicholas Güsken[1,2], Torsten Rieger[1,2], Mihail Ion Lepsa[1,2], Alexander Pawlis[1,2], Detlev Grützmacher[1,2], Martin Weides[3], and Thomas Schäpers[1,2] — [1]Peter Grünberg Institut 9, Forschungszentrum Jülich, Germany — [2]JARA - Fundamentals of Future Information Technologies — [3]Physikalisches Institut, Karlsruher Institut für Technologie

State-of-the-art qubits, like the Cooper pair box, are typically tuned in frequency by a magnetic field. Our goal is to fabricate an electrically tunable qubit, using a semiconductor nanowire Josephson junction as nonlinear element. If a gate voltage is applied to the nanowire, the charge carrier concentration is changed, which effectively leads to a change in the critical current and the kinetic inductance of the junction. Thereby it is possible to tune the resonance frequency of the qubit into the excitation frequency of the microwave cavity without a flux bias. The main limitation for the qubit performance is the semiconductor-superconductor interface. Here, the InAs nanowires grown by molecular beam epitaxy were in-situ covered by an Al shell. This procedure ensures a clean interface without any contamination. The electrical properties of the InAs nanowires was tuned by means of Te doping. Based on these InAs/Al core/shell nanowires Josephson junctions were fabricated. Subsequently, the junctions were electrically characterized at low temperature. Finally, implementations as building blocks for 3-dimensional transmon qubits will be shown.

Coffee Break

HL 69.6 Thu 11:15 POT 151

Optimal feedback control of a single-electron transistor. — •Timo Wagner[1], Philipp Strasberg[2], Johannes C. Bayer[1], Eddy P. Rugeramigabo[1], Tobias Brandes[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität, Appelstr. 2, D-30167 Hannover, Germany — [2]Institut für Theoretische Physik, TU Berlin, Hardenbergstr. 36, D-10623 Berlin, Germany

Recently we reported the strong suppression of shot noise in a closed-loop feedback controlled single-electron transistor [1]. The implemented feedback loop compensates the time-dependent fluctuations between the single electron-tunneling events, leading to a highly accurate and stable tunneling current [1,2]. Our technique is analog to the generation of squeezed light in quantum optics, using in-loop photo detection [3]. Here we investigate the optimal feedback response, achieving the maximum suppression of shot-noise. For the optimal response the saturation value of the second cumulant of the full counting statistics [4] is found to be given by the electron target number. Astonishingly the feedback works even for target numbers much smaller than one.

[1] T. Wagner, et al. Nature Nanotech. (doi:10.1038/nnano.2016.225)
[2] T. Brandes, Phys. Rev. Lett. 105, 06060 (2010)
[3] S. Machida, Y. Yamamoto, Opt. Commun. 57, 290 (1986)
[4] S. Gustavson, et al., Surf. Sci. Rep. 64, 191 (2009)

HL 69.7 Thu 11:30 POT 151

Time-resolved optical detection of electron tunneling into a single self-assembled quantum dot — •Annika Kurzmann[1], Jens Kerski[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, Germany. — [2]Chair of Applied Solid State Physics, Ruhr-University Bochum, Germany.

Self-assembled quantum dots (QDs) as artificial atoms are promising building blocks for QD lasers and single photon sources and have been intensively investigated in optical and transport measurements. While transport measurements are still limited to measurements of ensembles of self-assembled QDs, optical measurements give access to single QDs [1].

We demonstrate here an optical detection scheme to observe quantum jumps for single electron tunneling into a single self-assembled QD. The detection scheme is based on driving the excitonic transition into resonance fluorescence [2], which is quenched in the presence of an additional electron. The observed random telegraph signal of single electron tunneling is evaluated using counting statistics. This reveals the interactions and correlations between excitons and electrons and gives direct access to the statistics 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 between the electron tunneling events.

[1] A. Kurzmann et al., Phys. Rev. Lett. **117**, 017401 (2016).
[2] C. Matthiesen et al., Nat. Commun. **4**, 1600 (2013).

HL 69.8 Thu 11:45 POT 151

Low dimensional transport phenomena in modulation-doped GaAs-based core-multishell nanowire field-effect transistors — •Jonathan Becker[1], Dominik M. Irber[1,2], Nari Jeon[2], Jakob Seidl[1], Damon J. Carrad[1], Stephanie Morkötter[1], Bernhard Loitsch[1], Sonja Matich[1], Markus Döblinger[3], Gerhard Abstreiter[1], Jonathan J. Finley[1], Lincoln J. Lauhon[2], Matthew Grayson[4], and Gregor Koblmüller[1] — [1]Walter Schottky Institut, Garching, 85748, Germany — [2]Dept. of Materials Science & Engineering, Northwestern Univ., Evanston, Il 60208, U.S.A. — [3]Dept. of Chemistry, LMU München, Munich 81377, Germany — [4]Dept. of Electrical Eng. & Computer Sci., Northwestern Univ., Evanston, Il 60208, U.S.A.

In this work we present evidence of 1D quantization in the electronic subband-structure of novel δ-doped GaAs/AlAs core-multishell Ω-

gated NWFET devices at low-temperature. The device is adapted from our previous studies of Si-δ-doped GaAs-AlGaAs core-shell NWFETs, which exhibit sharp switching characteristics (SS of 70 mV/dec at 300K) and low-temperature electron mobilities of $\approx$5000 cm^2/Vs of the 2DEG channel confined at the core-shell interface. We find a series of clear conductance steps of distinct subbands in the diffusive regime. Self-consistent Schrödinger-Poisson calculations of the electronic structure reveal a series of quantized degenerate and non-degenerate subbands in good agreement with the experimentally observed degeneracies and level spacings.

HL 69.9 Thu 12:00 POT 151

Heavy-hole states in Ge hut wires — •Hannes Watzinger[1], Christoph Kloeffel[2], Lada Vukušić[1], Marta Rossell[3,4], Violetta Sessi[5], Josip Kukučka[1], Raimund Kirchschlager[1], Elisabeth Lausecker[1], Alisha Truhlar[1], Martin Glaser[6], Friedrich Schäffler[6], Armando Rastelli[6], Andreas Fuhrer[4], Daniel Loss[2], and Georgios Katsaros[1] — [1]IST Austria, 3400 Klosterneuburg, Austria — [2]University of Basel, 4056 Basel, Switzerland — [3]Empa, 8600 Dübendorf, Switzerland — [4]IBM Research Zürich, 8803 Rüschlikon, Switzerland — [5]TU Dresden, 01062 Dresden, Germany — [6]JKU, 4040 Linz, Austria

Holes confined in group IV quantum dots are promising candidates for the realization of spin qubits. In our group we study holes which are confined in SiGe self-assembled nanostructures [1]. Here we focus on transport measurements through so called Ge hut wires [2]. The g-factors, obtained from magnetic field spectroscopy, show a high in-plane and out-of-plane anisotropy of up to 18, which depends on the number of holes confined in the quantum dot. Numerical simulations are in very good agreement with our experimental findings and reveal a heavy-hole character of the low energy states [3]; such is important for achieving long dephasing times. This work is supported by the EC FP7 ICT project no. 323841, the ERC Starting Grant no. 335497 and the FWF-I-1190-N20 project.

[1] Katsaros, G. et al., Nature Nano. 5, 458-464 (2010); [2] Zhang, J. J. et al. PRL 109, 085502 (2012); Watzinger, H. et al. APL Mater. 2, 076102 (2014) [3] Watzinger, H. et al. Nanolett. 16, 6879-6885 (2016)

HL 69.10 Thu 12:15 POT 151

Toward a metrological quantification of the conversion efficiency in GaAs nanowire based photodetectors — •Davide Cammi[1], Beatrice Rodiek[2], Kseniia Zimmermann[1], Martin Friedl[3], Nick Morgan[3], Anna Fontcuberta i Morral[3], Stefan Kück[2], and Tobias Voss[1] — [1]Institut für Halbleitertechnik (IHT) und Laboratory for Emerging Nanometrology (LENA), TU Braunschweig, Hans-Sommer-Straße 66, 38106 Braunschweig — [2]Physikalisch-Technische Bundesanstalt (PTB), Bundesallee 100, 38116 Braunschweig — [3]Laboratory of Semiconductor Materials (LMSC), Ecole Polytechnique Fédérale de Lausanne (EPFL), Route Cantonale, 1015 Lausanne, Schweiz

The design of novel photodetectors based on semiconductor nanowires with diameters of few hundred nanometers or below may lead to a significant enhancement of the photoconductive gain and an increase of the detection speed in comparison to the corresponding planar technology. However, a precise quantification of the photodetection performance of such devices requires the development of a metrological procedure for their calibration. In this contribution, we discuss the main challenges and the steps which are required, in order to achieve this goal. In particular, we propose an experimental approach which combines optical and electrical methods for the determination of a two-dimensional, spatially resolved mapping of the device*s photoresponse. We focus the investigation in particular on contacted single GaAs nanowires, which act as photodetectors in the near infrared spectral range.

HL 70: Topological Insulators I (joined session with TT)

Time: Thursday 9:30–12:45 Location: POT 251

Invited Talk HL 70.1 Thu 9:30 POT 251

Sub-nm probing of Topological insulators and Rashba systems — •Markus Morgenstern — II. Institute of Physics and JARA-FIT, RWTH Aachen, D-52074 Aachen, Germany

Spin-orbit interactions in solids are the key for many anticipated new functionalities ranging from the meanwhile traditional Datta-Das transistor to topological quantum computation using Majorana excitations. Local probes can provide crucial information on this interaction down to the nm scale. Within this talk, I will show how scanning tunneling spectroscopy reveals the presence of topologically protected edge states provided by a spin-orbit induced band inversion of heavy metal graphene [1], how the detrimental fluctuations of the spin-orbit interaction can be probed down to the nm length scale [2], and that ferroelectricity induces Rashba-type spin-orbit interaction within the bulk of the simple binary material GeTe [3].

[1] C. Pauly et al., Nat. Phys. 11, 338 (2015); ACS Nano 10, 3995 (2016). [2] J. R. Bindel et al., Nat. Phys. 12, 920 (2016). [3] M. Liebmann et al., Adv. Mat. 20, 560 (2016); H. J. Elmers et al., Phys. Rev. B 94, 201403 (2016).

HL 70.2 Thu 10:00 POT 251

2D Topological Insulators: Trends in Chemical Space — •Carlos Mera Acosta[1,2], Christian Carbogno[1], Adalberto Fazzio[2], Luca M. Ghiringhelli[1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Instituto de Física, Universidade de São Paulo, SP, Brazil

2D topological insulators (TI) have attracted considerable scientific interest in recent years [1]. The search for new TIs has often focused on elements with strong spin-orbit coupling (SOC) [2], which can induce the necessary topological transition. In this work, we have computed the topological invariant Z_2 for 200 functionalized honeycomb-lattice systems using our recent Wannier center of charge (WCC) [3] implementation in the FHI-aims electronic structure code. Besides confirming the TI character of well-known materials, e.g., functionalized stanene [1], our study found several other yet unreported TIs. This reveals that also elements with relatively low SOC can form TIs. To analyze the observed trends in chemical space we relate the WCCs to the atomic features of the constituent atoms using a compressed-sensing approach. For this purpose, the LASSO and ℓ_0 minimization of Ref. [4] is extended from learning scalar properties to functions.

This work received funding from The Novel Materials Discovery (NOMAD) Laboratory, a European Centre of Excellence.

[1] Y. Ren, Z. Qiao, and Q. Niu, *RPP* **79**, 6 66501 (2016).
[2] M. Z. Hasan and C. L. Kane, *Rev. Mod. Phys.* **82**, 3045 (2010).
[3] R. Yu, *et al.*, *Phys. Rev. B* **84**, 075119 (2011).
[4] L. M. Ghirighelli, *et al.*, *Phys. Rev. Lett.* **114**, 105503 (2015).

HL 70.3 Thu 10:15 POT 251

Occupied topological surface states in strained α-Sn — Victor Rogalev[1], •Tomáš Rauch[2], Markus Scholz[1], Felix Reis[1], Lenart Dudy[1], Andrzej Fleszar[3], Vladimir Strocov[4], Jürgen Henk[2], Ingrid Mertig[2,5], Jörg Schäfer[1], and Ralph Claessen[1] — [1]Physikalisches Institut und Röntgen Center for Complex Material Systems, Universität Würzburg, 97074 Würzburg, Germany — [2]Institute of Physics, Martin Luther University Halle-Wittenberg, 06099 Halle (Saale), Germany — [3]Institut für Theoretische Physik und Astronomie, Universität Würzburg, 97074 Würzburg, Germany — [4]Swiss Light Source, Paul Scherrer Institute, CH-5232 Villigen, Switzerland — [5]Max Planck Institute for Microstructure Physics, 06120 Halle (Saale), Germany

Unstrained α-Sn is a semimetal with a non-trivial band ordering at the Γ point of the bulk Brillouin zone: $E(\Gamma_8^+) > E(\Gamma_7^-) > E(\Gamma_7^+)$. Strain in (001) direction lifts the degeneracy of the Γ_8^+ level at the Fermi energy. We demonstrate that compressive strain turns the system into a strong topological insulator, whereas tensile strain causes a transition into the topological Dirac semimetal phase.

I will present the results of calculations carried out along experimental findings obtained by soft X-ray angle-resolved photoemission. I will show that the existence of a previously unknown surface state located in the occupied projected bulk band structure of α-Sn is unveiled by both experimental and theoretical methods. In addition, its topological origin was confirmed by calculating the topological invariants of the bulk bands.

HL 70.4 Thu 10:30 POT 251

Engineering topological phases in crystalline symmetry-protected monolayers — •Chengwang Niu, Patrick M. Buhl, Gustav Bihlmayer, Daniel Wortmann, Stefan Blügel, and Yuriy Mokrousov — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The properties that distinguish topological crystalline insulators (TCIs) and topological insulators (TIs) rely on crystalline symmetry and time-reversal symmetry, respectively, which encodes different surface/edge properties. Here, we predict theoretically that TlM, thallium chalcogenide, (M = S and Se) (110) monolayers realize a family of two-dimensional (2D) TCIs characterized by mirror Chern number $\mathcal{C}_M = -2$ with an even number of band inversions. [1] Remarkably, under uniaxial strain ($\approx 1\%$), a topological phase transition between 2D TCI and 2D TI is revealed in TlM. In contrast, for Na_3Bi, the band inversion occur at single k point, thus a coexistence of 2D TI and 2D TCI is obtained. [2] Finally, we show different edge-state behaviors, especially at the time reversal invariant points.

This work was supported by SPP 1666 of the DFG.

[1] C. Niu, P. M. Buhl, G. Bihlmayer, D. Wortmann, S. Blügel, and Y. Mokrousov, Nano Lett. **15**, 6071 (2015).

[2] C. Niu, P. M. Buhl, G. Bihlmayer, D. Wortmann, S. Blügel, and Y. Mokrousov, submitted.

HL 70.5 Thu 10:45 POT 251

Anisotropy of Magneto-Transport on the Surface of Topological Insulators — •Alexey Taskin[1], Henry Legg[2], Fan Yang[1], Andrea Bliesener[1], Satoshi Sasaki[3], Yasushi Kanai[3], Kazuhiko Matsumoto[3], Achim Rosch[2], and Yoichi Ando[1] — [1]Institute of Physics II, University of Cologne — [2]Institute for Theoretical Physics, University of Cologne — [3]Scientific and Industrial Research, Osaka University

Recent advances in MBE growth and microfabrication technique allow to obtain Topological Insulator (TI) systems where the transport is dominated by the surface. Here we report a magneto-transport study of high-quality bulk-insulating $Bi_{2-x}Sb_xTe_3$ thin films, which were fabricated into devices with electrostatic gates on both bottom and top surfaces. For magnetic fields applied parallel to the surface of a TI, we found a clear anisotropy in magnetoresistance and related planar Hall effect that originates from the fundamental property of the surface Dirac fermions, the locking of their spin and momentum. The key signature of anisotropic magnetoresistance is a strong dependence on the gate voltage with a characteristic two-peak structure near the Dirac point. The observed anisotropy is related to a modification of the topological protection of the Dirac electrons against backscattering from impurities in the in-plane magnetic field and provides an example of a controllable time-reversal breaking on the surface of TIs.

Coffee Break

HL 70.6 Thu 11:30 POT 251

Topological insulator - superconductor hybrid devices — •Peter Schüffelgen, Daniel Rosenbach, Michael Schleenvoigt, Tobias W. Schmitt, Martin Lanius, Christian Weyrich, Tristan Heider, Benjamin Bennemann, Stefan Trellenkamp, Elmar Neumann, Gregor Mussler, Thomas Schäpers, and Detlev Grützmacher — Peter Grünberg Institute 9, Forschungszentrum Jülich & JARA-FIT, 52425 Jülich, Germany

3D topological insulators (TIs) possess metallic surface states with a spin-locked momentum. Therefore, in proximity to an s-wave superconductor, Majorana zero modes (MZMs) are predicted to occur at the surface of TIs. We found first signatures of 4π-periodic Josephson supercurrents in our topological Josephson junctions. The TI thin film was 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 pristine surface states during ex-situ fabrication. To increase the 4π-periodic contribution we fabricated quasi 1D Josephson junctions on pre-patterned silicon substrates. By covering the Si-111 surface partly with a thin layer of Si3N4/SiO2 we made the topological insulator grow only on the silicon surface. In this way we were able to realize 1D trenches by predefining the MESA structure before MBE growth. To further improve the quality of our hybrid devices we developed a process, which allows to deposit superconducting contacts via stencil lithography. Combining this technique with selective area growth allows to fabricate complex devices in-situ.

HL 70.7 Thu 11:45 POT 251

Ultrafast mid-IR pump, THz probe spectroscopy investigating of the topological insulator BSTS — •Matteo Montagnese, Jingy Zhu, Chris Rheinhoffer, Yoichi Ando, and Paul H. M. van Loosdrecht — II. Physikalishes Institut der Universität zu Köln, Zülpicher str 77, D-25127 Köln

We present ultrafast pump-probe measurements on the topological insulator BSTS. We employed a high-intensity tunable mid-IR pulse (2-10 microns) as a pump, generated by difference-frequency mixing in an optical parametric amplifier to excite the BSTS system below the onset of the bulk optical electronic continuum. Upon excitation, the far-IR (0.1-3 THz) response of the system has been probed by a single-cycle coherent THz pulse, generated by optical rectification of a near-IR pulse. The time-resolved transmittance of the THz spectra have been measured employing optical sampling and time-domain techniques. By tuning the pump energy, the impurity states leading to charge puddle formation and the surface state are selectively populated, with the aim of disentangling their respective contributions to the dynamic optical conductivity.

HL 70.8 Thu 12:00 POT 251

Observation of the Quantum Anomalous Hall Effect depending on structural properties of $(VBiSb)_2Te_3$ layers — •Martin Winnerlein, Steffen Schreyeck, Stefan Grauer, Sabine Rosenberger, Kajetan Fijalkowski, Charles Gould, Karl Brunner, and Laurens W. Molenkamp — Physikalisches Institut, Experimentelle Physik III, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The quantum anomalous Hall effect is observed in thin V-doped $(BiSb)_2Te_3$ layers, a magnetic topological insulator. Thin layers revealing quantization are reproducibly deposited by molecular beam epitaxy at growth conditions effecting a compromise between controlled layer properties and high crystal quality. The influence of Sb content, layer thickness, structural quality, used substrates and cap layers is studied.

The Sb content is the main layer parameter to be optimized in order to approach charge neutrality. The Sb content is reliably determined from the in-plane lattice constant measured by X-ray diffraction even in thin layers. Within a narrow range at about 80% Sb content, the Hall resistivity reveals a maximum at 4 K and quantizes at mK temperatures [1]. Under these conditions thin layers grown on Si(111) or InP(111) and with or without a Te cap layer exhibit quantization. The quantization persists independently from the substrate, cap layer, the limited crystal quality and the degradation of the layer. This proves the robustness of the quantum anomalous Hall effect.

[1] S. Grauer *et al.*, Phys. Rev. B **92**, 201304 (2015).

HL 70.9 Thu 12:15 POT 251

Quantum Hall effect in three-dimensional Bi_2Se_3 single crystals — •Olivio Chiatti[1], Marco Busch[1], Sergio Pezzini[2], Steffen Wiedmann[2], Oliver Rader[3], Lada V. Yashina[4], 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]Helmholtz-Zentrum-Berlin für Materialien und Energie, 12489 Berlin, Germany — [4]Department of Chemistry, Moscow State University, 119991 Moscow, Russia

Topological insulators present surface (or edge) states of helically spin-polarized Dirac fermions, which are readily identified by spectroscopic methods. However, they are not so easily identified in transport, because they can be masked by bulk states. Bi_2Se_3 is one of the prototype topological insulators, but investigating transport by surface states has been hampered by residual bulk charge carriers. We have investigated nominally undoped, high-quality Bi_2Se_3 single crystals, with bulk electron densities of $n \approx 1.8 \cdot 10^{19}$ cm^{-3} and mobilities of up to $\mu \approx 10^3$ cm^2/Vs. Surface states have been confirmed by ARPES measurements [1]. We have measured magnetotransport between $T = 0.3$ K and $T = 72$ K, for tilted magnetic fields up to $B = 33$ T. We observe both Shubnikov-de Haas (SdH) effect and quantum Hall effect (QHE). The SdH oscillations appear dominated by 3D bulk charge carriers. However, the scaling of the QHE with sample thickness can be interpreted as transport over layered 2D states in the bulk.

[1] Chiatti *et al.*, Sci. Rep. **6**, 27483 (2016)

HL 70.10 Thu 12:30 POT 251

The electronic structure of few-quintuple-layer bismuth selenide from first-principles calculations — •Jae Young Kim

and Cheol-Hwan Park — Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea

Topological insulators are materials that behave as insulators in the interior, but have conducting surface states protected by time-reversal symmetry [1]. Bi2Se3, a prototypical example of a three-dimensional topological insulator, is a layered material composed of five-atom layers arranged along the z-direction, known as quintuple layers [2]. In this presentation, we will discuss the results of our first-principles calculations on the electronic properties of few-quintuple-layer Bi2Se3 and their relevance to device applications based on topological insulators.

[1] Hasan, M. Z., & Kane, C. L. (2010). Colloquium: topological insulators. Reviews of Modern Physics, 82(4), 3045.

[2] Zhang, H., Liu, C. X., Qi, X. L., Dai, X., Fang, Z., & Zhang, S. C. (2009). Topological insulators in Bi2Se3, Bi2Te3 and Sb2Te3 with a single Dirac cone on the surface. Nature physics, 5(6), 438-442.

HL 71: Transport Properties

Time: Thursday 9:30–11:30 Location: POT 112

HL 71.1 Thu 9:30 POT 112

Indirect excitons in (111) GaAs double quantum wells — •Colin Hubert, Alberto Hernández-Mínguez, Klaus Biermann, and Paulo Santos — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

We study the dynamics of indirect (or dipolar) excitons (IXs) in GaAs (111) double quantum wells (DQWs) subjected to a transverse electric field. In comparison with single (111) QWs, these DQWs can store, for a comparable applied fields and optical excitation density, a density of IXs much larger than in SQWs, thus leading to stronger IX-IX repulsive interactions. We show by means of spatially-resolved optical spectroscopy that IXs in (111) DWQs can be transported over distances exceeding 60 micrometers. From the spectral dependence of the IX spatial distribution profiles, we show that the long transport distances are due to drift forces arising from the strong IX-IX interactions.

HL 71.2 Thu 9:45 POT 112

Snake-orbit induced magnetoresistance oscillations in 2D electron gases — Andreas Leuschner[1], •Jakob Schluck[1], Mihai Cerchez[1], Thomas Heinzel[1], Klaus Pierz[2], and Hans Werner Schumacher[2] — [1]Heinrich Heine University Düsseldorf, Universitätsstr. 1, D-40225 Düsseldorf — [2]Physikalisch-Technische Bundesanstalt, Bundesallee 100, D-38116 Braunschweig

Localized magnetic fields of alternating sign in 2D electron gases give rise to snake- orbits. This may be realized in a Hall bar by the superposition of a homogeneous perpendicular magnetic field and a localized magnetic barrier of opposite sign [1]. The snake orbits redirect the edge states coming from source to the magnetic barrier from one edge of the Hall bar to the other, where, depending on the incident position they can be further directed back to source, or transmitted across the barrier. This has a commensurate periodic character, leading to oscillations in magnetoresistance. Experimental results and simulations are presented.

[1] S. Hugger, M. Cerchez, H. Xu, and T. Heinzel, Phys. Rev. B 76, 195308 (2007)

HL 71.3 Thu 10:00 POT 112

Thermal conductivity in intermetallic clathrates: A first-principles perspective on the phonon-glass concept — •Daniel Lindroth, Mattias Ångqvist, and Paul Erhart — Chalmers University of Technology, Department of Physics, Gothenburg, Sweden

Clathrates exhibit a very low thermal conductivity, which is a key factor for their very good thermoelectric properties and has been attributed to "phonon-glass" conduction behavior. Here, we present a computational analysis of the conduction mechanism using Ba8X16Y30 (X={Al,Ga}, Y={Si,Ge}) as model systems. Contributions to the thermal conductivity from both electrons as well as phonons are computed with Boltzmann transport theory.

The calculations are in good agreement with experimental data and in particular reproduce the experimentally observed ordering of the lattice thermal conductivity between the different systems. We demonstrate that these rather non-intuitive trends can be traced to the presence (or lack thereof) of dispersed higher frequency optical phonon modes, which provide a surprisingly large contribution to the lattice thermal conductivity. The "phonon-glass" behavior manifests itself in our calculations in the form of very short lifetimes, which indicate that already at room temperature the majority of modes is overdamped.

In terms of the electronic thermal conductivity, our results provide insight into the applicability of the Wiedemann-Franz law. While the latter is regularly used to separate lattice and electronic contributions to the thermal conductivity, our data show that the choice of pre-factor can incur an error of up to 50% for the electronic thermal conductivity.

HL 71.4 Thu 10:15 POT 112

Ab-initio phonon scattering by dislocations using Atomic-Green's function approach — •Tao Wang[1], Jesus Carrete Montaña[2], Natalio Mingo[2], and Georg K. H. Madsen[1,3] — [1]ICAMS, Bochum, Germany — [2]CEA-Grenoble, Grenoble, France — [3]Institute of Materials Chemistry, Wien, Austria

Predicting the thermal conductivity of modern semi-conductor architectures is an inherent multi-scale problem. It requires the quantification of phonon scattering strength caused by various types of defects e.g. vacancies, interfaces and dislocations, inside the materials. We introduce the atomic-Green's-function approach as an efficient way to evaluate the phonon scattering of dislocations with ab-initio precision. The three-dimensional Brillouin Zone (BZ) is divided into parallel planes perpendicular to the defect line direction. A triangulation mesh is adopted to discretize each of the two-dimensional BZ planes. By summing the Green's function results of all the linearly interpolated triangular elements on the planar sub-domains, the T-matrix and scattering cross section are obtained.

We will illustrate this strategy by setting up an atomic model of a quadrupolar arrangement of edge dislocations in silicon using linear elasticity theory. The frequency dependence of the scattering rate is calculated and discussed. Dislocation density influenced thermal conductivity evaluated from the Boltzmann-transport-equation is further analyzed to reveal how the long range elastic deformation field and short range dislocation core will modify lattice thermal transport behavior.

Coffee Break

HL 71.5 Thu 10:45 POT 112

Pressure-induced conduction band convergence in the thermoelectric ternary chalcogenide, $CuBiS_2$ — •Najebah Alsaleh, Elvis Shoko, and Udo Schwingenschlogl — King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia

The pressure dependence of electronic and thermoelectric properties of four ternary chalcogenides with space group Pnma, namely, $CuSbS_2$, $CuSbSe_2$, $CuBiS_2$, and $CuBiSe_2$ are investigated up to 10 GPa by using density functional theory combined with semiclassical Boltzmann theory. The effects of Van der Waals interactions are included in all calculations since these compounds have layered structures. All the compounds have indirect band gaps which decrease monotonically with increasing pressure except for $CuBiS_2$. For this compound, an indirect-indirect band gap switching occurs around 3 GPa leading to a conduction band convergence which appears to have important implications for thermoelectric properties. From a detailed examination of the structural changes in the different compounds, the unusual properties of $CuBiS_2$ are explained.

HL 71.6 Thu 11:00 POT 112

Electron pairing in nonlinear nanoelectromechanical systems — •Matthias Droth[1], Gábor Széchenyi[2], and András Pályi[1,2] — [1]Budapest University of Technology and Economics (Budapest, Hungary) — [2]Eötvös University (Budapest, Hungary)

Despite the success of BCS-theory, the underlying mechanism for electron-pairing remains elusive for many superconducting materials. For $SrTiO_3$, it has been shown [1] that electron-pairing outside the superconducting regime can be explained with an effectively negative charging energy $U<0$. Here, we show theoretically that a quantum dot

on a non-linear mechanical resonator supports electron-pair tunneling through the device by means of $U<0$ while its system parameters lie within reach of current experiments. We describe the system as a capacitor network model and discuss its relation to the Anderson-Holstein model [2]. Restricting the mechanical resonator potential to quadratic and quartic terms, we find that the system always possesses a phase that supports electron-pair tunneling. This phase can be achieved with a quantum dot on a suspended graphene resonator.

[1] Guanglei Cheng *et al.*, *Electron pairing without superconductivity*, Nature (London) **521**, 196 (2015).

[2] J. Koch, M. E. Raikh, and Felix von Oppen, *Pair tunneling through single molecules*, Phys. Rev. Lett. **96**, 056803 (2006).

HL 71.7 Thu 11:15 POT 112

Gaussian beam electron optics with quantum point contacts — •Jaan Freudenfeld[1], Sergey Platonov[1,2], Max Geier[3], Piet Brouwer[3], Vladimir Umansky[4], and Stefan Ludwig[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Deutschland — [2]Ludwig-Maximilians-Universität, München, Deutschland — [3]Freie Universität, Berlin, Deutschland — [4]Weizmann Institute of Science, Tel Aviv, 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. Quantum point contacts (QPCs) are fundamental building blocks of nanoscale circuits and characterized by quantized conductance. The emission of electrons from these one-dimensional constrictions happens within an aperture angle and is subject to diffraction. We experimentally study the diffraction pattern of QPCs with confinement potentials resembling parabolic saddle point potentials. In contrast to usual hard wall single slit experiments our parabolic "slits" emit electrons in Hermite functions. As a consequence the ballistic electron dynamics is described by Gaussian beam electron optics yielding a very different diffraction pattern compared to the usual single slit plane wave approach. We experimentally explore the diffraction pattern by combining magnetic deflection with electrostatic focusing using a field effect lens and compare the results with model calculations. The observed diffraction pattern and focusing properties of our electrostatic lens clearly indicate Gaussian beam electron optics, a crucial information for the design of future quantum circuit applications.

HL 72: Nitrides: Devices

Time: Thursday 9:30–11:45 Location: POT 06

HL 72.1 Thu 9:30 POT 06

Fabrication and characterization of hybrid n-GaN/p-PEDOT structures for optoelectronic applications — •Linus Krieg[1], Priya Moni[2], Karen Gleason[2], and Tobias Voss[1] — [1]Institute of Semiconductor Technology and Laboratory for Emerging Nanometrology, Braunschweig University of Technology, 38092 Braunschweig — [2]Department of Chemical Engineering, Massachusetts Institute of Technology, 02139 Cambridge, USA

Hybrid structures consisting of an inorganic and organic layer are promising for the development of cheap, versatile and tailored electronic and optoelectronic devices. The structures are supposed to combine the advantages of inorganic and organic components such as a high structural stability whilst maintaining a high flexibility. One method to conformally deposit polymer layers even on both, planar and 3D-structured substrates, is the oxidative chemical vapor deposition (oCVD). The oCVD process is dry and solventless as the polymer is deposited from the gas phase. Therefore, etching of fragile surfaces can be minimized. On the way towards a hybrid GaN/PEDOT LED, the oCVD of PEDOT on n-type GaN substrates is studied. In particular, the effect of different substrate temperatures on the resulting hybrid layer structures is investigated. The IV-characteristics of the hybrid p-n-junctions are analyzed and compared to that of structures containing an additional insulating tunnel barrier of poly(divinylbenzene) (pDVB) between the GaN and PEDOT. First results show pronounced diode characteristics of the hybrid devices and allow us to determine the relevant conduction mechanism at the inorganic/organic interface.

HL 72.2 Thu 9:45 POT 06

Optoelectronic Characterization of AlGaN-based MSM-UV-Photodetectors — •Sebastian Walde, Moritz Brendel, Sylvia Hagedorn, Frank Brunner, Ute Zeimer, and Markus Weyers — Ferdinand-Braun-Institut, Leibniz-Institut fuer Hoechstfrequenztechnik, Gustav-Kirchhoff-Straße 4, 12489 Berlin, Germany

The alloy $Al_xGa_{1-x}N$ used as absorber material in photodetectors (PD) offers a high sensitivity in the UV with cut-off wavelength between 200 nm (AlN) and 365 nm (GaN), adjustable by the Al-content x. A metal-semiconductor-metal (MSM) design has the advantage of a relatively simple layout, which makes it easy to fabricate and suitable for analyzing material properties of the underlying epitaxial layers.
We present results of bottom-illuminated MSM-UV-PD with $Al_{0.5}Ga_{0.5}N$ absorber layers of different thicknesses t_{abs}. The structures grown on AlN/sapphire exhibit a saturation of the external quantum efficiency (EQE) above specific saturation voltages. Two different carrier collection mechanisms can be observed and they are distinguished by different saturation regimes. The first is dependent on t_{abs} and can be explained by the extension of the space charge region below the biased electrode. In that case, EQE at a wavelength of 250 nm saturates above 40 V for $t_{abs} = 500$ nm. The second mechanism is independent of the absorber thickness showing EQE saturation already above 15 V. This is most likely related to crystal defects penetrating through the absorber layer and forming electrically active channels between the electrodes and the carrier collection volume.

HL 72.3 Thu 10:00 POT 06

Beyond classical band offsets: Employing multiquantum barriers for electron blocking in group III-nitride devices — •Anton Muhin[1], Martin Guttmann[1], Christoph Reich[1], Konrad Bellmann[1], Johannes Enslin[1], Norman Susilo[1], Luca Sulmoni[1], Tim Wernicke[1] und Michael Kneissl[1,2] — [1]Technische Universität Berlin , Institute of Solid State Physics — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Berlin

Electron leakage current is one of the major loss mechanisms in AlGaN-based light emitting devices (UV LEDs). This can be reduced by inserting a layer with a larger band gap into the heterostructure, an electron blocking layer (EBL), with a conduction band offset of typically 0.3-0.8 eV. By stocking multiple EBLs on a nanometer scale, an additional virtual barrier (VB) can be created by a so-called multiquantum barrier (MQB) structure. Numerical calculations were performed of AlGaN-MQBs in order to quantify the VB, the optimal structure parameters and their robustness to fluctuations. Polarization fields and the band profile have been modeled by solving the Poisson's equation. Transfer matrix method and the Esaki-Tsu current formula were applied to compute the reflection probabilities and the current-voltage-characteristics, respectively. The simulations show an increase of the effective barrier height of 66% when employing on optimized $Al_{0.2}Ga_{0.8}N$/GaN-MQB compared to a $Al_{0.2}Ga_{0.8}N$ EBL of the same thickness on GaN. Approaches to verify the VB experimentally will be discussed in this talk.

HL 72.4 Thu 10:15 POT 06

Enhanced light extraction and internal quantum efficiency for UVB LEDs with UV-transparent p-AlGaN superlattices — •Martin Guttmann[1], Martin Hermann[1], Johannes Enslin[1], Sarina Graupeter[1], Luca Sulmoni[1], Christian Kuhn[1], Tim Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Berlin

Light emitting diodes (LEDs) in the UVB spectral range (280 nm - 315 nm) are of particular interest for applications such as plant growth lighting and phototherapy. State-of-the-art devices utilize highly absorbing p-GaN contacts and low aluminum mole fraction p-AlGaN layers to enable low operating voltages. The exploitation of UV-transparent p-AlGaN layers together with highly UV-reflective metal contacts may significantly increase the light extraction efficiency (LEE). In this paper, the light output of LEDs emitting around 310 nm with UV-transparent and absorbing Mg-doped AlGaN superlattices is compared. A three-fold increase of the external quantum efficiency (EQE) was observed for LEDs with UV-transparent p-AlGaN layers.

To investigate these findings, LEDs with low-reflectivity Ni/Au and high-reflectivity Al contacts were fabricated, characterized, and ray tracing simulations were performed. The increased EQE can be partially ascribed to an two-fold improved LEE in combination with a 50% increase of the injection and internal quantum efficiency when using a UV-transparent p-$Al_{0.4}Ga_{0.6}N/Al_{0.6}Ga_{0.4}N$-superlattice.

Coffee Break

HL 72.5 Thu 11:00 POT 06

Influence of the GaN:Mg contact layer on the electro-optical properties of UVB LEDs — •Norman Susilo[1], Johannes Enslin[1], Luca Sulmoni[1], Martin Guttmann[1], Ute Zeimer[2], Tim Wernicke[1], Markus Weyers[2], and Michael Kneissl[1,2] — [1]Institute of Solid State Physics, Technische Universität Berlin — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Berlin

Light emitting diodes (LEDs) in the UVB spectral range (280 nm - 320 nm) are ideally suited for applications such as phototherapy and plant growth lighting. In order to improve the external quantum efficiency of UVB LEDs GaN:Mg contact layers were investigated to achieve UV-reflective and low resistance ohmic contacts. UVB LED heterostructures were grown by metal organic vapour phase epitaxy and fabricated into LED devices by standard lithography and metalization techniques. From transmission line measurements (TLM) we found that the p-contact resistivity increases rapidly with decreasing GaN:Mg thickness and exhibits a clear Schottky behaviour for layer thicknesses below 40 nm. At the same time, the emission power increases from 0.1 to 1.5 mW at 20 mA with decreasing GaN:Mg thickness. The electro-optical and the structural properties of the LEDs show that a 40 nm thick GaN:Mg cap layer is the best compromise due to the low p-contact resistivity ($3.5{\cdot}10^{-4}$ Ωcm^2) and low absorption resulting in UVB-LEDs with external quantum efficiencies of more than 2 %, measured on-wafer.

HL 72.6 Thu 11:15 POT 06

Time-resolved spectral characterization of white LEDs for car-to-x communication — •Vanessa Simon, Matthias Wachs, and Ulrich T. Schwarz — Chemnitz University of Technology, Experimental Sensor Science, Reichenhainer Str. 70, 09126 Chemnitz

Sensor development, car-to-car and car-to-environment (car-to-x) commonucation became a fast growing research area over the last years. A new approach could be car-to-x communication by means of white LEDs. This principle of data transmission was demonstrated by H.L. Minh et al. [1] in their Visible Light Communication (VLC) System. They achieved a bandwidth of about 50 MHz.

The aim of our attempt is to examine this system for different LEDs of their suitability for car-to-x communication. Therefore we investigate the switching behavior of gallium nitride and the phosphor converter with a time-resolved spectroscopy setup using a streak camera as detector. This measurement setup allows to determine the rise and fall time of the blue LED and the phosphor converter separately. The studied devices are warm-white and cold-white LEDs from Osram and Nichia. The measured rise and fall time of gallium nitride and the phosphor converter are compared to measurements similar to the experiment from H.L. Minh et al. [1] using a photodiode and band pass filters.

References: [1] H.L. Minh et al., IEEE Photonic Tech L. 21, 1063 (2009).

HL 72.7 Thu 11:30 POT 06

Molecular control over Ni/GaN Schottky barrier diode using Thiol Porphyrin — •Manjari Garg[1], Tejas R. Naik[2], Subramaniyam Nagarajan[3], V. Ramgopal Rao[1], and Rajendra Singh[1] — [1]Wide Bandgap Semiconductor Lab, Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi-110016 — [2]Indian Institute of Technology Bombay — [3]Aalto University Finland

The present work aims to investigate the control of self-assembled monolayers SAM of Thiol- Porphyrin on the electrical characteristics of GaN based Schottky barrier diode. In this work, SAM of Thiol-Porphyrin TTPSH organic molecules were sandwiched between Nickel metal and GaN semiconductor to tune the work function. The chemisorption of TTPSH SAM on GaN surface was confirmed by using Water contact angle measurements, XPS and AFM. KPFM revealed that the GaN surface potential was reduced from 950 mV to 750 mV after the adsorption of SAM on GaN. A decrease in the surface potential of semiconductor side of the metal-semiconductor interface implies decrease in workfunction of semiconductor which may lead to an increase in Schottky barrier height. Ni metal was deposited on the molecularly modified GaN surface and was electrically characterized by current-voltage measurements. A significant increase in Schottky barrier height and a decrease in reverse bias leakage current by four orders of magnitude was obtained. An increase in the photoluminescence intensity of GaN at 365 nm wavelength shows that surface passivation of GaN is occurring, which leads to the improvement of electrical characteristics of the diodes.

HL 73: Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - VI

Time: Thursday 10:30–13:45 Location: GER 38

HL 73.1 Thu 10:30 GER 38

Implicit solvation functionality in FHI-aims: Kirkwood multipole expansion model — •Markus Sinstein, Karsten Reuter, and Harald Oberhofer — Technische Universität München, Germany

Implicit solvation models describe a liquid environment in form of a dielectric continuum. Used within first-principles calculations for the solute such models provide a numerically most efficient way to effectively capture solvation effects. To this end we have implemented the multipole expansion (MPE) model introduced originally by Kirkwood into the full-potential density-functional theory (DFT) code FHI-aims. This implementation fully exploits the optimized multi-center multipole decomposition of the density performed within FHI-aims and therewith leads generally to an insignificant overhead as compared to the underlying DFT calculation for the solute.

Aiming to minimize the number of free parameters inevitably connected with such implicit models, we use an iso-density definition of the solvent cavity. As to the other parameters, we present an efficient parametrization scheme based on experimentally measured hydration energies of small organic molecules. Finally, we discuss extensions of the solvation model to address extended solid-liquid interfaces.

HL 73.2 Thu 10:45 GER 38

Using Dipsersion-Corrected Density Functional Theory to Understand the Phase Diagram of Alkanethiolates on Gold — •Joakim Löfgren, Henrik Grönbeck, Kasper Moth-Poulsen, and Paul Erhart — Chalmers University of Technology, Gothenburg, Sweden

A key challenge in modern computational materials chemistry is the description of van der Waals interactions in density functional theory simulations, where the failure of conventional exchange-correlation functionals is well-known. While, in the recent years, several methods have been proposed for overcoming these difficulties, the applications are becoming increasingly more demanding as well. An important example is that of ligand-protected nanoparticles, which typically feature metallic, covalent as well as dispersive interactions that should all, ideally, be treated on an equal footing. In this work we show that significant progress can be made in this direction: with the aid of the recently-developed vdW-DF-cx functional we study the phase diagram of self-assembled monolayers of alkanethiolates on gold. This system is important for practical applications and as a general representative of self-assembly at a metal surface. In particular, a quantitative description of the dispersion-driven phase transition between a lying-down and a standing-up monolayer is obtained using an ab inito thermodynamics framework. The results are shown to be in good agreement with experimental data and highlight that accurately accounting for dispersive interactions is both feasible and a crucial part of modeling self-assembled systems.

HL 73.3 Thu 11:00 GER 38

Finite-temperature properties of the thermoelectric clathrate $Ba_8Al_xSi_{46-x}$ — •Maria Troppenz, Santiago Rigamonti, and Claudia Draxl — Humboldt-Universität zu Berlin

Intermetallic clathrate compounds are promising candidates for high-efficiency thermoelectric (TE) applications. Here, we study $Ba_8Al_xSi_{46-x}$ in the composition range $x \in [6, 16]$ [1]. Recent theoretical studies [2] show a strong dependence of the electronic properties on configuration, i.e. the atomic arrangement of the substitutional Al atoms in the crystal framework. At the Zintl composition ($x = 16$), the ground-state configuration is semiconducting. However, configurations higher in energy are metallic. Understanding this metal-semiconductor transition is essential, as semiconducting behavior is a prerequisite for TE applications. In this work, we employ the cluster expansion technique combined with Monte-Carlo simulations and the Wang-Landau method [3] to access finite-temperature properties. We find that the transition is driven by a partial order-disorder transition of the substituents. Most importantly, it is found that the transition temperature (~ 800 K) at the Zintl composition is close to the typical temperatures at which the figure of merit of TE clathrates is maximal. Signatures of the transition in the entropy, order parameter, specific heat, and canonical distribution are analyzed for the full composition range.

[1] J. H. Roudebush *et al.*; *Inorg. Chem.* **51**, 4161 (2012)
[2] M. Troppenz, S. Rigamonti and C. Draxl; preprint.
[3] F. Wang and D. P. Landau, *Phys. Rev. Lett.* **86**, 2050 (2001)

HL 73.4 Thu 11:15 GER 38

Electronic structure and solid-state optical properties of indigo from time-dependent optimally tuned range-separated hybrid functional theory — •Bernd Kollmann[1], Arun Kumar Manna[2], Daniel Lüftner[1], Leeor Kronik[2], and Peter Puschnig[1] — [1]Institute of Physics, NAWI Graz, University of Graz, Austria — [2]Department of Materials and Interfaces, Weizmann Institute of Science, Israel

Indigo is a natural dye with a long history in organic chemistry. Recent applications of indigo as a functional building block for organic electronics, like in solar cells or field effect transistors, have renewed the interest in the chemical and physical properties of this molecule. We report on its electronic structure for the isolated molecule as well as for the alpha- and beta- bulk molecular crystal phases. Further we investigate the optical properties of the bulk molecular crystal phases. For the molecule we employ an optimally tuned range-separated hybrid functional (OT-RSH) within density functional theory. Comparing the theoretical results obtained with different levels of theory and with experiment emphasizes the need for going beyond simple semi-local DFT-functionals in order to obtain the correct orbital ordering. For the bulk crystals we take into account the screening in the bulk by using an optimally tuned screened range-separated hybrid (OT-SRSH) approach. Regarding the optical properties of the bulk molecular phases we employ time-dependent density functional theory (TDDFT) to calculate the absorption spectra, whereby TDDFT represents an accurate low-cost substitute to many-body perturbation theory.

HL 73.5 Thu 11:30 GER 38

Thermodynamic properties from ab-initio calculations - Ti as a case study — •Guy Makov — Materials Dept, Ben-Gurion University of the Negev, Beer Sheva, Israel

Ab-initio calculations of thermophysical properties and of phase stability as a function of pressure and temperature are considered in titanium as a case study. Ti is of interest due to its multiple phases and unusual thermophysical properties. At low temperatures Ti has been reported to exhibit negative anisotropic thermal expansion. In addition, there have been reports of two additional phases at high pressure and room temperature, and a possible transition to a bcc phase at very high pressures.

Despite extensive studies there remains both experimental and theoretical uncertainty in determining the phase diagrams and selected properties. Density Functional Theory total energy calculations complemented by Density Functional Perturbation Theory (DFPT) calculations of phonon spectra are obtained as a function of pressure. The free energy and thermal properties (heat capacity and thermal expansion) of Ti phases, phase equilibria and high pressure phase sequence are determined. The contribution of phonon modes to the thermal expansion is analyzed and the negative thermal expansion is shown to be dominated by negative mode Gruneisen parameters at specific points on the Brillouin zone boundaries. The elastic (Debye) theory for negative thermal expansion is shown to be irrelevant for these phenomena. Uncertainties in the calculated results are discussed in light of experimental observations & motivating further experimental studies.

HL 73.6 Thu 11:45 GER 38

Molecular orbitals in the bismuth perovskites — •Kateryna Foyevtsova[1,2], Arash Khazraie[1,2], Ilya Elfimov[1,2], and George A. Sawatzky[1,2] — [1]Department of Physics and Astronomy, University of British Columbia, Vancouver, BC, Canada V6T 1Z1 — [2]Stewart Blusson Quantum Matter Institute, Vancouver, BC, Canada V6T 1Z4

The bismuth perovskites $SrBiO_3$ and $BaBiO_3$ become superconducting upon hole doping, with the transition temperatures as high as 30 K. The origin of the superconductivity in these compounds has remained unidentified for more than three decades. The BCS mechanism alone is not sufficient to account for such a high T_c due to the small electron-phonon coupling that is being consistently found in numerous experimental and theoretical studies. Further effects must therefore be of key importance, such as, for example, formation of bipolarons.

In this talk, we will focus on the insulating state of the pristine $SrBiO_3$. Peculiarly, this state is associated with a structural distortion whereby the Bi-O bonds disproportionate, resulting in a three-dimensional array of alternating small and large BiO_6 octahedra. This "breathing" distortion melts away with doping and is believed to be competing with superconductivity. We will show using DFT calculations that the microscopic state in the pristine bismuthates corresponds to a lattice of frozen bipolarons. More specifically, the holes, intrinsically present in the material, condense pairwise into the A_{1g}-symmetric molecular orbitals formed from the O-p_σ atomic orbitals of the small BiO_6 octahedra. This is facilitated by the strong hybridization between the O-2p states and the Bi-6s states.

HL 73.7 Thu 12:00 GER 38

Ab initio calculations and strain-dependent scaling of excitons in carbon nanotubes — •Christian Wagner[1,3], Jörg Schuster[2], Michael Schreiber[3], and André Schleife[4] — [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, UIUC, USA

Optical transitions in carbon nanotubes (CNTs) show a strong strain sensitivity, which makes them suitable for optical strain sensing at the nano-scale and for strain-tunable emitters. The origin of this effect is the band-gap change, depending on strain and chirality, which is well explored. However, there is no quantitative model for the strain dependence of optical transitions — as they are subject to strong excitonic effects due to the quasi one-dimensional structure of CNTs.

One approach towards such a model is the scaling relation of CNT excitons with respect to dielectric constant, reduced mass, and CNT radius given by Perebeinos *et al.* However, the description of screening in this model is insufficient, since for CNTs, a one-dimensional wave-vector dependent dielectric function $\epsilon(q)$ is needed instead of an effective-medium dielectric constant ϵ_0.

We achieve this by combining the scaling relation with the wave-vector dependent screening model by Deslippe *et al.* The strain-dependent scaling is fitted to electronic-structure calculations within many-body perturbation theory as a reference. This enables us to quantitatively predict the strain dependence of optical transitions for any CNT.

HL 73.8 Thu 12:15 GER 38

Dzyaloshinskii-Moriya-interaction energy, where it is located? Real and reciprocal spaces views. — •Leonid Sandratskii — Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

Recently Dzyaloshinskii-Moriya interaction (DMI) attracted new wave of intense attention stimulated by its role in the stabilization and fast dynamics of skyrmions. Numerous approaches have been suggested for the estimation of the the DMI parameters. Many efforts are devoted to reveal the electronic properties responsible for the strength of the DMI and, in this way, to help to engineer the materials with desired DMI characteristics. Although there is full consensus with respect to the most fundamental reasons of the DMI, the SOC and broken inversion symmetry, in details the physical pictures suggested by different authors differ strongly. In particular, this concerns the role of the avoiding crossings in the electronic structure, the spatial location of the DMI energy, the role of the orbital moments. This stimulated us to perform detailed study of the DMI in CoPt bilayer focusing on the open questions. We used both the approximate calculations for spin spirals with arbitrary wave vectors and more precise but also more time and resources consuming full relativistic calculations for super-

cells with the magnetic structures of opposite chirality. The results of the calculations are presented and analyzed.

HL 73.9 Thu 12:30 GER 38

***Ab-initio* study of the Raman spectra of strained graphene** — •Albin Hertrich, Caterina Cocchi, Pasquale Pavone, and Claudia Draxl — Department of Physics, Humboldt-Universität zu Berlin, Germany

Raman spectroscopy is an important non-destructive method for characterizing graphene-based materials. The main features of Raman spectra of pristine graphene are the first-order G-band at $\approx 1580\,\mathrm{cm}^{-1}$ and the dispersive second-order 2D-band at $\approx 2700\,\mathrm{cm}^{-1}$. In this work, we perform a systematic analysis on the effect of strain on both bands. All calculations are done using the full-potential all-electron code `exciting` [1]. Phonon properties are computed within the frozen-phonon approximation, the frequency-dependent dielectric tensor within the random-phase approximation. Raman-scattering intensities are calculated from vibrational matrix elements and derivatives of the dielectric tensor with respect to the phonon normal coordinates [2]. Under biaxial strain both Raman bands are shifted, while uniaxial strain leads to a splitting of the G-band by lifting the degeneracy of the optical in-plane Γ-point phonons. Further, we explore the effect of different types of inhomogeneous strain on the optical phonon frequencies and Raman-scattering intensities.

[1] A. Gulans *et al.*, J. Phys.: Condens. Matter **26**, 363202 (2014).
[2] C. Ambrosch-Draxl *et al.*, Phys. Rev. B **65**, 064501 (2002).

HL 73.10 Thu 12:45 GER 38

DFT meets Landau Theory: The High Pressure Phase Transition of Lead Titanate — •Andreas Tröster — Vienna University of Technology, Institute of Material Chemistry, Getreidemarkt 9 A-1060 Wien, Austria

Landau theory (LT) coupled to infinitesimal strain is a cornerstone of the theory of structural phase transitions. At high pressures, however, this approach breaks down due to the appearance of large strains and the accompanying nonlinear elastic energy contributions. In density functional theory (DFT), on the other hand, stress and strain are easy to control, but entropic effects are difficult to incorporate since DFT is a genuine zero temperature method. Recently we have shown how to combine the strengths of these two antipodal approaches by constructing a high pressure extension of conventional LT with the help of DFT. Essential for the success of this approach is the ab initio calculation of pressure-dependent elastic constants. This theory yields a concise numerical description of the high pressure phase transition in strontium titanate, and also allows to resolve a number of severe and long-standing discrepancies between the experimental data and the theoretical description of the ferroelectric high pressure phase transition of the perovskite lead titanate, a material which is also of considerable technological interest.

HL 73.11 Thu 13:00 GER 38

Ground-State and Excitation Properties of Orthorhombic $MAPbI_3$ — •Claudia Rödl and Silvana Botti — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Hybrid organic-inorganic halide perovskites are one of the most promising candidates for the next generation of photovoltaic devices with high power-conversion efficiencies. Despite the amazing progress in device fabrication, many of the fundamental properties of these materials are not yet understood. The flexibility in composition of hybrid perovskites permits to tune physical properties like band gap, dielectric constant, or optical absorption which renders them interesting also from a fundamental point of view and for applications beyond photovoltaics. The most intensively studied compound, methylammonium lead iodide ($MAPbI_3$), condenses in a low-temperature orthorhombic phase which undergoes a phase transition to a tetragonal structure at 162.2 K and transforms into a cubic high-temperature phase above 327.4 K. These phase transitions go along with a change in the optical properties. Here, we focus on the orthorhombic phase of $MAPbI_3$. We have studied the ground-state atomic structure, and in particular the orientation of the MA^+ ion within the inorganic cage, within density-functional theory. We investigate the one-particle excitation properties (band gap, photoemission spectrum) within the GW approximation of many-body perturbation theory. Moreover, we calculate optical and loss spectra using time-dependent density-functional theory and solving the Bethe-Salpeter equation.

HL 73.12 Thu 13:15 GER 38

Structure, nonstoichiometry, and geometrical frustration of α-tetragonal boron — •Jens Kunstmann[1], Naoki Uemura[2], Hagen Eckert[1], and Koun Shirai[2] — [1]TU Dresden, Germany — [2]Osaka University, Japan

It is currently believed that boron in the α-tetragonal structure is not an elemental crystal. Here we contradict this view and resolve the structural and thermodynamic characteristics of pure α-tetragonal boron via density functional theory calculations. The conditions for stable covalent bonding are almost fulfilled at a stoichiometric composition B_{52}. This phase is an elemental crystals with geometrical frustration. Furthermore, our thermodynamic considerations show that small, positive deviations from the stoichiometric composition occur at finite temperatures. [Uemura, Shirai, Eckert, Kunstmann, Phys. Rev. B 93, 104101 (2016)]

HL 73.13 Thu 13:30 GER 38

Magnetic response properties of thin films using Kubo's linear response formalism — •Andreas Held, Sebastian Wimmer, Sergiy Mankovsky, and Hubert Ebert — Department Chemie, Ludwig-Maximilians-Universität München

We have applied the fully relativistic spin-polarized Korringa-Kohn-Rostoker method to investigate various magnetic response properties of two-dimensional systems such as free-standing mono- and multilayers, surfaces and thin films on surfaces. Our approach is based on an implementation of Kubo's linear response formalism within the tight-binding (or screened) KKR framework that allows introducing layer-resolved response coefficients τ_{ij}^{IJ}. Extending previous work [1] focusing on the symmetric part of the electrical conductivity tensor, we are able to describe the full response tensors connected to charge and spin transport, Gilbert damping, spin-orbit torque and the Edelstein effect. An implementation of the Coherent Potential Approximation for layered systems allows the treatment of disorder effects including the Vertex Corrections to the response coefficients [2]. This can be used to study chemical disorder in alloys but also to include the effect of finite temperatures. For the latter the so-called Alloy-Analogy Model [3] is employed to treat vibrations and spin fluctuations.

[1] W.H. Butler *et al.*, *Phys. Rev. B* **52**, 13399 (1995). [2] W.H. Butler, *Phys. Rev. B* **31**, 3260 (1985); K. Palotás *et al.*, *Phys. Rev. B* **67**, 174404 (2003). [3] H. Ebert *et al.*, *Phys. Rev. B* **91**, 165132 (2015).

HL 74: Group IV: Si/Ge/SiC

Time: Thursday 12:00–13:15 Location: POT 06

HL 74.1 Thu 12:00 POT 06

The silicon path to a new kilogram: Impact of the isotopic composition of Si determined by high resolution mass spectrometry — •Axel Pramann and Olaf Rienitz — Physikalisch-Technische Bundesanstalt (PTB), Braunschweig, Germany

The planned re-definition of the SI unit kilogram will be performed via the Planck constant h and in a complementary approach via the Avogadro constant N_A applying the X-ray-crystal-density XRCD method (Avogadro-project) by counting the silicon atoms in single-crystalline Si spheres[1]. One key experiment is the mass spectrometric determination of the molar mass M of Si with lowest uncertainty by developing new analytical techniques (isotope ratio calibration) and modifying e.g. isotope dilution mass spectrometry (IDMS) in combination with a high resolution multicollector-ICP-mass spectrometer (HR-MC-ICP-MS) [2]. This resulted in u_rel(M) < 5 x 10-9 routinely, when applied to silicon material enriched in 28Si with x(28Si) > 0.9999 mol/mol. New Si crystals even higher enriched in 28Si recently produced in Russia exhibit a strong reduction of u(M). Already u_rel(M) < 1 x 10-9 can be obtained when using crystals with x(28Si) > 0.999 99 mol/mol. An estimation of the correlation between enrichment and decrease of uncertainty is given, stimulated by an uncertainty reduction of M by approximately three orders of magnitude in ten years [3].

[1] Y. Azuma et al., Metrologia, 52, 360 (2015). [2] O. Rienitz, A. Pramann, D. Schiel, Int. J. Mass Spectrom., 289, 47 (2010). [3] K. Fujii et al. Metrologia, 53, A19 (2016).

HL 74.2 Thu 12:15 POT 06

Modulation Doping of Si using Al-induced Acceptor States in SiO2 — Dirk König[1], •Daniel Hiller[2], Sebastian Gutsch[2], Margit Zacharias[2], and Sean Smith[1] — [1]University of New South Wales (UNSW), Sydney, Australia — [2]Laboratory for Nanotechnology, IMTEK, University of Freiburg, Germany

Silicon nanovolumes suffer from effects that impede conventional doping due to fundamental physical principles such as out-diffusion, statistics of small numbers, quantum- or dielectric confinement. Efficient and reliable control over the majority charge carriers by impurity doping is infeasible for ultra-small Si crystals [1].

In this work, we demonstrate a heterostructure modulation doping method for Si, similar to the concept of modulation doping originally invented for III-V semiconductors [2]. Our approach utilizes a specific acceptor state of Al-atoms in SiO2, which is located 0.5 eV below the Si valence band, to generate holes as majority carriers in adjacent Si [3]. The relocation of the impurity dopants from Si to SiO2 circumvents all nanoscale doping problems. We present successful Si modulation doping from the theoretical background (density functional theory simulations, DFT) to experimental evidence by capacitance-voltage (C-V), Hall-measurements and deep level transient spectroscopy (DLTS). In addition, we demonstrate how modulation doping of bulk-Si enables passivating hole selective tunnelling contacts as required for high-efficiency photovoltaics [3].

[1] Sci. Rep. 5, 09702 (2015) [2] Appl. Phys. Lett. 33, 665 (1978) [3] D. König & D. Hiller et al., Sci. Rep., under review (2016)

HL 74.3 Thu 12:30 POT 06

Investigation of 3C-SiC/SiO2 interfacial point defects from ab initio g-tensor calculations and electron paramagnetic resonance measurements — •T. A. Nugraha[1,2], M. Rohrmüller[2], U. Gerstmann[2], S. Greulich-Weber[3], A. Stellhorn[2], J. L. Cantin[4], J. Von Bardeleben[4], W. G. Schmidt[2], and S. Wippermann[1] — [1]Max-Planck-Institut für Eisenforschung — [2]University of Paderborn — [3]Solar Weaver GmbH — [4]Pierre and Marie Curie University

SiC is widely used in high-power, high-frequency electronic devices. Recently, it has also been used in nanocomposites as light absorbers in solar energy conversion devices. Analogous to Si, SiC features SiO2 as native oxide that can be used for passivation and insulating layers. However, a significant number of defect states are reported to form at SiC/SiO2 interfaces, limiting mobility and increasing recombination of free charge carriers. We investigated the growth of oxide on different 3C-SiC surfaces from first principles. Carbon antisite Csi defects are found to be strongly stabilized in particular at the interface, because carbon changes its hybridization from sp3 in the SiC-bulk to sp2 at the interface, creating a dangling bond inside a porous region of the SiO2 passivating layer. Combining ab initio g-tensor calculations and electron paramagnetic resonance (EPR) measurements, we show that Csi defects explain the measured EPR signatures, while the hyperfine structure allows to obtain local structural information of the oxide layer. Financial support from BMBF NanoMatFutur grant 13N12972 and DFG priority program SPP-1601 is gratefully acknowledged.

HL 74.4 Thu 12:45 POT 06

Direct band gap and strain-related properties of germanium under high uniaxial stress — •Kevin Guilloy[1], Alban Gassenq[1], Nicolas Pauc[1], S. Tardif[1], F. Rieutord[1], Y.M. Niquet[1], J.M. Escalante[1], I. Duchemin[1], L. Milord[2], G. Osvaldo Dias[2], D. Rouchon[2], J. Widiez[2], J.M. Hartmann[2], J. Aubin[2], A. Chelnokov[2], R. Geiger[3], T. Zabel[3], E. Marin[3], H. Sigg[3], J. Faist[4], V. Reboud[2], and Vincent Calvo[1] — [1]Université Grenoble Alpes, CEA-INAC, Grenoble, France — [2]Université Grenoble Alpes, CEA-LETI Minatec, Grenoble, France — [3]Laboratory for Micro- and Nanotechnology, Paul Scherrer Institut, Villigen, Switzerland — [4]Institute for Quantum Electronic, ETH Zurich, Switzerland

The induction of high tensile strain is predicted to make germanium a direct band gap semiconductor. We present here an experimental study of the dependence of such a tensile stress on the direct optical transitions and the Raman strain-induced shift.

Using germanium-on-insulator (GeOI) substrates, we fabricated micro-membranes amplifying the residual stress of the germanium layer. Laue X-ray diffraction measurements at the BM32 beamline (ESRF) showed the strain reaches 4.9 %. We studied the relationship between the strain measured by XRD and the Raman shift and observed a unexpected nonlinear behaviour.

We finally performed electro-absorption spectroscopy on micro-bridges to determine the energy of its optical transitions, showing that the relation between strain and the energy of these transitions differs significantly from previous models.

HL 74.5 Thu 13:00 POT 06

Defect-induced magnetism in SiC probed by nuclear magnetic resonance — •Zhitao Zhang[1,2], Daryna Dmytriieva[2,3], Sebastian Molatta[2,3], J. Wosnitza[2,3], Yutian Wang[1], Manfred Helm[1,3], Shengqiang Zhou[1], and Hannes Kühne[2] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden, Germany — [2]Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden, Germany — [3]TU Dresden, D-01062 Dresden, Germany

We give evidence for intrinsic, defect-induced bulk paramagnetism in SiC by means of ^{13}C and ^{29}Si nuclear magnetic resonance (NMR) spectroscopy. The temperature dependence of the internal dipole-field distribution, probed by the spin part of the NMR Knight shift and the spectral linewidth, follows a Curie law and scales very well with the macroscopic DC susceptibility. In order to quantitatively analyze the NMR spectra, a microscopic model based on dipole-dipole interactions was developed. The very good agreement between these simulations and the NMR data establishes a direct relation between the frequency distribution of the spectral intensity and the corresponding real-space volumes of nuclear spins. The presented approach by NMR can be applied to a variety of similar materials and, thus, opens a new avenue for the microscopic exploration and exploitation of diluted bulk magnetism in semiconductors.

HL 75: Quantum Dots: Transport Properties II

Time: Thursday 14:45–16:15 Location: POT 151

Invited Talk HL 75.1 Thu 14:45 POT 151

Spectroscopy on self-assembled quantum dots: Transport meets optics — •Martin Geller — Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

Self-assembled quantum dots (QDs) are nanoscopic semiconductor islands in a crystalline matrix material. After more than 20 years, these "artificial atoms" are still of great interest to study fundamental physics in low-dimensional systems. They have entered commercially available products and have visionary future perspectives in quantum information processing.

After a general introduction, I will summarize the transport (like capacitance-voltage spectroscopy) and optical methods (like microphotoluminescence) on self-assembled QDs. Afterwards, I will introduce the time-resolved conductance spectroscopy [1] and show a combination of "transport and optics". In an optical detection scheme, based on resonance fluorescence, the electron tunneling (and quantum jumps), photo-induced electron capture and Auger-recombination can be observed time-resolved on a single self-assembled dot [2].

[1] B. Marquardt, et al., Nature Commun. **2**, 209 (2011); A. Beckel, et al., Phys. Rev. B **89**, 155430 (2014). [2] A. Kurzmann, et al., Phys. Rev. Lett. **117**, 017401 (2016); A. Kurzmann, et al., Appl. Phys. Lett. **108**, 263108 (2016); A. Kurzmann, et al., Nano Lett. **16**, 3367 (2016).

HL 75.2 Thu 15:15 POT 151

Thermal energy and charge currents in multi-terminal nanorings — •Christian Riha[1], Tobias Kramer[1,2], Christoph Kreisbeck[1], Olivio Chiatti[1], Sven S. Buchholz[1], Andreas D. Wieck[3], Dirk Reuter[4], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, D-12489 Berlin — [2]Zuse-Institut für Informationstechnik, D-14195 Berlin — [3]Angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum — [4]Optoelektronische Materialien und Bauelemente, Universität Paderborn, D-33098 Paderborn

We study thermal energy and charge transfer close to the quantum limit in a ballistic nanodevice experimentally [1] and theoretically [2]. The device consists of multiply connected one-dimensional electron waveguides and is based on an AlGaAs/GaAs heterostructure. A global top-gate steers the thermal energy and charge transfer in the presence of a temperature gradient, which is established by a heating current. Thermal noise measurements allow to estimate the heat transfer and shows the device to act as a switch for charge and thermal energy transfer. Wave-packet simulations, that are based on the multi-terminal Landauer-Büttiker approach, confirm the experimental finding of a mode-dependent redistribution of the thermal energy current, if a scatterer breaks the device symmetry.

[1] C. Riha *et al.*, Appl. Phys. Lett. **106**, 083102 (2015)
[2] T. Kramer *et al.*, AIP Advances **6**, 065306 (2016)

HL 75.3 Thu 15:30 POT 151

Comparison of the carrier transfer properties between an electrolyte and GaInN- and GaNP-nanowires — •Jan Philipps[1], Sara Hölzel[1], Pascal Hille[1], Jörg Schörmann[1], Jan Stehr[2], Irina Buyanova[2], Charles Tu[3], Detlev Hofmann[1], and Martin Eickhoff[1] — [1]I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Germany — [2]Department of Physics, University of Linköping, Sweden — [3]Department of Electrical and Computer Engineering, University of California, San Diego, USA

$Ga_{1-x}In_xN$ nanowires with In concentrations x of about 0.3 and GaP/GaN_xP_{1-x} core/shell nanowires (x $\sim$ 0.08) show interesting properties for the charge carrier transfer from the semiconductor into an electrolyte, which might be used for sensing applications or catalytic water splitting. The transfer can be initiated by visible light and depending on an applied bias electron- or hole-transfers are achieved. The processes can be monitored by photocurrent measurements or in more detail by electron paramagnetic resonance experiments using spin trapping agents. We find that the processes strongly affect the near bandgap emission in $Ga_{1-x}In_xN$ nanowires but have only minor effect on the emission of GaP/GaN_xP_{1-x} nanowires. The results will be discussed in the frame of the surface band bending model of the semiconductor/electrolyte interface.

HL 75.4 Thu 15:45 POT 151

Electron transport through coupled semiconductor quantum dots — •Simon Liebing, Torsten Hahn, and Jens Kortus — TU Bergakademie Freiberg, Institute for Theoretical Physics, Germany

The electronic structure for single- (CdS, ZnSe) and coupled-quantum dots (CdS-ZnSe) were calculated by means of density functional theory (DFT)[1]. Additionally, for the coupled dots we investigated transport characteristics based on NEGF transport theory [2]. We observe that the coupling strength depends strongly on the relative orientation of the dots with respect to the atoms which model the contact.

In contrast to single dots, the current-voltage curves in case of the coupled dot system shows clearly rectification behavior. The rectification can be understood in detail based on our electronic structure calculation, which also show that weak coupling between the dots is a requirement for the found rectification behavior.

[1] M. Pederson et. al., Phys. Status Solidi b 217, 197. (2000).
[2] J. Enkovaara et al., JOP: Condensed Matter 22, 253202 (2010).

HL 75.5 Thu 16:00 POT 151

Determining tunneling times in Ge hut wires via single-shot measurements — •Lada Vukušić, Josip Kukučka, Hannes Watzinger, Elisabeth Lausecker, and Georgios Katsaros — IST Austria

Group IV semiconductors are an attractive platform for spin qubits, with electron spin coherence times in isotopically purified Si exceeding 0.5 s [1]. Nevertheless, for fast gate manipulation, holes should be more suitable due to the stronger spin-orbit coupling. Purely HH states have been predicted to show long dephasing and, under certain conditions, relaxation times [2]. Here we work with Ge hut wires, a system which has been recently shown to confine almost purely HH states [3]. For determining the hole-spin relaxation time, a charge sensor is needed. Recently, we have realized for the first time charge sensing in Ge hut wires, which is based on both capacitive and tunnel coupling between two hut wires [4]. For achieving a fast readout, the charge sensor has been connected to a radio frequency reflectometry setup [5]. With this configuration we have measured the single-hole tunnel time between the two quantum dots to be about 10 us, which is two orders of magnitude smaller than the predicted spin relaxation time [6]. Thus, it is perfectly suitable for performing spin readout measurements.

[1] J. T. Muhonen et al., Nature Nano 9, 986 (2014); [2] D. V. Bulaev and D. Loss, PRL 95, 076805 (2005); [3] H. Watzinger et al., Nano Letters 16, 6879 (2016); [4] A. Morello et al., Nature 467 (2010); [5] N. Ares et al., PR Applied 5, 034011 (2016); [6] A. F. Zinov'eva et. al., Jetp Lett. 82, 302 (2005);

HL 76: Topological Insulators II (joined session with TT)

Time: Thursday 14:45–16:45 Location: POT 251

HL 76.1 Thu 14:45 POT 251

Visualizing the response of Weyl semimetals to Coulomb and magnetic perturbations — •Thomas Bathon[1], Paolo Sessi[1], Yan Sun[2], Florian Glott[1], Zhilin Li[3], Hongxiang Chen[3], Liwei Guo[3], Xialong Chen[3], Markus Schmidt[2], Claudia Felser[2], Binghai Yan[2], and Matthias Bode[1] — [1]Experimentelle Physik II der Universität Würzburg, Würzburg — [2]Max Planck Institute for Chemical Physics of Solids, Dresden — [3]Institute of Physics at the Chinese Academy of Sciences, Peking

Weyl semimetals are a new class of topological materials which led to the emergence of Weyl physics in condensed matter. While photoemission successfully identified Weyl surface states with unique Fermi arcs, their fundamental microscopic properties, such as scattering mechanisms, persistence of spin-coherence, and the reaction to external perturbations, have not been widely investigated so far.
Here, we use TaAs to address these important aspects at the atomic scale by scanning tunneling microscopy and spectroscopy. We deliberately introduce external adatoms to test the response of this class of materials to well-defined Coulomb and magnetic perturbations. We demonstrate that, contrary to topological insulators, they are effectively screened in Weyl semimetals. Our analysis demonstrates that intra- as well as inter-Fermi arc scattering events are strongly suppressed. Additionally, we show that the existence of large parallel segments of spin-split trivial states facing each other makes possible, through scattering, to revert both the propagation direction while simultaneously flipping the spin state, strongly limiting its coherence.

HL 76.2 Thu 15:00 POT 251

Investigation of topological states in proximitized superconducting 2d materials — •Petra Högl, Denis Kochan, Tobias Frank, Martin Gmitra, and Jaroslav Fabian — Insitute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

Recently, the appearance of helical edge states in graphene in transition-metal dichalcogenides has been predicted [1]. The presence of these quantum spin Hall states is a precursor for topological insulators. We theoretically investigate such 2d systems proximitized to a s-wave superconductor. As predicted by Fu and Kane [2] the combination of 2d topological insulators and superconductors can lead to the formation of Majorana states. This work has been supported by the Int. Doctorate Program Topological Insulators of the Elite Network of Bavaria, DFG SFB 689, GRK 1570, and by the EU Seventh Framework Programme under Grant Agreement No. 604391 Graphene Flagship.

[1] M. Gmitra, D. Kochan, P. Högl, J. Fabian, Phys. Rev. B 93, 155104 (2016)

[2] L. Fu and C. L. Kane, Phys. Rev. B 79, 161408(R) (2009)

HL 76.3 Thu 15:15 POT 251

Tuning Quantum Transport and Interference in Topological Nanowires — •Vincent Sacksteder[1] and Quansheng Wu[2] — [1]W155 Wilson Building, Royal Holloway University of London, Egham Hill, Egham, TW20 0EX, United Kingdom — [2]Theoretical Physics and Station Q Zurich, ETH Zurich, 8093 Zurich, Switzerland

We study the magnetoconductance of topological insulator nanowires in a longitudinal magnetic field, including Aharonov-Bohm, Altshuler-Aronov-Spivak, perfectly conducting channel, and universal conductance fluctuation effects. We show that changing the Fermi energy can tune a wire from from ballistic to diffusive conduction and to localization. In both ballistic and diffusive single wires we find both Aharonov-Bohm and Altshuler-Aronov-Spivak oscillations with similar strengths, accompanied by quite strong universal conductance fluctuations (UCFs), all with amplitudes between 0.3 and 1 conductance quanta. This contrasts strongly with the average behavior of many wires, which shows Aharonov-Bohm oscillations in the ballistic regime and Altshuler-Aronov-Spivak oscillations in the diffusive regime, with both oscillations substantially larger than the conductance fluctuations. We also show that in long wires the perfectly conducting channel is visible at a wide range of energies within the bulk gap. We present typical conductance profiles at several wire lengths, showing that conductance fluctuations can dominate the average signal. Similar behavior will be found in carbon nanotubes.

Coffee Break

HL 76.4 Thu 16:00 POT 251

time-reversal-breaking topological phases in anti-ferromagnetic Sr_2FeOsO_6 films — •Xiao-Yu Dong[1,2], Sudipta Kanungo[3,4], Binghai Yan[2,3], and Chao-Xing Liu[5] — [1]Department of Physics and State Key Laboratory of Low-Dimensional Quantum Physics, Tsinghua University, Beijing 100084, P.R.China — [2]Max-Planck-Institut für Physik komplexer Systeme, 01187, Dresden, Germany — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany — [4]Center for Emergent Matter Science (CEMS), RIKEN, 2-1, Hirosawa, Wako, Saitama 351-0198, Japan — [5]Department of Physics, The Pennsylvania State University, University Park, Pennsylvania 16802-6300, USA

In this work, we studied time-reversal-breaking topological phases as a result of the interplay between anti-ferromagnetism and inverted band structures in anti-ferromagnetic double perovskite transition metal Sr_2FeOsO_6 films. By combining the first principles calculations and analytical models, we demonstrate that the quantum anomalous Hall phase and chiral topological superconducting phase can be realized in this system. We find that to achieve time-reversal-breaking topological phases in anti-ferromagnetic materials, it is essential to break the combined symmetry of time reversal and inversion, which generally exists in anti-ferromagnetic structures. As a result, we can utilize an external electric gate voltage to induce the phase transition between topological phases and trivial phases, thus providing an electrically controllable topological platform for the future transport experiments.

HL 76.5 Thu 16:15 POT 251

Surface state-dominated photoconduction and THz-generation in topological Bi_2Te_2Se-nanowires — •Marinus Kundinger[1], Paul Seifert[1], Kristina Vaklinova[2], Klaus Kern[2,3], Marko Burghard[2], and Alexander Holleitner[1] — [1]Walter Schottky Institut and Physics-Department, Technical University of Munich, Am Coulombwall 4a, D-85748 Garching, Germany — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart, Germany — [3]Institut de Physique, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

Topological insulators constitute a fascinating class of quantum materials with non-trivial, gapless states on the surface and trivial, insulating bulk states. In revealing the optoelectronic dynamics in the whole range from femto- to microseconds, we demonstrate that the long surface lifetime of Bi_2Te_2Se-nanowires allows to access the surface states by a pulsed photoconduction scheme and that there is a prevailing bolometric response of the surface states. The interplay of the surface state dynamics on the different timescales gives rise to a surprising physical property of Bi_2Te_2Se-nanowires: their pulsed photoconductance changes polarity as a function of laser power. Moreover, we show that single Bi_2Te_2Se-nanowires can be used as THz-generators for on-chip high-frequency circuits at room temperature. Our results open the avenue for single Bi_2Te_2Se-nanowires as active modules in optoelectronic high-frequency and THz-circuits.

We acknowledge financial support by the DFG priority program SPP 1666 'topological insulators'.

HL 76.6 Thu 16:30 POT 251

THz radiation induced helicity sensitive photocurrents in type-II GaSb/InAs quantum well structures — •Helene Plank[1], Johanna Pernul[1], Tanja Hummel[1], Georg Knebl[2], Pierre Pfeffer[2], Martin Kamp[2], Susanne Mueller[3], Thomas Tschirky[3], Sergey A. Tarasenko[4], Werner Wegscheider[3], Sven Höfling[2,5], and Sergey D. Ganichev[1] — [1]Terahertz Center, University of Regensburg, Regensburg, Germany — [2]Technische Physik University of Würzburg, Würzburg, Germany — [3]ETH Zurich, Solid State Physics Laboratory, Zurich, Switzerland — [4]Ioffe Institute, St.Petersburg, Russia — [5]University of St. Andrews, St. Andrews, United Kingdom

We report on the observation of terahertz radiation induced helicity sensitive photocurrents in GaSb/InAs quantum wells in the inverted regime. The photocurrent reverses its direction upon switching the circular polarization from left- to right-handed. The origin of the photocurrent depends on the experimental geometry and the Fermi energy

position. For illuminating the sample centre, it stems from asymmetric scattering of free carriers excited by electric THz field [1]. At normal incidence or for Fermi energies in the gap it vanishes. The situation changes at the sample edges, where is it observed for both cases. We show that this edge current is caused by optical excitation of helical edge states in 2D topological insulators. The observed sign inversion upon changing the photon helicity is attributed to selection rules of optical transitions. We discuss the photocurrent behaviour and present microscopic models. [1] H. Plank *et al.*, Physica E **85**, 193 (2017).

HL 77: Transport in High Magnetic Fields

Time: Thursday 14:45–16:30 Location: POT 112

HL 77.1 Thu 14:45 POT 112

Topological Entanglement in Two-Dimensional Electron Gases Under Perpendicular Magnetic Fields — •Daniel Hernangómez-Pérez[1,2], Thierry Champel[2], and Serge Florens[3] — [1]Institut für Theoretische Physik, Universität Regensburg, D-93053 Regensburg, Germany — [2]Université Grenoble Alpes/CNRS, Laboratoire de Physique et Modélisation des Milieux Condensés, B.P. 166, 38042 Grenoble Cedex 9, France — [3]Institut Néel, CNRS and Université Grenoble Alpes, B.P. 166, 38042 Grenoble Cedex 9, France

Inspired by a recently developed single-particle vortex state formalism, we pinpoint a non-trivial long-range bipartite entanglement of electron cyclotron motions which can occur in two-dimensional electron gases under perpendicular magnetic fields. The entanglement is achieved through the introduction of bicomplex spinorial eigenstates of the clean Hamiltonian describing a four-dimensional (4D) singular hydrodynamic flow. We show that the topological origin of the entanglement, as well as the winding and parity quantum numbers describing the quantum states, suggests that 4D vortices of electron pairs are good candidates for stable quasiparticles at high magnetic fields. The relevance of this approach is discussed in the context of the fractional quantum Hall effect.

HL 77.2 Thu 15:00 POT 112

Geometrically disordered network models, quenched quantum gravity, and critical behavior at quantum Hall plateau transitions — Ilya A. Gruzberg[1], •Andreas Klümper[2], Win Nuding[2], and Ara Sedrakyan[3] — [1]Ohio State University, USA — [2]Wuppertal University, Germany — [3]Yerevan Physics Institute, Armenia

Recent results for the critical exponent of the localization length at the integer quantum Hall transition (IQHT) differ considerably between experimental ($\nu_{\text{exp}} \approx 2.38$) and numerical ($\nu_{\text{CC}} \approx 2.6$) values obtained in simulations of the Chalker-Coddington (CC) network model. The difference is at least partially due to effects of the electron-electron interaction present in experiments. Here we propose a mechanism that changes the value of ν even within the single-particle picture. We revisit the arguments leading to the CC model and consider more general networks with structural disorder. Numerical simulations of the new model lead to the value $\nu \approx 2.37$. We argue that in a continuum limit the structurally disordered model maps to free Dirac fermions coupled to various random potentials (similar to the CC model) but also to quenched two-dimensional quantum gravity. This explains the possible reason for the considerable difference between critical exponents for the CC model and the structurally disordered model. We extend our results to network models in other symmetry classes.

HL 77.3 Thu 15:15 POT 112

Phase transition induced by impurities in GaAs/AlGaAs single quantum wells — •Eddy P. Rugeramigabo, Lina Bockhorn, and Rolf J. Haug — Institute for Solid State Physics, Leibniz Universität Hannover

We report on a phase transition in two-dimensional electron gases (2DEG) interacting with specific background impurities. These are silicon atoms which have been intentionally incorporated in high quality single GaAs/AlGaAs quantum wells confining the 2DEG. The reference 2DEG, without any additional impurities, has an electron mobility μ_E of $3.2 \cdot 10^6\,\text{cm}^2/\text{Vs}$ and a 2D electron density n_E of $2.9 \cdot 10^{11}\,\text{cm}^{-2}$ at low temperature. The incorporated impurities induce a decrease in the sample quality, observed in the lowering of μ_E. However at high magnetic fields they induce a phase transition. The new phase has a metastable equilibrium between 7 T and 13 T ($2 < \nu > 1$). It is characterized by better developed fractional filling factors, e.g. $\nu = 5/3$ and $\nu = 4/3$. The phase transition is shown to be related to nuclear spin polarization.

Coffee Break

HL 77.4 Thu 15:45 POT 112

Interlayer magnetotransport phenomena of double quantum wells — •Gunnar L. Schneider[1], Rolf J. Haug[1], and Werner Dietsche[2] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Germany — [2]Max Planck Institut für Festkörperphysik, Stuttgart, Germany

We study the transport phenomena of two parallel 2-dimensional electron systems in a magnetic field, especially at the v_T=1 state of excitonic condensation. These systems are realized by a GaAs/AlGaAs double quantum well separated by an AlAs isolation layer and defined by the ratio of the layer-to-layer distance d to the magnetic length l_B. Hallbar geometry in combination with selective field gating allow an independent characterization of each layer's magnetotransport properties, investigating the interlayer electron-electron Coulomb interaction and measuring the magneto dependent interlayer I/V tunnel current [1].

The existence of a BEC excitonic state was raised over 40 years ago and our used sample geometry has been proven to contain such a condensate [2]. Our measurements show evidences that we are able to create a BEC excitonic state and the signals correlate to the d/l_B -value. In addition we performed highly resolved magneto dependent I/V tunnel characteristics from zero up to two Tesla at which we see the v_T=1 BEC excitonic state and an underlying pattern due to the Coulomb interaction between the layers and quantum Hall physics.

[1] L. Tiemann et al., New J. of Phys. 10, 045018 (2008)
[2] J. P. Eisenstein and A. H. MacDonald, Nature 432, 691 (2004)

HL 77.5 Thu 16:00 POT 112

Calculations of Quantum Capacitance of The Two Dimensional Electron System — •Eren Güvenilir[1], Özge Kiliçoğlu[2], Afif Siddiki[3], and Deniz Eksi[4] — [1]Istanbul Technical University, Istanbul, Turkey — [2]Işik University, Istanbul, Turkey — [3]Mimar Sinan Fine Arts University, Istanbul, Turkey — [4]Yeni Yuzyil University, Istanbul, Turkey

In this work we investigate the electrostatic properties of two dimensional electron system (2DES) in the integer quantum Hall regime. The alternating screening properties of the compressible and the incompressible strips are formed due to edge effects. We consider the effects of impurities on the 2DES via density of states calculations. As it is well known, the Landau Levels emerge due to strong perpendicular magnetic field and the levels are broadened which stem from impurities. At a first order approximation the density of state takes two different forms when considering impurities, these are the Gaussian and the semi-elliptic forms calculated within the self consistent Born approximation. Having in hand the density of states, we calculate both the longitudinal and Hall conductivities utilizing Thomas-Fermi-Poisson approximation. Since, the definition of capacitance is closely related with the charging energy; the compressibility of 2DES is extremely important. Here we numerically simulate the experimental observations and can predict local capacitance. We obtained numerically the local capacitances of a 2DES subject to perpendicular magnetic field. Our findings are in perfect agreement with the experiment which is based on a dynamic scanning capacitance microscopy.

HL 77.6 Thu 16:15 POT 112

THz radiation induced analog of microwave-induced resistance oscillations in GaAs heterostructures — •Tobias Herrmann[1], Ivan A. Dmitriev[1,2], Dmitriy A. Kozlov[2], Martin Schneider[1], Bruno Jentzsch[1], Ze Don Kvon[4], Peter Olbrich[1], Vasily V. Bel'kov[3], Andreas Bayer[1], Dieter Schuh[1], Dominique Bougeard[1], Thomas Kuczmik[1], Martin Oltscher[1], Dieter Weiss[1], and Sergey D. Ganichev[1] — [1]University of Regensburg, Regensburg, Germany — [2]Universitätsstr. 31 — [3]Rzhanov In-

stitute of Semiconductor Physics, Novosibirsk, Russia — [4]Novosibirsk State University, Novosibirsk, Russia

We report on the study of terahertz (THz) radiation induced oscillations of magneto-resistivity in AlGaAs/GaAs two dimensional electron systems, the THz analog of microwave induced resistivity oscillations (MIRO). Our experiments answer two most intriguing questions on MIRO, the effect of radiation helicity and the role of the edges yielding crucial information for understanding of the MIRO origin. We exploit the specific advantages of THz laser radiation not present in the MW regime, i.e., the possibility to focus it onto a spot smaller than the sample's size and easy control of the radiation's polarization. The most important features clearly detected on a large variety of samples are (i) a very weak dependence of the oscillations' amplitude on the photon helicity and (ii) the "bulk" nature of the effect. Moreover, our study shows that the MIRO oscillations can be excited at THz frequencies even in the samples with low mobility whereas in the MW range ultra-high mobility samples are needed for this type of experiments.

HL 78: Optics and Light-Matter Interaction with Excitons in 2D Materials (SYLM) (joined session DS, DY, HL, TT, organized by HL)

Time: Thursday 15:00–18:30 Location: HSZ 02

Invited Talk HL 78.1 Thu 15:00 HSZ 02

Light matter interaction in TMDs and their heterostructures — •Ursula Wurstbauer — Walter Schottky Institute and Physics-Department, TU Munich — Nanosystems Initiative Munich (NIM)

Transition metal dichalcogenides (TMDs) such as MoS2 are of current interest for optoelectronic, sensing and energy harvesting applications, but also for studying fundamental aspects of light-matter interaction in strictly two-dimensional semiconductors [1,2]. These materials exhibit a high sun light absorbance of up to 15% in the monolayer limit [3], photocatalytic stability [4] and access to excitonic phenomena in van der Waals heterostructures. We access the complex dielectric function and their fine-structure by spectroscopic imaging ellipsometry [3]. The importance of excitonic effects emerge also in resonant Raman spectroscopy, where unexpected polarization dependence points towards strong exciton-phonon coupling in MoS2. We furthermore achieve strong signatures for interlayer coupling and the formation of presumably long-lived interlayer excitons in such van der Waals heterostructures.

We acknowledge support by BaCaTeC and DFG via Nanosystems Initiative Munich (NIM), and project WU 637/4-1.

[1] U. Wurstbauer et al. arXiv:1611.05255 (2016). [2] B. Miller, et al., Appl. Phys. Lett. 106, 122103 (2015). [3] S. Funke et al., J. Phys. Condens. Matter 28, 385301 (2016). [4] E. Parzinger et al. ACS Nano 9(11), 11302 (2015).

Invited Talk HL 78.2 Thu 15:30 HSZ 02

Quantum optics with deterministically positioned quantum emitters in a two-dimensional semiconductor — •Brian Gerardot — Institute of Photonics and Quantum Sciences, SUPA, Heriot-Watt University, Edinburgh EH14 4AS, UK

The emergence of single quantum emitters in layered transition metal dichalcogenide semiconductors offers new opportunities to construct a scalable quantum architecture with a coherent light-matter interface. Here I will present results taking steps in this direction. First, using nanoscale strain engineering, we deterministically achieve a two-dimensional lattice of quantum emitters in an atomically thin semiconductor. We create point-like strain perturbations in mono-and bilayer WSe2 which locally modify the band-gap, leading to efficient funnelling of excitons towards isolated strain-tuned quantum emitters that exhibit high-purity single photon emission. Next, we perform resonance fluorescence and high-resolution photoluminescence excitation spectroscopy of these isolated, localized 2D excitons to reveal near ideal single photon fluorescence and uncover dark exciton states ~ 5meV blue-shifted from the bright exciton states. The high-purity single photon emission is stable and bright, yielding detected count rates up to 3 MHz. These results yield a route for intriguing investigations of the spin and valley coherence of localized excitons in 2D-transition metal dichalcogenide semiconductors.

Invited Talk HL 78.3 Thu 16:00 HSZ 02

Light-matter coupling with atomic monolayers in microcavities — •Christian Schneider — Technische Physik, University of Wuerzburg, Germany

Transition metal dichalcogenides represent a novel emerging class of materials which seems almost ideal to study light-matter coupling in solid state. In this talk, I address the case of a single atomic monolayer embedded in dielectric and metal-based photonic structures. I will discuss the formation of exciton-polaritons from cryogenic temperatures up to ambient conditions in compact and flexible Tamm-structures. I will also discuss peculiarities which arrise from the moderate quality factors in these structures, yielding significantly different anticrossings in luminescence and reflection. Finally, a focus is set on the interplay of excitons and trions, both in the weak and strong coupling limit.

Coffee Break

Invited Talk HL 78.4 Thu 17:00 HSZ 02

Properties of Synthetic 2D Materials and Heterostructures — •Joshua Robinson — Pennsylvania State University, University Park, PA, USA

The last decade has seen nearly exponential growth in the science and technology of two-dimensional materials. Beyond graphene, there is a huge variety of layered materials that range in properties from insulating to superconducting. Furthermore, heterogeneous stacking of 2D materials also allows for additional dimensionality for band structure engineering. In this talk, I will discuss recent breakthroughs in two-dimensional atomic layer synthesis and properties, including novel 2D heterostructures and novel 2D nitrides. Our recent works include development of an understanding of substrate impact on 2D layer growth and how we can tune the substrate to acheive near-single crystal 2D materials over large areas. I will also dsicuss doping of 2D materials with magentic elements, selective area synthesis of 2D materials, and the first demonstration of 2D gallium nitride (2D-GaN). Our work and the work of our collaborators has lead to a better understanding of how substrate not only impacts 2D crystal quality, but also doping efficiency in 2D materials, and stabalization of nitrides at their quantum limit.

Invited Talk HL 78.5 Thu 17:30 HSZ 02

Exciton spectroscopy in transition metal dichalcogenide monolayers and van der Waals heterostructures — •Bernhard Urbaszek — CNRS - Toulouse University, France

Excitons in transition metal dichalcogenide monolayers (MLs) provide exciting opportunities for applications and new frontiers in physics: (i) with binding energies of several hundred meV, excitons dominate optical properties even at room temperature, (ii) strong exciton oscillator strength leads to absorption of up to 20 % per ML, and (iii) the interband selection rules are valley selective. In combination with strong spin-orbit splittings this allows studying spin-valley physics. Although ML samples on Si/SiO2 substrates are widely studied in the literature, conclusive measurements on the excited exciton states and fine structure (2s/2p) are still missing. In hBN / ML WSe2 / hBN samples we measure for the linewidth of the neutral and charged exciton emission values down to 1.6 meV at T=4K, close to the homogenous limit. This allows us to perform 1 and 2-photon spectroscopy which reveal details previously masked by inhomogeneous broadening. Also, we demonstrate control of the exciton valley coherence in ML WSe2 on SiO2 by tuning the applied magnetic field B perpendicular to the ML plane. Linearly polarized laser excitation prepares a coherent superposition of valley states and the induced valley Zeeman splitting between K+ and K- results in a change of the oscillation frequency of the superposition of valley states. This corresponds to a rotation of the exciton valley pseudo-spin by angles as large as 30 degrees for fields up to B=9T.

Invited Talk HL 78.6 Thu 18:00 HSZ 02

Strain-induced single-photon emitters in layered semiconductors — •Rudolf Bratschitsch — Westfälische Wilhelms-Universität Münster, Münster, Deutschland

Single-photon sources are important building blocks for quantum information technology. Emitters based on solid-state systems provide a viable route for their integration in photonic devices. Recently, we have found single-photon emitters in the atomically thin semiconductor WSe2 [1]. We show that the quantum light sources are strain-induced and demonstrate deterministic positioning of the emitters on the nanoscale [2]. Finally, we present single-photon emission from the layered semiconductor GaSe and provide evidence that the incorporated non-classical light sources are also strain-induced [3].

[1] P. Tonndorf et al., Optica 2, 347 (2015)
[2] J. Kern et al., Advanced Materials 28, 7101 (2016)
[3] P. Tonndorf et al., 2D Materials (2016)

HL 79: Poster: New Materials

Time: Thursday 15:00–19:00 Location: P2-OG3

HL 79.1 Thu 15:00 P2-OG3

Exciton recombination dynamics of graphene nanoribbons probed by time-resolved Raman spectroscopy — •Raphael German, Jinghi Zhu, Boris Senkovskiy, Alexander Grüneis, and Paul H.M. van Loosdrecht — II.Physikalisches Institut Köln, Zülpicher Str. 77, 50937 Köln

Graphene based materials show remarkable chemical, electrical and optical properties. Recently, it has been shown that one can grow atomically precise one-dimensional graphene nanoribbons. Here, we investigate armchair graphene nanoribbons of N=7 carbon atoms width transferred onto the insulating substrate, using steady state and time-resolved spontaneous Raman spectroscopy. The Raman signal shows a resonance near 2.2 eV, consistent with the energy level structure. The time-dependent Raman data is interpreted in terms of exciton recombination dynamics, indicating that exciton recombination occurs mainly through exciton-exciton annihilation which is limited by one-dimensional diffusion.

HL 79.2 Thu 15:00 P2-OG3

Comparison of the electrical conductivity between H terminated and heated electronic grade diamonds — •Sven Graus[1], Stefan Borgsdorf[1], Ulrich Köhler[1], Nikolas Wöhrl[2], Dennis Oing[2], Volker Buck[2], Tanmoy Chakraborty[3], and Dieter Suter[3] — [1]Experimentalphysik IV, AG Oberflächen, Ruhr- Universität Bochum, Germany — [2]Experimentalphysik, AG Lorke, Universität Duisburg-Essen, Germany — [3]Experimentelle Physik IIIA, Technische Universität Dortmund, Germany

Color centers in diamond, especially nitrogen vacancy (NV) centers, are practical single photon emitters due to RT operation and are candidates for applications in quantum computing and are elements for quantum information technologies. We create the NV centers with low energy nitrogen implantation in electronic grade diamonds. To prevent charging effects on the surface which defocus the ion beam it is common to use hydrogen terminated diamonds. The termination in combination with water adsorbates leads to a surface conductivity which is induced by a two dimensional hole gas (2DHG) close to the surface. For implantation experiments at high temperatures (up to 900 °C) the termination and also the 2DHG is destroyed but the conductivity induced by charge carriers from boron impurities and intrinsic charge carries is rising with the temperature. We compared the conductivity by van der Pauw measurements of the terminated diamond at RT and the diamond at 900 °C in UHV. The appearance of any defocusing effects on the hot diamond while implantation were also checked.

HL 79.3 Thu 15:00 P2-OG3

UHV nanopositioning system for close to surface nitrogen implantation in diamond — •Stefan Borgsdorf[1], Ulrich Köhler[1], Tanmoy Chakraborty[2], and Dieter Suter[2] — [1]Experimentalphysik IV, AG Oberflächen, Ruhr- Universität Bochum, Germany — [2]Experimentelle Physik IIIA, Technische Universität Dortmund, Germany

Color centers in diamond, especially nitrogen vacancy (NV) centers, are practical single photon emitters due to RT operation and are candidates for applications in quantum computing and are elements for quantum information technologies. We present a setup for low energy implantation of NV centers near to the surface with a lateral resolution from micrometer to nanometer scale. The lateral resolution is achieved by a closed loop nanopositioning system combined with an exchangeable aperture with diameters between a micrometer down to a few nanometer. The system allows us to heat the sample up to 900 °C in UHV while implanting with nitrogen without any graphitization on the surface.

HL 79.4 Thu 15:00 P2-OG3

Macro- and micro-scale investigation of diamond etching — •Meng Ge, Christian Osterkamp, Fedor Jelezko, and Alexander Kubanek — Institute for Quantum Optics, Ulm University, D-89081 Ulm, Germany

Diamonds have special usage in quantum information science and technology. The existence of the negatively charged nitrogen-vacancy (NV) centers in diamond, whose electron spin can be coherently manipulated by microwave, are very good candidates for single photon sources, nano-scale magnetic and electric field sensors, and quantum bits (qubits). For many applications good optical and spin properties are required in micro-and nanostructured diamond devices. In order to fulfill this aim and provide a smooth and uniform method, plasma processes are employed. During our research, we focus on both the SF6 and the O2 inductively coupled plasma (ICP) processes.We optimize etching process towards fabrication of diamond nano-structures. A confocal microscope is used for characterizing NV centers in our diamond before and after the diamond structuring procedure.

HL 79.5 Thu 15:00 P2-OG3

Robust optically pumped nuclear spin polarization — •Jochen Scheuer[1], Ilai Schwartz[2], Samuel Müller[1], Qiong Chen[2], Martin B Plenio[2], Boris Naydenov[1], and Fedor Jelezko[1] — [1]Institute of Quantum Optics, Ulm University, Ulm, Germany — [2]Institute of Theoretical Physics, Ulm University, Ulm, Germany

Dynamical nuclear polarisation (DNP) can enhance the sensitivity of magnetic nuclear resonance imaging (MRI) by several orders of magnitude. Nanodiamonds are candidates for novel MRI tracers with particle sensitivity and long coherence times. There are several techniques which perform well for hyperpolarization in aligned magnetic fields, however, they are not applicable for randomly oriented nanodiamonds at ambient conditions. Here polarization and read out of a ^{13}C nuclear spin bath is demonstrated by using a single nitrogen-vacancy (NV) center in a macroscopic diamond.

Our polarization methods use microwave dressed states and semi-adiabatic passages to transfer the NV's electron spin polarization to the surrounding carbon nuclear spins, whereas the NV is repeatedly polarized optically.

We show that using integrated solid effect both for single and double quantum transitions a nuclear spin polarization can be achieved for broadened NV-ESR lines e.g. when the static magnetic field is not aligned along the NV's crystal axis [1]. Our results can be applied for DNP in nanodiamonds, which would find a wide application in magnetic resonance imaging and could revolutionize the field.

[1] Chen, Q., et al., Phys Rev B 92.18 (2015): 184420.

HL 79.6 Thu 15:00 P2-OG3

Sensing Properties of Carbon-Nanotube/Boron-Nitride-Nanotube Heterojunction towards Carbon Monoxide: A First Principles Study — •Shahim Vedaei and Ebrahim Nadimi — Center for Computational Micro and Nanoelectronics, Faculty of Electrical Engineering, K. N. Toosi University of Technology, Tehran, Iran

Detection of carbon monoxide (CO), known as silent killer, is of great importance. Nanotubes could be considered as useful materials for gas sensing applications due to their large surface to volume ratio. But carbon nanotubes (CNT) have almost no interaction with CO molecule and boron nitride nanotubes (BNNT) shows small binding energy of about 0.2 eV. However, we find that, the CNT/BNNT/CNT heterojunctions with appropriate BNNT length show binding energies with CO of the order of 1 eV. The calculations have been performed within pseudopotential density functional theory (DFT) as implemented in SIESTA code. Non-stoichiometric BNNT layers as well as interface

bonding (N-C or B-C) could strongly influence the adsorption energy and consequently the sensing behavior. The results show that such heterojunction could be a promising candidate for CO detection.

HL 79.7 Thu 15:00 P2-OG3

Nanostructured water and carbon dioxide inside collapsing carbon nanotubes at high pressure — •Wenwewn Cui[1], Tiago Cerqueira[2,1], Silvana Botti[2,3], and Miguel Marques[4,3] — [1]Institut Lumière Matière, UMR5306 Université Lyon 1-CNRS, Université de Lyon, F-69622 Villeurbanne Cedex, France — [2]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [3]European Theoretical Spectroscopy Facility — [4]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

We present simulations of the collapse under hydrostatic pressure of carbon nanotubes containing either water or carbon dioxide. We show that the molecules inside the tube alter the dynamics of the collapse process, providing either mechanical support and increasing the collapse pressure, or reducing mechanical stability. At the same time the nanotube acts as a nanoanvil, and the confinement leads to the nanostructuring of the molecules inside the collapsed tube. In this way, depending on the pressure and on the concentration of water or carbon dioxide inside the nanotube, we observe the formation of 1D molecular chains, 2D nanoribbons, and even molecular single and multi-wall nanotubes. The structure of the encapsulated molecules correlates with the mechanical response of the nanotube, opening opportunities for the development of new devices or composite materials. Our analysis is quite general and it can be extended to other molecules in carbon nanotube nanoanvils, providing a strategy to obtain a variety of nanoobjects with controlled features

HL 79.8 Thu 15:00 P2-OG3

EPR spectroscopy of Yb3+ in lithium yttrium borate (LYB) single crystals — •Sara Arceiz Casas[1], Gábor Corradi[2], László Kovács[2], Éva Tichy-Rács[2], and Sigmund Greulich-Weber[1] — [1]Paderborn University, Warburger Str. 100, 33098 Paderborn, Germany — [2]Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungarian Academy of Sciences, Konkoly-Thege u. 29-33, 1121 Budapest, Hungary

Lithium yttrium borate Li6Y(BO3)3 is an excellent nonlinear optical material with a wide UV range of transparency. Due to the easy incorporation of rare earth ions at Y sites LYB is a prospective laser host material. Yb3+ ions are especially interesting for near-infrared laser pulse applications, indeed, mode-locked and Q-switched laser operation near 1042 nm in Yb-doped LYB has already been realized. EPR studies of Yb+3 in LYB have only been reported in powdered materials. Here single-crystal results on the EPR and its temperature dependence characterizing the Stark-split ground state of Yb+3 in the low symmetry crystal field of LYB are presented.

LYB crystals doped with 1 mol% Yb were grown by the Czochralski method. EPR was measured at low temperature on samples oriented by X-ray diffraction and cut perpendicular to the crystallographic twofold symmetry axis b. Angular dependent EPR spectra near 5K have been taken for the magnetic field in four crystallographic planes required for a full and unambiguous determination of the g-tensor and the hyperfine-tensor of the 171Yb and 173Yb isotopes. The results show reasonable agreement with theoretical results published recently.

HL 79.9 Thu 15:00 P2-OG3

Theoretical and experimental investigation of Iron doped hexagonal $BaTiO_3$ — •Waheed A. Adeagbo[1], Sanjeev K. Nayak[2], Hichem B. Hamed[1], Hans T. Langhammer[3], Wolfram Hergert[1], and Thomas Müller[4] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, 06120 Halle, Germany — [2]Department of Materials Science and Engineering, University of Connecticut, USA — [3]Institute of Chemistry, Martin Luther University Halle-Wittenberg, 06120 Halle, Germany — [4]Faculty of Physics and Earth Sciences, Leipzig University, 04103 Leipzig, Germany

EPR measurements on Fe-doped hexgonal $BaTiO_3$ (h-BTO), with Fe concentration between 0.5−2.0 mol%, show the detection of isolated Fe^{3+} which occupies only one of the two crystallographic different Ti sites, that could be the exclusively corner-sharing octahedron, in all different annealing prepared samples. Also, there is speculation about EPR non-detectable states of Fe^{2+} and Fe^{4+} presence, but Fe^{5+} formation is completely ruled out. Recent further defect center detected is identified as Fe^{3+} associated with an oxygen vacancy (V_O) in the first coordination sphere. The exact Fe^{3+} and V_O occupation sites and the V_O roles in the complex are still unknown. Thus, we have used the first principles approach to study the defect properties of substitutionally doped Fe in h-BTO and to examine the role played by the V_O in structure, electronic and magnetic properties due to the introduced defects in the pure crystal. Our theoretical analysis of the defect formation energy derived from the total energies of defective supercells in various charge states will be presented with respect to available EPR-data.

HL 79.10 Thu 15:00 P2-OG3

structural engineering of electrode materials for Na-ion batteries — •Benrong Hai[1,2], Yang Xu[1], Min Zhou[1], Chengliang Wang[1], Liying Liang[1], Yan Mi[1], and Yong Lei[1] — [1]TU-ilmenau, Ilmenau, Germany — [2]Northeastern University, Shenyang, P. R. China

In response to the increased demands of energy storage, Na-ion batteries (SIBs) appear as alternatives to lithium ion batteries. However, because of large radius of Na ions, more complex requirements for the intrinsic properties raise the difficulties in finding a suitable material. Structural engineering is a promising approach to enhance sodium storage, of which amorphization and introduction of oxygen vacancies are two efficient methods to allow the crystalline features of active materials more suitable for large sodium ions. For the former method, TiO2 electrodes with different orderliness of atomic arrangement are employed as the state-of-the art example. Corresponding results prove that the disordering at the surface is benefit for the faradaic contribution from surface processes, which is particularly significant to the electrode materials with poorer affinity of transporting ions. With regard to the influences of oxygen vacancies (OVs), the SIB performance of MoO3 and amorphous SnO2 with and without OVs both evidence that the OVs can increase the electric conductivity and Na-ion diffusion coefficient, leading to the promotion of sodium storage.

HL 79.11 Thu 15:00 P2-OG3

A New Concept for Doping Silicon and its Nanostructures: Modulation Doping using Al-induced Acceptor States in SiO2 — •Daniel Hiller[1] and Dirk König[2] — [1]Laboratory for Nanotechnology, IMTEK, University of Freiburg, Germany — [2]University of New South Wales (UNSW), Sydney, Australia

Silicon nanostructures are omnipresent in fundamental research (quantum dots, nanowires) but are also approached in future technology nodes of the microelectronics industry. Several fundamental physical principles based on diffusion, statistics, and quantum confinement, impede efficient and reproducible impurity doping of nano-Si with e.g. P or B.

In this presentation, we highlight a novel concept: Heterostructure modulation doping of Si using an acceptor state of Al-atoms in SiO2. This state is located 0.5 eV below the Si valence band and captures electrons from the Si over a distance of several nanometers, leaving behind holes as majority carriers [1]. We demonstrate experimental evidences of this mechanism: fixed negative charges and increased tunnelling currents in SiO2:Al thin films, induced holes in modulation doped Si quantum wells, and PL quenching of modulation doped Si nanocrystals.

[1] D. König & D. Hiller et al., Sci. Rep., under review (2016)

HL 79.12 Thu 15:00 P2-OG3

Designing Locally Symmetric Eigenstates in Planar Discrete Systems — •Malte Röntgen, Christian V. Morfonios, and Peter Schmelcher — Zentrum f. Optische Quantentechnologien, Luruper Chaussee 149, 22761 Hamburg

Local symmetries are spatial symmetries that are only present in a spatially finite subdomain of a system. Contrary to the usual case of global symmetries, the effects of local symmetries on the system's eigenstates are not obvious and thus have not been investigated thoroughly in the past. However, in this paper we show that it is indeed possible to gain knowledge about the structure of the eigenstates of systems possessing local symmetries. To this end, we use and extend a framework of so-called non-local currents that has been established recently. The then-extended framework is applicable to all kinds of discrete planar Schrödinger systems, including those with non-uniform connectivity. We use the framework both to derive general identities as well as to investigate two locally symmetric subsystems in detail. These subsystems are closed-loops and one-dimensional open ended chains. We find that, depending on the local symmetry and the type of subsystem, some or all amplitudes within the subsystem to be related by a constant factor. Since these effects can easily be understood using our framework of non-local currents, we expect it to help researchers

finding and understanding more effects of local symmetries.

HL 79.13 Thu 15:00 P2-OG3

Optical properties of (CuI)-based inorganic-organic hybrid materials as active semiconductor in planar microcavities — •Lukas Trefflich[1], Gabriele Benndorf[1], Rüdiger Schmidt-Grund[1], Harald Krautscheid[2], and Marius Grundmann[1] — [1]Institute for Experimental Physics II, University of Leipzig, 04103 Leipzig, Germany — [2]Institute for Inorganic Chemistry, University of Leipzig, 04103 Leipzig, Germany

We have investigated electronic and optical properties as well as temporal dynamics of (CuI)-based inorganic-organic hybrid materials using photoluminescence spectroscopy and ellipsometry. By changing the chemical composition bright light emission in the visible spectral range can be tuned from approximately 450 nm to 650 nm . We found the luminescence decay time to be in the microsecond range. Furthermore, we have determined the dielectric function from the far UV to mid IR range in order to design planar microcavities for possible laser and LED application. This is of particular interest because white light LEDs usually contain rare-earth elements. [1] Their mining is difficult and expensive. Because of the facile synthesis, high quantum yield (up to 95%), thermal stability and optical tunability [2], (CuI)-based inorganic-organic hybrid materials are promising alternatives.

[1] H. Höppe, Angew. Chem., Int. Ed. 2009, 48, 3572
[2] W. Liu et al., J. Am. Chem. Soc. 2015, 137, 9400-9408

HL 79.14 Thu 15:00 P2-OG3

Structural and optical properties of TiN/MgO superlattices — •Florian Jung, Vitaly Zviagin, Michael Bonholzer, Chris Sturm, Jörg Lenzner, Rüdiger Schmidt-Grund, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Leipzig, Germany

We present an investigation of structural and optical properties of TiN/MgO superlattices grown by pulsed laser deposition on MgO(100)-substrates. Multilayers and superlattices are grown in an argon atmosphere and their growth is in-situ monitored using reflection high energy electron diffraction. The films' structural properties are evaluated using X-ray diffraction, X-ray reflectometry, atomic force microscopy and reciprocal space mapping techniques. Systematic studies of the dependence of optical properties of the films on process parameters are performed using ellipsometry.

Periodic metal/dielectric planar metamaterials are known to be adjustable such that they exhibit a hyperbolic dispersion and thus anisotropic optical behaviour. Material stacks on a sub-wavelength scale realising such a dispersion are referred to as hyperbolic metamaterials (HMMs). Titanium nitride has already been applied as a plasmonic component in previous studies[1]. Our results show, that MgO/TiN superlattices are promising for application as HMMs.

[1] G. V. Naik et al., PNAS, Vol. 111, No. 21, 7546-7551 (2014)

HL 79.15 Thu 15:00 P2-OG3

Band Offset in (Ga,In)As/GaAs/Ga(As,Sb) heterostructures — Sebastian Gies[1], •Benjamin Holz[1], Maria Weseloh[1], Christian Fuchs[1], Wolfgang Stolz[1], Jörg Hader[2,3], Jerome Moloney[2,3], Stephan Koch[1], and Wolfram Heimbrodt[1] — [1]Department of Physics and Materials Science Center, Philipps-Universität Marburg, Renthof 5, 35032 Marburg, Germany — [2]Nonlinear Control Strategies Inc., 7040 Montecatina Dr., Tucson, AZ 85704, USA — [3]College of Optical Sciences, University of Arizona, Tucson, AZ 85721, USA

The (Ga,In)As/GaAs/Ga(As,Sb) material system is used for lasers operating over a wide spectral range in the infrared. To further optimize the design of such heterostructures, it is important to have exact knowledge of the band structure and the band offsets, in particular. Here, we present a thorough analysis of the optical properties of (Ga,In)As/Ga(As,Sb) type-II heterostructures by means of temperature- and power-dependent photoluminescence spectroscopy. In conjunction with a microscopic many-body theory we are able to determine the band offset between Ga(As,Sb) and GaAs with high precision. Furthermore, we reveal the temperature dependent band-alignment in these heterostructures. Additionally, we introduce a GaAs interlayer of variable thickness to influence the tunnel processes of the charge carriers. Here, the great importance of these tunneling processes on the optical spectra and the influence of the internal interfaces are investigated.

HL 79.16 Thu 15:00 P2-OG3

Calculation of forces in the KKR method — •Jonas Friedrich Schäfer, Michael Czerner, and Christian Heiliger — Justus-Liebig-Universität Gießen

Although the general method of calculating forces on atomic nuclei in the KKR formalism seems to be simple, a closer investigation reveals major challenges: First, Hellmann-Feynman forces are very sensitive to small deviations from a spherical core electron density. Given that spherical symmetry is a requirement for fast convergence of the angular momentum expansion, this contribution needs special treatment. Further, the expression for the interstitial space contribution (i.e., the space outside the Muffin-Tin spheres) is highly sensitive to the angular momentum cut-off, too. We present quantitative studies to the aforementioned problems and trace them back to the underlying mathematical expressions. Based thereupon, we discuss possible improvements to the calculational scheme.

HL 79.17 Thu 15:00 P2-OG3

Elastic strain relaxation and evolution in GaAs/InGaAs/GaAs radial nanowire heterostructures — •Ali Al Hassan[1], Ryan B. Lewis[2], Hanno Küpers[2], Emmanouil Dimakis[2], Arman Davtyan[1], Christian Sternemann[3], 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 — [3]Zentrum fuer Synchrotronstrahlung Technische Universitaet Dortmund, Maria-Goeppert-Mayer-Str. 2, 44227 Dortmund, Germany

The optical performance of nanowire based devices is strongly related to the sharpness of the hetero-interface and the homogeneity of atomic composition within the active volume. In GaAs/InGaAs/GaAs core-shell-shell nanowires, misfit strain can easily release towards NW side planes. However due to hexagonal geometry of the nanowires, the interfacial strain might differ towards different radial directions and requires careful analysis. Towards this goal, we report explicitly on the 3D investigation of the strain interaction and relaxation mechanisms in GaAs/InGaAs/GaAs core-shell-shell NW ensembles by means of high resolution x-ray diffraction (XRD) and finite element methods (FEM) as a function of InGaAs shell thickness and nominal indium concentration. In order to obtain a full 3D strain field map, special attention was paid to determine the strain impact along the azimuth and in-plane directions of the NW core shell system.

HL 79.18 Thu 15:00 P2-OG3

Transmission Electron Microscopy investigations on structural origins of cross hatching in $Si_{1-x}Ge_x$/Si — Florian Biebl, •Elisabeth Anna Zolnowski, Felix Schwarzhuber, Christian Neumann, Michaela Trottmann, Dominique Bougeard, and Josef Zweck — Institute of Experimental and Applied Physics, University of Regensburg, Germany

The occurrence of cross-hatched surfaces can be observed under certain growth conditions in various strain engineered semiconductor materials. This means, that a surface shows periodic ridges and trenches along specific growth directions. This phenomenon influences the electron mobility and other properties of the grown materials. Therefore, it is important to understand the origin of the cross-hatch pattern (CHP) in order to prevent unwanted effects in semiconductor devices. By Transmission Electron Microscopy (TEM) we investigated CHPs on epitaxially grown strain-relaxed $Si_{1-x}Ge_x$/Si by molecular beam epitaxy, prepared as a cross section specimen along a periodic direction of the CHP. The periodicity and depth of the CHP observed in our measurements are in good agreement with literature [1]. Further, we could show that there is a correlation between the occurrence of a trench and a so called 60° dislocation originating in the substrate. In addition, we will present results of nanodiffraction experiments, revealing that these dislocations may separate areas of slightly different crystallographic orientations.

[1] Lutz et al., Influence of misfit dislocations on the surface morphology of $Si_{1-x}Ge_x$ films, Applied Physics Letters 66, 724 (1995)

HL 79.19 Thu 15:00 P2-OG3

Effect of the different surface texture on the metal-insulator-silicon photoanodes performances for water photosplitting — •Haojie Zhang[1,2], Stefan L. Schweizer[1], Alexander Sprafke[1], and Ralf B. Wehrspohn[1,2] — [1]Institute of Physics, Martin-Luther-University Halle-Wittenberg, Germany — [2]Fraunhofer-Institut für Mikrostruktur von Werkstoffen und Systemen IMWS

Metallurgical grade (MG) silicon processed with the metal-assisted chemical etching(MaCE) can not only promote the purity, but also from the nanostructures in the bulk of the MG silicon. Since the surface texture of the silicon was dominated the optical (e.g. reflection, scattering, carries, bending gap and charge-transfer rate) and chemical (e.g. catalytic site, surface area and defects) characteristics. Moreover, the stability in extremely acidic and basic electrolytes was concerned and could be effectively enhanced by coating a thin and robust tunneling layer (such TiO2, ZnO). Herein, the different texture surfaces of Si were demonstrated by MaCE with different catalytic and other methods as a comparison. A protecting layer and catalytic particles were deposited by Atomic Layer Deposition (ALD) to promote the durable and catalytic performance in the photoelectrochemical(PEC).

HL 79.20 Thu 15:00 P2-OG3

Comparison of Cu, Ag and Pt assisted chemical etching for metallurgical silicon purification — •Junna Wang[1,2], Stefan L. Schweizer[1], Alexander Sprafke[1], and Ralf B. Wehrspohn[1,2] — [1]Institute of Physics, Martin-Luther-University Halle-Wittenberg, Germany — [2]Fraunhofer-Institut für Mikrostruktur von Werkstoffen und Systemen IMWS

The purity of metallurgical grade silicon can be improved during metal assisted chemical etching (MaCE). Since MaCE can form nanostructures in metallurgical silicon (MG Si), metal impurities are removed during the formation of porous silicon. We chose different catalytic metals and compared the resulting nanostructures moreover the catalyst selection results in different purification efficiency and application.

HL 79.21 Thu 15:00 P2-OG3

Effect of the different surface texture on the metal-insulator-silicon photoanodes performances for water photosplitting. — •Haojie Zhang[1,2], Stefan L. Schweizer[1], Alexander Sprafke[1], and Ralf B. Wehrspohn[1,2] — [1]Institute of Physics, Martin-Luther-University Halle-Wittenberg, Germany — [2]Fraunhofer-Institut für Mikrostruktur von Werkstoffen und Systemen IMWS

Metallurgical grade (MG) silicon processed with the metal-assisted chemical etching(MaCE) can not only promote the purity, but also from the nanostructures in the bulk of the MG silicon. Since the surface texture of the silicon was dominated the optical (e.g. reflection, scattering, carries, bending gap and charge-transfer rate) and chemical (e.g. catalytic site, surface area and defects) characteristics. Moreover, the stability in extremely acidic and basic electrolytes was concerned and could be effectively enhanced by coating a thin and robust tunneling layer (such TiO2, ZnO). Herein, the different texture surfaces of Si were demonstrated by MaCE with different catalytic and other methods as a comparison. A protecting layer and catalytic particles were deposited by Atomic Layer Deposition (ALD) to promote the durable and catalytic performance in the photoelectrochemical(PEC).

HL 79.22 Thu 15:00 P2-OG3

Anneal induced transforms of radiation defects in heavily irradiated Si detectors — •Dovile Meskauskaite, Tomas Ceponis, Eugenijus Gaubas, Vytautas Rumbauskas, and Juozas Vaitkus — Vilnius University Institute of Applied Research, Vilnius, Lithuania

In this research, transforms of the radiation defect induced by anneals have been studied in heavily irradiated Si. The n-type and p-type CZ and FZ Si material samples and detector structures, irradiated by high energy electrons (6.6 MeV), protons (26 GeV/c) and pions (300 MeV/c) using fluences up to 5×10^{16} cm^{-2}, have been studied. The deep level spectra have been examined by combining the capacitance and current deep level transient spectroscopy (DLTS) and using the optical injection techniques. The DLTS spectroscopy means has been combined with measurements of the temperature dependent carrier trapping lifetime (TDTL). The latter TDTL technique is a contact-less spectroscopy tool based on recording of the microwave-probed photoconductivity transients. This TDTL technique is preferential when radiation trap density approaches or exceeds the dopant concentration and when necessary to avoid modification of a detector structure due to anneals at elevated temperatures. A good agreement between the DLTS and TDTL spectra has been obtained. The dominant radiation defects and their transform paths under isochronal anneals have been revealed.

HL 79.23 Thu 15:00 P2-OG3

Micro-Raman spectroscopy of laser-annealed reheated SiO_x films on silica substrate — •Christian Gobert[1], Nan Wang[1], Thomas Fricke-Begemann[2], Jürgen Ihlemann[2], and Michael Seibt[1] — [1]IV. Physikalisches Institut, Universität Göttingen, Germany — [2]Laser-Laboratorium Göttingen, Germany

The development of Si-based opto-electronics for integrated circuits is still an unsolved problem as bulk-Si is an indirect semiconductor resulting in improbable optical transitions. Nanocrystalline silicon (nc-Si) is expected to be a feasible material for this purpose due to quantum confinement effects compassing the indirect band gap [1]. It was recently shown [2] that cw laser irradiation of substrate-bound silicon-rich silicon oxide (SRSO) is suitable to produce a phase separation reaction leading to strong room temperature photoluminescence (PL). The latter was attributed to small amorphous Si clusters in the remaining amorphous silicon oxide matrix, as indicated by Raman spectroscopy. Such particles, however, could not be confirmed by transmission electron microscopy.

In this work, the effect of subsequent low-temperature furnace annealing of laser-annealed SiO_x films on silica substrate is investigated by micro-Raman spectroscopy. In order to test the above hypothesis, changes in Raman spectra induced by low temperature (500-700°C) furnace annealing are followed to observe the selective crystallization of a-Si clusters. [1] T. Nikitin, L. Khriachtchev, Nanomaterials 5, 614-655 (2015) [2] T. Fricke-Begemann, N. Wang, P. Peretzki, M. Seibt, J. Ihlemann, J. Appl. Phys. 118, 124308 (2015)

HL 79.24 Thu 15:00 P2-OG3

Crystal structure and thermoelectric properties of some indium-based thiospinels — •Pawel Wyzga[1,2], Igor Veremchuk[2], Matej Bobnar[2], Tina Weigel[1], Tilmann Leisegang[1], Andreas Leithe-Jasper[2], and Roman Gumeniuk[1] — [1]TU Bergakademie Freiberg, Germany — [2]MPI Chemische Physik fester Stoffe, Dresden, Germany

Nowadays, a particular emphasis in thermoelectric research is put on the obtaining both high-performance and earth abundant materials. These requirements are perfectly suited in case of sulphur-containing materials. For instance, the nonstoichiometric chalcocite $Cu_{2-x}S$ ($x = 0.03$) reveals extremely high values of thermoelectric figure of merit $ZT_{max} = 1.9$ at 970 K [1]. The indium-containing thiospinels MIn_2S_4 (M = Cr, Mn, Fe, Co) [2], initially attracted a special attention due to their interesting magnetic behaviours. In this work, we focus on the study of thermoelectric properties of new $Ti_{0.8}In_{2.2}S_4$ and known $Fe_{0.9}In_{2.1}S_4$ compounds. Both of them show different transport properties: Ti-containing is a metal while that with Fe is a semiconductor. Despite relatively low thermal conductivities at elevated temperatures, both thiospinels show negligibly small ZT values (5×10^{-3} and 2×10^{-3} at 300 K, respectively). However, taking into account that the transport properties of Ti-Fe indium-thiospinels are ranging from metallic to semiconducting, a possibility of tuning of thermoelectric properties makes these sulphides promising materials.

[1] L. Zhao et al., J. Mater. Chem. A 3 (2015) 9432-9437
[2] H. Hahn, W. Klinger, Z. Anorg. Allg. Chem. 263 (1950) 177-190

HL 79.25 Thu 15:00 P2-OG3

Temperature-dependent Seebeck coefficient of silver nanowires — •Maximilian Kockert[1], Danny Kojda[1], Rüdiger Mitdank[1], Johannes Ruhhammer[2], Zhi Wang[2], Michael Kröner[2], Peter Woias[2], Toni Markurt[3], and Saskia F. Fischer[1] — [1]Group Novel Materials, Humboldt-Universität zu Berlin, D-12489 Berlin — [2]Laboratory for Design of Microsystems, University of Freiburg - IMTEK, D-79110 Freiburg — [3]Leibniz-Institute for Crystal Growth, D-12489 Berlin

Bulk silver has the highest electrical and thermal conductivity of all metals. The process of miniaturization and nanopatterning affects these two parameters. The electrical and thermal conductivity of individual silver nanowires were recently investigated in [1] and [2].

In this work, we present the temperature-dependent Seebeck coefficient of individual silver nanowires relative to platinum between temperatures of 10 K and 300 K. The silver nanowires were prepared by the reduction of high purity silver nitrate (99.9999 %). Four individual silver nanowires showed reproducable results. Above 160 K, the diffusive part of the Seebeck coefficent of silver nanowires relative to nanostructured platinum conducting lines $S^{NW}_{Ag,Pt}$ is in agreement with the Seebeck coefficent of bulk silver relative to bulk platinum $S^{Bulk}_{Ag,Pt}$. A change of sign of the Seebeck coefficent takes place at 160 K. Below 160 K, the Seebeck coefficent is dominated by the phonon drag effect.In this regime $S^{NW}_{Ag,Pt}$ differs from $S^{Bulk}_{Ag,Pt}$.

[1] D. Kojda *et al.*, Physical Review B **91**, 024302-1 (2015).
[2] D. Kojda *et al.*, Physica Status Solidi A **213**, 557 (2015).

HL 79.26 Thu 15:00 P2-OG3

Role of interlayer coupling for the power factor of $CuSbS_2$ and $CuSbSe_2$ — •Najebah Alsaleh, Nirpendra Singh, and Udo Schwingenschlogl — King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia

The electronic and transport properties of bulk and monolayer $CuSbS_2$ and $CuSbSe_2$ are determined by using density functional theory and semiclassical Boltzmann transport theory, in order to investigate the role of the interlayer coupling for the thermoelectric properties. The calculated band gaps of the bulk compounds are in agreement with experiments and significantly higher than those of the monolayers, which thus show lower Seebeck coefficients. Since also the electrical conductivity is lower, the monolayers are characterised by lower power factors. Therefore, interlayer coupling is found to be essential for the excellent thermoelectric response of $CuSbS_2$ and $CuSbSe_2$ even though it is weak.

HL 79.27 Thu 15:00 P2-OG3

Electronic properties of the thermoelectric Mg2X (X=Si,Ge,Sn)-based alloys — •Juan Guerra, Carsten Mahr, Marcel Giar, Michael Czerner, and Christian Heiliger — Justus Liebig University Giessen, Institut für Theoretische Physik, Giessen, Germany

Since there has been recent research interest in Mg2X based alloy systems for thermoelectric applications, we present an ab initio description of electronic properties in the cases of X=Si, Ge, and Sn. Due to a reported importance of spin-orbit coupling we model the system using a fully relativistic implementation of the density functional theory (DFT) based Korringa-Kohn-Rostocker (KKR) Green's function method in conjunction with the coherent potential approximation (CPA), which allows us to efficiently account for scattering processes in substitutional alloys. Using our calculation scheme we extract parameters important for transport modelling, e.g. band gaps, charge carrier effective masses and velocities

HL 79.28 Thu 15:00 P2-OG3

Magnetotransport experiments on Lorentz systems with varying scatterer shape — •Tabea Heckenthaler — Heinrich-Heine-Universität Düsseldorf

In the Lorentz model one usually assumes an array of randomly distributed hard disks to model scattering in solids. This has hitherto been discussed primarily from a theoretical point of view.

Due to advancements in semiconductor processing, one can nowadays realize systems with desired specifications in order to also study them experimentally.

We examine such samples based on high electron mobility Ga[Al]As heterostructures, where holes of varying shape are introduced via Ar - ion etching. The scattering at the artificial obstacles dominates the magnetoresistance at low magnetic fields, since background scattering is minimized. We show that these effects have a classical character, which is plausible due to the scatterer size in comparison to the Fermi wavelength.

In addition to the shape we vary the size and density of scatterers and study the effect on magnetoresistance at low temperatures.

HL 79.29 Thu 15:00 P2-OG3

Electron flow focusing with magnetic barriers in 2DEG — •Jan Steimann, Mihai Cerchez, and Thomas Heinzel — Heinrich Heine University Düsseldorf, Universitätsstr. 1, D-40225 Düsseldorf

Electrons in a 2DEG are forced to travel from source to drain through two parallel openings in a transversal potential wall, produced by local anodic oxidation. A magnetic barrier is positioned at the openings to control the electron flow. The magnetic barrier height can be tuned such that a number of electrons coming through one opening can be focused onto the second opening, leading to magnetoresistance fluctuations. Experimental results and simulations will be presented.

HL 79.30 Thu 15:00 P2-OG3

Electrical Measurements of Single As-Grown Semiconductor Core-Shell Nanowires — •Danial Bahrami[1], Jovana Colvin[2], Hanno Küpers[3], Rainer Timm[2], Lutz Geelhaar[3], and Ullrich Pietsch[1] — [1]University of Siegen, Solid State Physics department , Siegen, Germany — [2]Lund University, NanoLund and division of Synchrotron Radiation Research, Lund, Sweden — [3]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

Characterizing and controlling the electrical properties of core-shell nanowire (NW) heterostructures is fundamental for their implementation into device applications including photonics, sensors, and electronics. For typical conductivity studies, the NW, after removal from the original substrate, is deposited horizontally and contacted with electrodes in as-called field-effect transistor geometry. Here, we report on electrical measurements at single NWs in their as-grown geometry on the substrate by means of FIB/SEM and AFM systems. Using either a tungsten nano-manipulator probe installed inside the FIB/SEM chamber or a sharp metallic tip of a conductive AFM, the I-V curves and current maps along the side-wall and on the top of selected GaAs/InGaAs core-shell NWs have been measured. Similar to previous studies [1, 2], significant differences between the I-V characteristics from individual NWs grown on the same substrate are observed, confirming the necessity of thorough characterization at the single-NW level. The electrical characteristics of NWs can be correlated to their structural properties.

[1] R.Timm et al. Nano Lett. 2013, 13, 5182 -5189. [2] G.Bussone et al. Nano Lett. 2015, 15, 981-989.

HL 79.31 Thu 15:00 P2-OG3

Experimental study of Memory effects in Lorentz Gases — •Matthias Hund[1], Jakob Schluck[1], Thomas Heinzel[1], Klaus Pierz[2], and Hans W. Schumacher[2] — [1]Heinrich-Heine Universität — [2]PTB Braunschweig

The classical Lorentz model is a fundamental class of systems to study transport properties in disordered media. It consists of non-interacting point particles that move through randomly placed static scatterers with short range forces. For such systems, extensive predictions exist for the low density regime, while studies related to large scatterer densities are rare. Resistivity contributions due to scattering correlations are called memory effects. They are expected to modify in particular the magnetoresistivity. Here, we report magnetotransport measurements of Lorentz gases defined with various scatterer densities in high electron mobility $GaAs/Ga_xAl_{1-x}As$ and show that the systems have a characteristic magnetoresistivity which can be attributed to different types of memory contributions.

HL 80: Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - VII

Time: Thursday 16:00–18:30 Location: GER 38

Invited Talk HL 80.1 Thu 16:00 GER 38

Spectacular success of DFT in predicting novel topological phases — •Arun Bansil — Northeastern Univ, Boston USA

The revolutionary discovery of topological insulators has turned out to be the proverbial tip of the much larger iceberg of exotic phases of quantum matter driven by spin-orbit coupling effects. The consideration of electronic states protected by time-reversal, crystalline and particle-hole symmetries has led to the prediction of many novel materials that can support Weyl, Dirac and Majorana fermions, and to new types of topological crystalline and Kondo insulators, and quantum spin Hall insulators with large band gaps. The first-principles DFT-based band theory paradigm has been a key player not only in this discovery process but also in identifying salient characteristics of topological states, enabling direct and sharpened confrontation between theory and experiment. [1] I will discuss our recent theoretical work aimed at predicting topological materials and identify cases where the materials have been realized successfully. [2-10] I will also comment on the potential of topological materials as next generation platforms for manipulating spin and charge transport and other applications.

[1] Bansil, Lin and Das, Rev. Mod. Phys. 88, 021004 (2016). [2] Chang et al, Sci. Adv. 2, e1600295 (2016). [3] Huang et al., PNAS 113, 1180 (2016). [4] Zheng et al., ACS Nano 10, 1378 (2016). [5] Xu et al., Science 349, 613 (2015). [6] Zeljkovic et al., Nat. Mat. 14, 318 (2015). [7] He et al., Nat. Mat. 14, 577 (2015). [8] Xu et al., Nat. Phys. 11, 748 (2015). [9] Crisostomo et al., Nano Lett. 15, 6568 (2015). [10] Xu et al., Sci. Adv. 1, e1501092 (2015).

HL 80.2 Thu 16:30 GER 38

Interlayer excitons and Band Alignment in MoS_2/hBN/WSe_2 van der Waals Heterostructures — •Simone Latini — Technical University of Denmark, Copenhagen, Denmark

Van der Waals Heterostructures (vdWHs) are a unique platform for the realization of novel (opto)-electronic devices with embedded multifunctionality. Combining two-dimensional (2D) semiconductors with misaligned band edges can lead to the formation of photo-excited electrons and holes localized in distinct layers, which result into interlayer excitons. Understanding the energetics behind the formation of interlayer excitons is the first step towards the engineering of charge separation processes in photovoltaic devices and photodetectors. The contribution of our work is then twofold. (I) We calculate, for the first time, the interlayer exciton binding energies in complex vdWHs, specifically MoS_2/hBN/WSe_2 heterostructures, using a first-principles approach. The binding energy is of extreme technological importance as it is a measure of how strongly the electron-hole pair is bound and hence how easily it can be separated. (II) We obtain accurate electronic band edges at the interface between the layers of the vdWHs, a task which could not yet be accomplished with any available state of the art technique. Importantly, the accuracy of our calculated exciton binding energies and band edges is confirmed by a striking agreement with experimental data on photoluminesce of interlayer excitons in MoS_2/hBN/WSe_2 heterostructures.

HL 80.3 Thu 16:45 GER 38

Trionic effects in graphene nanoribbons and further nanomaterials — •Thorsten Deilmann and Kristian Sommer Thygesen — Center for Atomic-Scale Materials Design (CAMD), Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

Among low-dimensional materials armchair-edged graphene nanoribbons are very promising candidates with optical properties which are dominates by excitons. In the presence of additional charges, trions (i.e. charged excitons) can occur in the optical spectrum. With our recently developed first-principle many-body approach [1], we predict strongly bound trions in nanoribbons with decreasing binding energies of 660 to 140 meV for widths of 3.6 to 14.6 Å. We determine their optical spectra and identify several trions by their real-space wave functions.

[1] Phys. Rev. Lett. **116**, 196084.

HL 80.4 Thu 17:00 GER 38

Interface Structure Prediction using the Ab Initio Random Structure Searching Method — •Georg Schusteritsch and Chris Pickard — Department of Materials Science and Metallurgy, University of Cambridge, 27 Charles Babbage Road, Cambridge CB3 0FS, U.K.

First-principles structure prediction of bulk materials is now routinely performed, however the field of predicting the atomic structure of interfaces is still in its infancy. A detailed understanding of and ability to predict the atomic structure of interfaces is however of crucial importance for many technologies. Interfaces are very hard to predict due to the complicated geometries, crystal orientations and possible non-stoichiometric conditions involved and provide a major challenge to structure prediction. We present here the ab initio random structure searching (AIRSS) method and how it can be used to predict the structure of interfaces. Our method relies on generating random structures in the vicinity of the interface and relaxing them within the framework of density functional theory. The method is simple, requiring only a small set of parameters, and can be efficiently run on modern parallel computer architectures. We focus here on the prediction of grain boundaries, but application to heterostructure interfaces is straightforward. Examples for several grain boundary defects in technologically important materials will be presented: In particular grain boundaries in graphene, the prototypical two-dimensional material will be discussed, alongside with examples of grain boundaries in transition metal oxides, such as SrTiO3 and TiO2.

HL 80.5 Thu 17:15 GER 38

Predicting new materials and their properties with supercomputers: the example of perovskites — •Silvana Botti[1] and Miguel A.L. Marques[2] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller Universität Jena, Max-Wien-Platz 1, 07743 Jena — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

Can new materials with optimized properties be designed using supercomputers?

I will try to convince you through the example of the search of new perovskites that first-principles calculations can efficiently speed up the discovery of new materials.

Theoretical approaches based and going beyond density functional theory ally today accuracy and efficiency, and are therefore suitable tools for understanding the physics not only of simple perfect crystals, but also of nanostructured materials, doped semiconductors, interfaces, alloys, etc. As a result, ab initio simulations of spectroscopic properties can finally account for the complexity of "real" experimental samples, allowing accurate comparison of calculated and measured structural and excitation properties. The powerful combination of theoretical spectroscopy with high-throughput calculations, structural prediction and machine learning can therefore provide a precious guide to experimentalists in the search of new materials.

HL 80.6 Thu 17:30 GER 38

Spectral property prediction with artificial neural networks — •Annika Stuke[1], Milica Todorovic[1], Kunal Ghosh[2], Aki Vehtari[2], and Patrick Rinke[1] — [1]Department of Applied Physics, Aalto University, Finland — [2]Helsinki Institute of Information Technology, Department of Computer Science, Aalto University, Finland

The ability to efficiently design new and advanced optoelectronic materials is hampered by the lack of suitable methods to rapidly and accurately identify yet-to-be-synthesized materials that meet a desired application. To overcome such design challenges, a machine learning model based on a deep multi-task artificial neural network (ANN) is presented that can predict spectral properties of small organic molecules. The ANN is trained and validated on data generated by accurate state-of-the art quantum chemistry computations for diverse subsets of the GDB-13 and GDB-17 datasets [1,2]. The molecules are represented by a simple, easily attainable numerical description based on nuclear charges and cartesian coordinates and are mapped onto multiple excited-state properties simultaneously using a deep ANN trained by gradient descent and error backpropagation [3]. This on-demand prediction model can be used to infer spectral properties of various candidate molecules in an early screening stage for new optoelectronic materials at negligible computational cost, thereby completely bypassing conventional laborious approaches towards ma-

terials discovery.

[1] L. C. Blum et al., J. Am. Chem. Soc. 2009, 131, 8732, [2] R. Ramakrishnan et al., Scientific Data 2014, 1, 140022, [3] G. Montavon et al., New J. Phys. 2013, 15, 095003

HL 80.7 Thu 17:45 GER 38

Machine-Learning Based Interatomic Potential for Amorphous Carbon — •Volker Deringer and Gábor Csányi — University of Cambridge, Cambridge, UK

Machine-learning based interatomic potentials are currently of growing interest in the solid-state theory communities, as they enable materials simulations with close-to DFT accuracy but at much lower computational cost. Here, we present such an interatomic Gaussian approximation potential (GAP) model for liquid and amorphous carbon. We first discuss the maximum accuracy that any finite-range potential can achieve in carbon structures; then, we show how a hierarchical set of two-, three-, and many-body structural descriptors can be used to fit a GAP that indeed reaches the target accuracy. The new potential yields accurate energetic and structural properties over a wide range of densities; it also correctly captures the structure of the liquid phases, at variance with state-of-the-art empirical potentials. Exemplary applications to surfaces of "diamond-like" tetrahedral amorphous carbon (ta-C) will be presented, including simulations of high-temperature surface reconstructions ("graphitization"). The method appears to be promising for realistic and accurate simulations of nanoscale amorphous carbon structures.

HL 80.8 Thu 18:00 GER 38

High-throughput computational search for new high mobility transparent (semi)conducting materials — •Geoffroy Hautier[1], Joel Varley[2], Anna Miglio[1], David Waroquiers[1], Viet-Anh Ha[1], and Gian-Marco Rignanese[1] — [1]Université catholique de Louvain, Louvain-la-Neuve, Belgium — [2]Lawrence Livermore National Laboratory

Transparent conducting oxides (TCMs) are large band gap materials (to favor transparency) doped with electrons (n-type) or holes (p-type). TCMs are essential to many technologies from solar cell to transparent electronics and there is currently a large effort towards the discovery of new TCMs. I will present the results of a high-throughput computational search for new TCMs especially directed at p-type materials. Focusing on low effective masses (leading to high mobility), large band gaps and dopability, I will show how thousands of compounds can be screened using various ab initio techniques (from density functional theory to GW) to find new potential high performance TCMs. I will discuss several unsuspected compounds with promising electronic structures and when available link our findings to experimental results. Beyond the description of those novel TCM candidates, I will chemically rationalize our findings, highlighting several design strategies towards the development of future high mobility TCMs.

HL 80.9 Thu 18:15 GER 38

Cross-validation in the cluster expansion method — •Axel Hübner, Santiago Rigamonti, and Claudia Draxl — Humboldt-Universität zu Berlin

The cluster expansion technique allows the construction of model Hamiltonians for an efficient evaluation of the total energy of alloys. This technique relies on a fit to a small set of *ab-initio* calculations for selected atomic configurations. Key aspects to maximize the predictive performance of the model are the selection of a set of basis functions, i.e. clusters, and of configurations. To achieve this, the cross-validation technique is typically used [1]. In this work, an analytical formula for the calculation of the leave-many-out cross-validation score (CV) is derived. This formula exhibits numerical instabilities, whose analytical properties yield a criterion for structure selection in cluster expansions. Moreover, a relation between the noise in the data and the CV is outlined. This leads to a tool which allows us to estimate, for a given noise level, the size of the ab-initio data set upon which no improvements of the model are obtained. These results are exemplified for a cluster expansion of the thermoelectric clathrate alloy $Ba_8Al_xSi_{46-x}$, calculated with the `CELL` package [2].

[1] A. van d. Walle *et al.*, Journal of Phase Equilibria 23 (2002), Aug., Nr. 4

[2] M. Troppenz *et al.*, submitted (2016); S. Rigamonti *et al.*, in preparation.

HL 81: Transport: Spintronics, Spincalorics and Magnetotransport (jointly with DS, HL, MA)

Time: Friday 9:30–11:30 Location: HSZ 03

HL 81.1 Fri 9:30 HSZ 03

Search for magneto-hydrodynamics in the delafossite metals $PdCoO_2$ and $PtCoO_2$ — •Nabhanila Nandi[1], Pallavi Kushwaha[1], Seunghyun Khim[1], Philip J.W. Moll[1], Burkhard Schmidt[1], Thomas Scaffidi[2], Markus König[1], and Andrew P. Mackenzie[1,3] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany — [2]Department of Physics, University of California, Berkeley, California 94720, USA — [3]Scottish Universities Physics Alliance, School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, United Kingdom

Electrical resistance is conventionally determined by the momentum-relaxing scattering of electrons by the host solid and its excitations. Hydrodynamic fluid flow through channels, in contrast, is determined by geometrical factors, boundary scattering and the viscosity of the fluid, which is governed by momentum-conserving internal collisions. In almost all known materials, however, the signatures of viscosity in electron flow cannot be resolved, because the rate of momentum-relaxing collisions dominates that of the momentum-conserving ones that give the viscous term. In previously published work, we reported experimental evidence that there is a regime in restricted channels of the ultra-pure two-dimensional delafossite metal $PdCoO_2$ in which the resistance has a large viscous contribution. In this talk I will report on our current work in which we extend our experiments to magneto-hydrodynamics, discussing data both from $PdCoO_2$ and a second delafossite metal, $PtCoO_2$.

HL 81.2 Fri 9:45 HSZ 03

Fe_3O_4 thin films: controlling and manipulating an elusive quantum material — •xionghua liu, chun-fu chang, aurora diana rata, alexander christoph komarek, and liu hao tjeng — Max Planck Institute for Chemical Physics of Solids, Nöthnitzerstr. 40, 01187 Dresden, Germany

Fe_3O_4 (magnetite) is one of the most elusive quantum materials and at the same time one of the most studied transition metal oxide materials for thin film applications. The theoretically expected half-metallic behavior generates high expectations that it can be used in spintronic devices. Yet, despite the tremendous amount of work devoted to preparing thin films, the enigmatic first order metal-insulator transition and the hall mark of magnetite known as the Verwey transition, is in thin films extremely broad and occurs at substantially lower temperatures as compared to that in high quality bulk single crystals.

In this work, we investigate systematically the effect of oxygen stoichiometry, thickness, strain, and microstructure on the Verwey transition in epitaxial Fe_3O_4 thin films on a variety of substrates. We have been able to determine the factors that affect negatively the Verwey transition in thin films. We have succeeded in finding and making a particular class of substrates that allows the growth of magnetite thin films with the Verwey transition as sharp as in the bulk. Moreover, we are now able to tune the transition temperature and, using tensile strain, increase it to substantially higher values than in the bulk.

HL 81.3 Fri 10:00 HSZ 03

Spin-switching via quantum dot spin valves — •Niklas M. Gergs[1], Scott A. Bender[1], Rembert A. Duine[1,2], and Dirk Schuricht[1] — [1]Institute for Theoretical Physics, Utrecht University, Utrecht, The Netherlands — [2]Department of Applied Physics, Eindhoven University of Technology, Eindhoven, The Netherlands

We theoretically investigate a spin-valve transistor setup, ie, correlated transport through a quantum dot positioned between two spin-polarised nano magnets. This causes the dynamical generation of a magnetic field on the dot even in the absence of external fields [1].

Here we consider the back action of the quantum dot onto the attached nano magnets via exerted spin torques. This may be used to

switch the nano magnets reliably from a parallel to an anti-parallel alignment and vice versa. All operations are done in the Coulomb-blockade regime of the quantum dot, so that the charge transport through the setup is strongly suppressed.

[1] M. Braun, J. König, J. Martinek, Phys. Rev. B 70, 195345 (2004)

HL 81.4 Fri 10:15 HSZ 03

Strong non-equilibrium effects in spin torque systems — •Tim Ludwig[1], Igor S. Burmistrov[2,3], Yuval Gefen[4], and Alexander Shnirman[1] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany — [2]L.D. Landau Institute for Theoretical Physics RAS, Kosygina street 2, 119334 Moscow, Russia — [3]Laboratory for Condensed Matter Physics, National Research University Higher School of Economics, 101000 Moscow, Russia — [4]Department of Condensed Matter Physics, Weizmann Institute of Science, 76100 Rehovot, Israel

We consider a problem of persistent magnetization precession in a single domain ferromagnetic nano particle under the driving by the spin-transfer torque [1]. We find that the adjustment of the electronic distribution function in the particle renders this state unstable. Instead, abrupt switching of the spin orientation is predicted upon increase of the spin-transfer torque current. On the technical level, we derive an effective action of the type of Ambegaokar-Eckern-Schön action for the coupled dynamics of magnetization (gauge group SU(2)) and voltage (gauge group U(1)).

[1] T. Ludwig, I. S. Burmistrov, Y. Gefen, and A. Shnirman, arXiv:1610.09944 (2016)

HL 81.5 Fri 10:30 HSZ 03

Spin-charge coupled dynamics driven by a time-dependent magnetization — •Sebastian Tölle[1], Ulrich Eckern[1], and Cosimo Gorini[2] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Faculty of Physics, University of Regensburg, 93040 Regensburg, Germany

The spin-charge coupled dynamics in a thin, magnetized metallic system are investigated. The effective driving force acting on the charge carriers is generated by a dynamical magnetic texture, which can be induced, e.g., by a magnetic material in contact with a normal-metal system. We consider a general inversion-asymmetric substrate/normal-metal/magnet structure, which, by specifying the precise nature of each layer, can mimick various experimentally employed setups. Inversion symmetry breaking gives rise to an effective Rashba spin-orbit interaction. We derive general spin-charge kinetic equations which show that such spin-orbit interaction, together with anisotropic Elliott-Yafet spin relaxation, yields significant corrections to the magnetization-induced dynamics. To highlight their physical meaning, the spin pumping configuration of typical experimental setups is analyzed in detail. In the two-dimensional limit the build-up of a DC voltage is dominated by the spin galvanic (inverse Edelstein) effect. A measuring scheme that could isolate this contribution is discussed.

HL 81.6 Fri 10:45 HSZ 03

Emergent magnetic ordering in transition metal atomic contacts — •Martin Keller, Florian Strigl, Elke Scheer und Torsten Pietsch — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

MD simulations and DFT calculations predict the development of local magnetic order at reduced dimensions in some paramagnetic transition metals (Pt, Pd, Ir), especially in atomic configurations [1,2,3]. This unusual property allows us to investigate the influence of the local magnetic properties on the conductance of atomic contacts without the effect of magnetic leads. Therefore atomic contacts of these metals are a model system to understand the origin of magnetoconductance and the role of spin-polarization of the conduction electrons. Herein we discuss recent results of Pt, Pd and Ir in the context of a microscopic model that successfully describes the observed magnetoconductance signature in these atomic contacts and chains [4]. Additionally, electronic transport spectroscopy is used to evaluate magnetic excitations in the electronic system of the contact, i.e. the presence of i) a zero-bias anomaly which is described by Kondo physics and ii) conductance fluctuations in the atomic contact, which indicate the formation of a magnetically ordered state. We will compare the three transition metals with respect to their different electronic structure and the role of spin-orbit coupling in the contacts.

[1] Phys. Rev. Lett. 92, 057201 (2004)
[2] Phys. Rev. B 78, 014423 (2008)
[3] Phys. Rev. B 81, 054433 (2010)
[4] Nature Comm. 6, 6172 (2015); Phys. Rev. B 94, 144431 (2016)

HL 81.7 Fri 11:00 HSZ 03

Electron transport through the helical systems: chiral magnetoresistance effect — •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, the chirality-induced spin selectivity (CISS) effect [1] has been discovered in which electron transport through systems with helical symmetry shows the different transmission for the electrons with different spin-polarizations. In this work, we show that CISS can be utilized in the new class of magnetic field sensors via novel chiral magnetoresistance effect (CMR) [2]. We present a theoretical investigation of the electron transport through the poly-GLY in helical form placed between one magnetic and one nonmagnetic leads by using the DFT and NEGF approach. We obtain that MR of the order 2

[1] Göhler B., Hamelbeck V., Markus T. Z., Kettner M., Hanne G. F., Vager Z., Naaman R., and Zacharias H., Science 331, 894 (2011)
[2] Kiran V., Mathew S.P., Cohen S.R., Delgado I.H., Lacour J., Naaman R., Adv. Mater. 28, 1957 (2016)

HL 81.8 Fri 11:15 HSZ 03

A Landauer-Büttiker approach for hyperfine mediated electronic transport in the integer quantum Hall regime — •Aniket Singha[1], M. Hamzah Fauzi[2], Yoshiro Hirayama[2], and Bhaskaran Muralidharan[1] — [1]Department of Electrical Engineering, IIT Bombay, Powai, Mumbai-400076, India — [2]Graduate School of Science, Tohoku University, Aoba-ku, Sendai-980-8578, Japan

The interplay of spin-polarized electronic edge states with the dynamics of host nuclei in quantum Hall systems presents rich and non-trivial transport physics. Here, we develop a Landauer-Büttiker approach to understand various experimental features observed in integer quantum Hall set ups featuring quantum point contacts. Such approach entails a phenomenological description of spin resolved inter-edge scattering induced via hyperfine assisted electron-nuclear spin flip-flop processes along with a self consistent simulation framework between the nuclear spin dynamics and edge state electronic transport in order to gain insights into the nuclear polarization effects on electronic transport vice-versa. In particular, we show that the hysteresis noted experimentally in the conductance-voltage trace as well as in the resistively detected NMR lineshape results from a lack of quasi-equilibrium between electronic transport and nuclear polarization evolution. In addition, we present circuit models to further facilitate a clear understanding of the electronic transport processes occurring near the quantum point contact.

HL 82: Quantum Information Systems

Time: Friday 9:30–11:15 Location: POT 81

HL 82.1 Fri 9:30 POT 81

Resonant driving of silicon vacancies in 4H-SiC — •Matthias Widmann[1], Roland Nagy[1], Matthias Niethammer[1], Ilja Gerhardt[1,2], Ivan G. Ivanov[3], Sophia Economou[4], Takeshi Oshima[5], Nguyen Tien-Son[3], Cristian Bonato[6], Sang-Yun Lee[7], Erik Janzén[3], and Jörg Wrachtrup[1,2] — [1]3rd Institute of Physics, IQST and Research Center SCOPE, Stuttgart — [2]Max-Planck Institute, Stuttgart — [3]Department of Physics, Chemistry and Biology, Linkoeping University — [4]Department of Physics, Virginia Tech, Blacksburg — [5]National Institutes for Quantum and Radiological Science and Technology (QST), Takasaki — [6]Institute of Photonics and Quantum Science, Heriot-Watt University — [7]Center for Quantum Information, Korea Institute of Science and Technology (KIST), Seoul

Spins associated to atomic scale defects in solids are attractive as sensitive probes and are promising candidates for quantum information processing (QIP) [1]. Our research is based on spin defects in silicon carbide (SiC), a technologically-relevant wide-bandgap semiconductor which offers spin-active defects with long coherence times at room temperature [2]. In this work, we extend our previous single spin study [2] by investigating optical and spin properties of the silicon vacancy in 4H-SiC via resonant optical and spin driving and discuss their potential use for quantum computing and quantum communication [3].

[1] F. Jelezko et al, PRL 100, (2012).
[2] M. Widmann et al, Nat. Mater 14 (2015).
[3] Ö. Soykal et al, PRB 93 (2016).

HL 82.2 Fri 9:45 POT 81

Cavity mediated entanglement generation between the electron spins of two NV$^-$ centers — •Vladislav Shkolnikov[1], Guido Burkard[1], and David Awschalom[2] — [1]Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — [2]Institute for Molecular Engineering, University of Chicago, Chicago, IL 60637, USA

While long spin coherence times and efficient single-qubit quantum control have been implemented successfully in negatively charged nitrogen-vacancy (NV) centers in diamond, the controlled coupling of remote NV spin qubits remains challenging. Here, we propose and analyze a controlled-phase (CPHASE) gate for the spins of two NV-centers embedded in a common optical cavity and driven by two off-resonant lasers. The excitation of the first NV, generated by the laser, can later be emited into the cavity and then reabsorbed by the second NV. The excited states in this process are only virtually occupied and it allows to generate entangling gate between the NV-centers, that is not limited by the excited state lifetime. We derive an analytical model for the case when spin-spin interaction in the excited state can be neglected and perform a numerical simulation taking it into account. We predict entangling gates with the operation time 500 ns, which is much smaller than spin coherence time in the NVs. In combination with previously demonstrated single-qubit gates, CPHASE allows for arbitrary quantum computations.

HL 82.3 Fri 10:00 POT 81

High-resolution NMR spectroscopy on small spin ensembles using a hybrid spin sensor — •Matthias Pfender[1], Nabeel Aslam[1], Philipp Neumann[1], Hitoshi Sumiya[4], Shinobu Onoda[5], Carlos A. Meriles[3], Junichi Isoya[2], and Jörg Wrachtrup[1] — [1]3. Physikalisches Institut, Universität Stuttgart — [2]Research Center for Knowledge Communities, University of Tsukuba — [3]Department of Physics, CUNYCity College of New York — [4]Sumitomo Electric Industries Ltd., Itami, Japan — [5]Takasaki Advanced Radiation Research Institute, Takasaki, Japan

In the last few years, the nitrogen-vacancy defect in diamond has emerged as an exceptional quantum sensor for magnetic and electric fields, capable of detecting proton spins outside the diamond. However, the performance of the NV electron spin alone limits the achievable resolution of an NV NMR spectroscopy experiment to about 200 Hz [2,3]. By using the NV's inherent nitrogen nuclear spin we form a robust hybrid quantum sensor, capable of performing NMR spectroscopy on nanometer sized samples. The hereby obtained spectra are not limited by the electron spin lifetimes, but rather by the sample spins. We perform NMR spectroscopy on spins inside and outside the diamond, reaching a frequency resolution of 10 Hz and 100 Hz, respectively, enough to extract structural information of the molecule.

[1] Staudacher, T. et al. Science 339, 561-563 (2013).
[2] Kong, X., Stark, A., Du, J., McGuinness, L. P. & Jelezko, F. Phys. Rev. Applied 4, 24004 (2015).
[3] Zaiser, S. et al. Nat Commun 7, 12279 (2016).

Coffee Break

HL 82.4 Fri 10:30 POT 81

Defect Engineering in Silicon Carbide — •Christian Kasper[1], Hannes Kraus[1,2], Dimitrij Simin[1], Yoshinori Suda[3], Takeshi Ohshima[2], Wataru Kada[3], Shunsuke Kawabata[3], Tomoya Honda[2,4], Yasuto Hijikata[4], Georgy Astakhov[1], and Vladimir Dyakonov[1,5] — [1]Exp. Physics VI, Julius Maximilian University of Würzburg — [2]National Institutes for Radiological Science and Technology(QST, formerly Japan Atomic Energy Agency), Takasaki, Japan — [3]Gunma University, Kiryu, Japan — [4]Saitama University, Saitama, Japan — [5]ZAE Bayern, Würzburg

Because of their long spin lifetime[1] and their unique spin-preserving optical pumping mechanism[2], quantum centers in silicon carbide (SiC) are promising candidates for spin based quantum information processing. Well known methods to produce one of these quantum center species, the silicon vacancy, homogeneously in the bulk are electron or neutron[3] irradiation. In contrast, a method to implant silicon vacancies at a specific position would be a huge improvement in terms of defect engineering.

In this study, the generation of silicon vacancies in bulk SiC as a result of proton irradiation can be verified. By the use of confocal microscopy, we show that the implantation depth is tunable by varying the irradiation energy. Further, we verify that by proton beam writing silicon vacancies can be implanted at a specific position in a SiC crystal.

[1] Simin et al., arXiv:1602.05775v2 (2016)
[2] H. Kraus et al., Nature Phys. **10**, 157 (2014)
[3] F. Fuchs et al., Nature Commun. **6**, 7578 (2015)

HL 82.5 Fri 10:45 POT 81

Three-spin qubits under the influence of tunneling noise — •Maximilian Russ and Guido Burkard — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

We investigate the behavior of qubits consisting of three electron spins in double and triple quantum dots subject to external electric fields[1]. Our model includes two independent bias parameters, ε and ε_M, and two independent tunnel couplings, t_l and t_r, which all couple to external electromagnetic fields and can be controlled in experiments by gate voltages applied to the quantum dot structures. By varying the detuning parameters one can switch the qubit type by shifting the energies in the single quantum dots thus changing the electron occupancy in each dot resulting in different qubit encodings. We focus on random electromagnetic field fluctuations, i.e., "charge noise", at each gate resulting in dephasing of the qubit. We pay special attention to charge noise with respect to the tunnel couplings due to recent interest in symmetric gate operations where the tunnel barrier is controlled. We search for sweet spots and double sweet spots, working points which are least susceptible to noise and compare the results to detuning noise. As a result, we show the absence of non-trivial double sweet spots in the case for tunneling noise.

[1] M. Russ, F. Ginzel, and G. Burkard, Phys. Rev. B 94, 165411 (2016)

HL 82.6 Fri 11:00 POT 81

3-axis magnetometer utilizing silicon vacancy defect spins in 4H silicon carbide — •Matthias Niethammer[1], Matthias Widmann[1], Sang-Yun Lee[1,4], Pontus Stenberg[2], Olof Kordina[2], Takeshi Ohshima[3], Nguyen Tien-Son[2], Erik Janzén[2], and Jöerg Wrachtrup[1] — [1]3rd Institute of Physics, University of Stuttgart, IQST and Research Center SCoPE — [2]Department of Physics, Chemistry and Biology, Linköping University — [3]National Institutes for Quantum and Radiological Science and Technology, Takasaki — [4]Korea Institute of Science and Technology, Seoul

Due to their inherent nature spins are very sensitive to magnetic fields.

The Zeeman effect can thus be used to sense magnetic fields. Solid state systems as silicon carbide (SiC) can host defects with high spin states, which can be optically detected such as the silicon vacancy (V_{Si}) in 4H-SiC down to the single level at room temperature [1]. In our previous work we showed that the C_{3V} symmetry of this system together with the spin state of $S=\frac{3}{2}$ allows extraction of the magnetic field strength and polar angle [2,3]. Here we demonstrate that an analytical solution in combination with pulsed spin manipulation techniques can be used to measure the complete magnetic field vector even in a large dynamic range [4]. Combined with electrical readout such approaches can lead to highly sensitive and integrated quantum vector magnetometers [5].

1. Widmann et al, Nat. Mater 14(2), 164-168 (2014) 2. Simin et al, Phys Rev Appl 4(1), 014009 (2015) 3. Lee et al, Phys Rev B 92(11), 115201 (2015) 4. Niethammer et al, Phys Rev Appl 6(3), 034001 (2016) 5. Cochrane et al, Sci. Rep. 6, 37077 (2016)

HL 83: Oxide Semiconductors (joined session with CPP, DS)

Time: Friday 9:30–12:45 Location: POT 51

Invited Talk HL 83.1 Fri 9:30 POT 51

New Frontiers in Quantum Matter Heterostructures — •Jochen Mannhart — Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

Combining the power and possibilities of heterostructure engineering with the collective and emergent properties of quantum materials, quantum-matter heterostructures [1] open a new arena of solid-state physics. Here we provide a review of interfaces and heterostructures made of quantum matter. As we will show, unique electronic states can be engineered in these structures, giving rise to unforeseeable opportunities for scientific discovery and potential applications.

[1] Quantum-Matter Heterostructures, H. Boschker and J. Mannhart, Annual Reviews of Condensed Matter Physics, 8, April 2017.

HL 83.2 Fri 10:00 POT 51

Self-consistent hybrid functional calculations: Electronic and optical properties of oxide semiconductors — •Daniel Fritsch[1], Benjamin Morgan[1], and Aron Walsh[1,2] — [1]Department of Chemistry, University of Bath, BA2 7AY Bath, UK — [2]Department of Materials, Imperial College London, SW7 2AZ London, UK

Owing to limitations of existing approximate exchange-correlation functionals, band gaps of semiconductors and insulators are often severely underestimated in density functional theory calculations. 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.

A recent self-consistent hybrid functional [1] removes this empiricism and offers a new approach for parameter-free hybrid functional investigations. Moreover, it provides a better starting point for many-body perturbation calculations based on the *GW* approximation. Applying this approach to a range of oxide semiconductors, we report on the electronic and optical properties, and compare them to other theoretical and experimental data.

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

HL 83.3 Fri 10:15 POT 51

Influence of temperature on the creation of Rydberg excitons — •Peter Grünwald[1], Julian Heckötter[2], Marc Assmann[2], Dietmar Fröhlich[2], Manfred Bayer[2], Heinrich Stolz[1], and Stefan Scheel[1] — [1]Institut für Physik, Universität Rostock, Rostock, Germany — [2]Experimentelle Physik 2, TU Dortmund, Dortmund, Germany

Solid-state systems are heavily influenced by temperature, changing the crystal structure and thus shifting the energy bands [1,2]. Excitons in semiconductors additionally experience collision ionization, and a decrease of the band edge due to plasma interaction [3]. However, in most semiconductor systems, measuring these effects is difficult because of the limited number of exciton states available. This is different for Rydberg excitons [4], where states up to $n \gtrapprox 20$ can easily be generated. Hence, these states can be used to analyze the temperature influence on the excited states and the excitation limit set by finite temperature.

[1] T. Itoh and S. Narita, J. Phys. Soc. Japan **39**, 140 (1975).
[2] P. B. Allen and M. Cardona, Phys. Rev. B **23**, 1495 (1980).
[3] D. Semkat *et al.*, Phys. Rev. B **80**, 155201 (2009).
[4] T. Kazimierczuk *et al.*, Nature **514**, 343 (2014).

HL 83.4 Fri 10:30 POT 51

Excitonic Giant-Dipole Potentials in Cuprous Oxide — •Markus Kurz and Stefan Scheel — AG Quantenoptik makroskopischer Systeme, Institut für Physik, Universität Rostock

Wannier excitons are of great physical interest since they represent the fundamental optical excitation in semiconductors. Recently, the discovery of highly excited Rydberg excitons in Cuprous Oxide (Cu_2O) and their exposure to external fields have shown a plethora of complex physical phenomena [1]. In atomic physics an exotic species of Rydberg atoms in crossed electric and magnetic fields, so-called giant-dipole atoms, have been predicted for two decades [2]. These exotic objects are characterized by an electron-ionic core separation in the range of several micrometers.

In this work, we expand this concept and predict the existence of excitonic giant-dipole states in Cu_2O. Performing a gauge-independent pseudoseparation of the center of mass motion we derive an effective single-particle description of the field-dressed excitonic system obtaining a spatial dependent electron-hole interaction potential. For specific field strengths and field orientations this potential exhibits an outer potential well providing bound excitonic states. Furthermore, we show that the giant-dipole interaction potential gives rise to Abelian and non-Abelian gauge fields acting on the relative motion of the two excitonic constituents.

[1]T. Kazimierczuk *et al.*, Nature (London) **514**, 343 (2014)
[2]O. Dippel, *et al.*, Phys. Rev. A **49**, 4415 (1994)

HL 83.5 Fri 10:45 POT 51

Excitons at $SrTiO_3$ and ZnO interfaces in ellipsometry spectra — •Stefan Zollner[1], C. Rodriguez[1], N. Samarasingha[1], J. Moya[1], N. Fernando[1], P. Ponath[2], K. Kormondy[2], A.A. Demkov[2], and S. Chattopadhyay[3] — [1]New Mexico State University, Las Cruces, NM, USA — [2]University of Texas, Austin, TX, USA — [3]Indian Institute of Technology, Indore, India

Excitonic features in optical spectra of semiconductors and insulators have been studied for many years. In an epitaxial layer on a substrate with a different band gap, the wave functions of electron and hole are strongly modified. In a type-I quantum well, consisting of a narrow-gap semiconductor grown on a large-gap substrate, both electron and hole are confined, which leads to an increase in the dipole overlap matrix element. Therefore, the dominant absorption peak at 4.2 eV is larger in a 20 nm thick $SrTiO_3$ layer on $LaAlO_3$ than in bulk $SrTiO_3$. (The band gap of $LaAlO_3$ is larger than that of $SrTiO_3$.) On the other hand, in a staggered type-II quantum well, either the electron is confined, or the hole, but not both. Therefore, the overlap dipole matrix element (and the excitonic absorption) is strongly reduced, because one quasiparticle resides in the quantum well and the other in the substrate. If a $SrTiO_3$ layer is grown on Si or Ge, the valence band maximum occurs in the substrate, while the conduction band offset is very small. Therefore, the exciton wave function is delocalized, which reduces the dipole overlap matrix element. The real and imaginary part of thin SrTiO3 layers on Si or Ge are much smaller than in the bulk and decrease monotonically with decreasing thickness.

Coffee Break

HL 83.6 Fri 11:30 POT 51

Tuning the refractive index of transparent conducting oxides via oxide/oxide periodic heterostructures — David Caffrey, Emma Norton, Cormac Ó Coileáin, Christopher M. Smith, Igor V. Shvets, and •Karsten Fleischer — School of Physics and CRANN, Trinity College Dublin, The University of Dublin, Ireland

Superlattice structures are a novel method of improving upon the op-

toelectronic properties of Transparent Conducting Oxide (TCO) structures. The invariability of the refractive index of TCO materials leads to reflection losses cells. The development of a transparent material or structure of tuneable refractive index at the interfaces of transparent devices such as solar would allow for the integration of anti-reflective coatings which would reduce such losses significantly, thus improving device efficiency. Previous attempts to modify the refractive index have been marred by the degradation of the electrical or optical properties of the tuned material. We demonstrate the novel use of a TCO/dielectric superlattice structure to achieve an effective medium of altered refractive index, while maintaining high values of transparency, conductivity and mobility. We demonstrate the efficacy of these superlattice structures on both amorphous $InGaZnO_4$ and ZnO:Al via TCO/SiO_2 and TCO/TiO_2 superlattices. The effective refractive indices of the films were successfully tuned over a range of $\Delta n \approx -0.2$ (SiO_2 inclusion) to $+0.4$ (TiO_2 inclusion) with a decrease in conductivity of less than an order of magnitude. Mobility of the films was also well conserved. We also discuss differences in the carrier injection from the TCO into the dielectric for the SiO_2 and TiO_2 case.

HL 83.7 Fri 11:45 POT 51

Hybrid functional calculations of oxygen mono- and di- vacancies in SrTiO3 — •Masud Alam, Liverios Lymperakis, and Jörg Neugebauer — Computational Material Design department, Max-Planck-Institut für Eisenforschung GmbH, Max-Planck Str. 1, 40237 Düsseldorf, Germany

Perovskite-type oxides ABO3 have attracted considerable interest for their large variety of technologically appealing characteristics such as ferroelectricity, magnetism, as well their dielectric properties. Among these materials, SrTiO3 (STO) serves as a representative model for the class of large bandgap perovskites. Nevertheless, the properties of this material are dominated by the presence of oxygen vacancies which act as n-type dopants. In the present work we investigate the energetics, atomic geometry and electronic structures of oxygen mono- and divacancies by employing Heyd, Scuseria, Ernzerhof (HSE) hybrid density functional calculations. Based on these calculations we identify the energy levels and the formation energies of aforementioned point defects as well as the binding energies of the point defect complexes. Our calculations reveal that interactions between single and doubly ionized defects as expected are strongly repulsive. Based on the aforementioned results we will further discuss in details the effect of oxygen vacancies as a function of growth conditions and doping level on the electronic properties of STO.

HL 83.8 Fri 12:00 POT 51

Low temperature absorption study of ferromagnetic EuO thin films — •Marcel Ney[1], Günther Prinz[1], Timm Gerber[2], Martina Müller[1,2], and Axel Lorke[1] — [1]Faculty of Physics and CENIDE, Universität Duisburg-Essen, D-47048 Duisburg — [2]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich GmbH, D-52428 Jülich

Europium Oxide is a ferromagnetic semiconductor with the Curie temperature of 69K. When it is used as a tunnel barrier, it can create up to 100% spin polarized electron currents, for use in spintronic research. This remarkable property raises the question, how the magnetic order at low temperatures affects the band structure of a thin EuO layer.

Thin EuO-layers were grown by molecular beam epitaxy on yttria-stabilized-zirconia-substrates, with different thicknesses. A fourier-transform-infrared spectrometer equipped with a liquid helium continuous-flow cryostat was used to measure the transmission through the EuO thin films.

Spectra measured for decreasing EuO thickness (30nm-3nm) show a shift of the absorption edge of EuO to higher energies due to an increasing quantum confinement along the growth direction. For low temperature measurements below the Curie temperature of EuO, we observed a red shift of the bandgap energy of about $E_a = (0.27 \pm 0.02)$eV. This energy shift is in good agreement with theoretical values and experimentally determined exchange splitting energies for thin europium-oxide layers, already published in the literature.

HL 83.9 Fri 12:15 POT 51

Ozone, oxygen and water interaction with In_2O_3(111) surfaces — •Theresa Berthold[1], Stefan Krischok[1], Marcel Himmerlich[1], Vladimir Polyakov[2], Volker Cimalla[2], Julius Rombach[3], and Oliver Bierwagen[3] — [1]Institut für Mikro- und Nanotechnologien MacroNano, Technische Universität Ilmenau — [2]Fraunhofer-Institut für Angewandte Festkörperphysik, Freiburg — [3]Paul-Drude-Institut für Festkörperelektronik, Berlin

In_2O_3 films are widely used in conductometric gas sensors based on their surface electron accumulation layer (SEAL) whose conductance is influenced by gas adsorption [1]. In this study the chemical composition and electronic surface properties of undoped and Mg-doped In_2O_3(111) films grown by plasma-assisted molecular beam epitaxy are analyzed by photoelectron spectroscopy. We analyze the formation or desorption (by UHV annealing or UV illumination) of adsorbates, the generation of defects as well as the variation in surface band bending, electron concentration, and surface dipole. Towards understanding the gas sensitivity under realistic conditions we study the effect of humidity on the sensor properties by experiments combining water interaction with ozone or oxygen surface oxidation. H_2O partially reverses the depletion/reduction of the SEAL after surface oxidation. Complete depletion of the SEAL is found after plasma oxidation [2]. The experimental results are combined with Schrödinger-Poisson calculations to establish a quantitative analysis of the electron density profile and the density of surface states. [1] J. Rombach et al., Sens. Actuators B, 236, 909 (2016) [2] T. Berthold et al., J. Appl. Phys. (submitted)

HL 83.10 Fri 12:30 POT 51

Gas sensing with sub-micrometer Pt/TiO_2 sensors — •Svenja Herbertz, Mihai Cerchez, and Thomas Heinzel — Solid State Physics Laboratory, Heinrich-Heine-Universität Düsseldorf

Pt/nanoporous TiO_2 hydrogen sensors with active sizes in the millimeter regime 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 this disordered system. The quest for miniaturization as well as for improved spatial resolution drives the search for sensors operational at the microscale. Here we present a sub-micrometer-sized lateral sensor for atmospheric hydrogen with planar geometry and full compatibility with Si processing technology. A titanium dioxide line of 200 nm width, written with the tip of an atomic force microscope, separates a thin Ti film on an insulating substrate into two metallically disconnected electrodes and forms the active area. It is sensitized by a sub-monolayer platinum sputtering step such that the two Ti electrodes remain disconnected. The device shows a large, selective sensitivity to hydrogen gas.

HL 84: Heterostructures and Interfaces

Time: Friday 9:30–12:45 Location: POT 151

HL 84.1 Fri 9:30 POT 151

Recombination dynamics of excitons in (Ga,In)As/Ga(As,Sb) type-II heterostructures — •Sebastian Gies, Benjamin Holz, Christian Fuchs, Wolfgang Stolz, and Wolfram Heimbrodt — Department of Physics and Materials Science Center, Philipps-Universität Marburg, Renthof 5, 35032 Marburg, Germany

(Ga,In)As/Ga(As,Sb) heterostructures are a material system widely used as an active medium in IR-lasers. It is necessary to have profound knowledge about the basic relaxation and recombination processes to improve this material. We present a thorough study of these properties by continuous-wave (cw-) and time-resolved (TR-) photoluminescence spectroscopy (PL) at various temperatures. Therefore, we investigate (Ga,In)As/GaAs/Ga(As,Sb) type-II structures with GaAs interlayers of different thicknesses to modify the type-II transition. Upon changing temperature a complex interplay of relaxation, tunneling and thermal reactivation is found, that changes the PL spectra drastically. Furthermore, the TRPL reveals, that the relaxation of holes has a tremendous influence on the transients of the type-II PL. A rate-equation model is developed to quantify the relaxation.

HL 84.2 Fri 9:45 POT 151

Investigation of the growth of the organic semiconductor F4-TCNQ on inorganic substrates — •Hannah Schamoni, Michael Haugeneder, Martin Hetzl, Oliver Bienek, and Martin Stutzmann — Walter Schottky Institut und Physik-Department, Technische Universität München, Deutschland

The combination of organic and inorganic semiconductors is one promising approach towards new materials for applications like solar cells and light emitting devices, as they open up the possibility to benefit from the advantages of both material types. In order to identify the most promising hybrid systems, a detailed understanding of the properties of the organic/inorganic interface is essential. In this work, we focus on the growth of the small-molecule organic semiconductor 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4-TCNQ) by organic molecular beam deposition on various inorganic substrates like Si, diamond, graphene on Si or GaN nanowire arrays. We are able to confirm a Stranski-Krastanov growth mode of the organic layer on most substrates by means of AFM, REM and XPS measurements. The size, shape and density of the molecular clusters depend on the inorganic material, which we attribute to the differences in binding energy between F4-TCNQ and the various substrates. Furthermore, our data reveal monotonic dependencies of the density of the F4-TCNQ clusters on the diameter of the GaN nanowires and the spacing in between the nanowires, respectively.

HL 84.3 Fri 10:00 POT 151

A band-offset study on NiO/SnO_2 heterojunctions using X-ray photoelectron spectroscopy (XPS) — •Fabian Michel, Benedikt Kramm, Martin Becker, Robert Hamann, Angelika Polity, Detlev M. Hofmann, and Martin Eickhoff — Justus-Liebig Universität, Gießen, Deutschland

The band discontinuities of NiO/SnO_2 pn-heterojunctions were evaluated by X-ray photoelectron spectroscopy. The heterojunctions were produced by ion beam sputtering. Using the common method of E.A. Kraut and J.R. Waldrop considering the position of the different core level signals and especially the related energy difference in the vicinity of the heterointerface the valence band and conduction band discontinuities of NiO/SnO_2 were investigated. For that the band gaps of the fabricated heterojunctions were determined via UV-VIS spectroscopy. A qualitative analysis of the interfacial chemical state by estimating the modified Auger parameter and the relative concentrations of the photoelectron signals using depth profiling via in situ Ar^+ ion etching was done. 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 such as NiO/ZnO, NiO/TiO and more.

HL 84.4 Fri 10:15 POT 151

$NiSi_2$-Si interfaces as building blocks for reconfigurable field-effect transistors: from the atomic structure to device characteristics — •Florian Fuchs[1,2,3], Jörg Schuster[2,4], and Sibylle Gemming[1,2,3] — [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 (ENAS), Chemnitz, Germany

The electron transport across metal-semiconductor interfaces is crucial for the functionality of reconfigurable field-effect transistors, which can be switched between electron and hole current. Devices were already fabricated experimentally, however, a profound understanding of the underlaying mechanism is not yet available.

This study focuses on the $NiSi_2$-Si interface, which is studied using the NEGF formalism. Based on the calculated transmission spectra, the transfer characteristic of a reconfigurable transistor is obtained using a simplified approach. Even though this model strongly simplifies the electrostatic environment in a transistor, very good agreement with experimental devices is demonstrated. The impact of strain on the device characteristic is studied as well. It is shown that the magnitude of electron and hole current can be altered successfully. They can also be tuned to be symmetric, which fits to experimental observations. Finally, new insight into the device functionality is gained based on our calculations of the work functions and effective masses of the isolated $NiSi_2$ and Si.

HL 84.5 Fri 10:30 POT 151

Iron-based Nitrogen doped Graphene Aerogels Derived from Seaweed Waste as Electrocatalysts for Efficient Electrochemical Energy Conversion and Storage — •Long Liu[1], Huaping Zhao[1], Rui Xu[1], Huanming Zhang[1], Yi Wang[1], Dongjiang Yang[2], and Yong Lei[1] — [1]Institut für Physik & IMN MacroNano, 98693 Ilmenau, Germany — [2]School of Environmental Science and Engineering, 266071 Qingdao, China

Advanced electrocatalysts are critical towards boosting the performance of electrochemical energy storage and conversion devices (e.g., lithium ion batteries, fuel cells). Here, we report our recent achievement about preparing bulky hierarchical Fe-based nanoparticles (NPs)/N-doped graphene aerogels (NGAs) through seaweed-derived biomass conversion strategy as highly-efficient electrocatalysts for electrochemical energy storage and conversion applications. The as-prepared unique Fe2N core-shell/NGAs exhibit highly desirable performance in oxygen reduction reaction (ORR), which is superior to costly commercial Pt/C electrocatalysts. Meanwhile, when transforming Fe2N core-shell / NGAs into Fe2O3 hollow nanoparticles (HNPs) / NGAs via the nanoscale Kirkendall effect, the as-obtained HNPs/NGAs display excellent energy storage performance in lithium ion batteries with high specific capacity, excellent rate capability and good cycle stability. These results demonstrate a sustainable approach to synthesize efficient and multifunctional electrocatalysts based on seaweed waste for electrochemical energy storage and conversion applications.

HL 84.6 Fri 10:45 POT 151

Charge Transport in Hexathiophene - Silicon Hybrid Systems — •Felix Eckmann, Hannah Schamoni, and Martin Stutzmann — Walter Schottky Institut und Physik Department, Technische Universität München, München, Deutschland

Hybrid structures containing organic and inorganic semiconductors are attractive material systems for applications such as light emitting devices and solar cells due to their potential of combining the high mobility and stability of inorganic semiconductors with the organic semiconductors' low production cost and flexibility. In order to gain insight into the fundamental electronic properties of such structures' interfaces, a model system containing a hexathiophene thin film deposited by organic molecular beam deposition onto variously doped silicon substrates has been chosen for thorough investigation. Current - voltage as well as capacitance - voltage measurements have been performed in order to compare different contacting methods to the thin film, such as Au lift-off float-on and Hg-droplet contacts. Our data yields good agreement to space charge limiting current theory, showing strong diode characteristics with rectification ratios of up to four orders of magnitude, a switch in forward direction as well as significantly varying barrier heights from n- to p-type substrates.

Coffee Break

HL 84.7 Fri 11:30 POT 151

Magnetic quantum ratchet effect in CdTe and Cd(Mn)Te quantum wells with dual grating top gate structure — •Philipp Faltermeier[1], Jan Unverzagt[1], Stefan Hubmann[1], Alexander Pfaller[1], Zbigniew Adamus[2], Grzegorz Karczewski[2], Thomasz Wojtowicz[2], Vasily. V. Bel'kov[3], Leonid Golub[3], Eougenious Ivchenko[3], Grigory Budkin[3], Vyacheslav Popov[4], Denis V. Fateev[4], Dieter Weiss[1], and Sergey D. Ganichev[1] — [1]University of Regensburg, Regensburg, Germany — [2]Institute of Physics, Polish Academy of Sciences, Warsaw, Poland — [3]Ioffe Institute, St. Petersburg, Russia — [4]Institute of Radio Engineering and Electronics (Saratov Branch), Saratov, Russia

We report on the observation of terahertz radiation induced magnetic-ratchet effects in CdTe and (Cd,Mn)Te quantum well structures superimposed with lateral superlattice. The in-plane potential was tuned by applying gate voltages. Irradiating the QW at normal incidence while applying a magnetic field B along the growth direction we observed that the terahertz-induced ratchet current exhibits sign-alternating $1/B$ periodic oscillations. The magnitude of the oscillations was by orders of magnitude larger than the ratchet photoresponse at zero magnetic field. The oscillation period corresponds to that of the Shubnikov-de-Haas effect. Our results reveal the existence of magnetic ratchet effects characterized by magnetic quantum photocurrent oscillations caused by Landau quantization and giant Zeeman effects in diluted magnetic heterostructures.

HL 84.8 Fri 11:45 POT 151

Spectroscopic studies of buried GaP/Si(100) heterointerfaces — •Oliver Supplie[1], Oleksandr Romanyuk[2], Toma Susi[3], Matthias M. May[1,4], and Thomas Hannappel[1] — [1]TU Ilmenau, Institute of Physics, D — [2]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, CZ — [3]Vienna University, Institute of Physics, AU — [4]Department of Chemistry, Cambridge University, UK

Pseudomorphic virtual GaP/Si substrates are attractive for III/V-on-Si integration for microelectronics, photovoltaics, and water-splitting applications. Adequate preparation of the GaP/Si(100) heterointerface is of particular interest since its atomic and electronic structure highly impacts crystal quality. Here, we study the formation of the GaP/Si(100) heterointerface *in situ* during preparation in metalorganic vapor phase epitaxy by means of reflection anisotropy spectroscopy and develop a dedicated nucleation sequence, which yields about 2 nm thin GaP layers on Si(100) with atomically well-ordered surfaces free of antiphase disorder, as evidenced by low energy electron diffraction [1]. Furthermore, we apply photoelectron spectroscopy (PES) on very thin GaP nucleation layers to conclude on the chemical structure of the heterointerface [1]. Density functional theory (DFT) calculations of chemical shifts caused by interfacial bonds support our findings of Si-P bonds being present at the interface [2]. With DFT, we also find interface states in the common band gap above the VBM [2]. Their predicted dispersion is anisotropic and provides distinct features for further experimental PES-based investigation [2]. [1] Supplie et al., *JPCL* 6, 464 (2015). [2] Romanyuk et al., *PRB* 94, 155309 (2016).

HL 84.9 Fri 12:00 POT 151

The importance of interface step configurations in the GaP/Si(111):As system: Towards a growth model for twin domain formation — •Christian Koppka, Lars Winterfeld, Matthias Steidl, Agnieszka Paszuk, Peter Kleinschmidt, Erich Runge, and Thomas Hannappel — TU Ilmenau, Institute of Physics, D-98693 Ilmenau, Germany

V-III epitaxy on (111) oriented semiconductors is an increasingly relevant topic for innovative optoelectronic devices. In particular, the combination of (111) oriented epilayers with the growth of nanowire-based structures is a subject of intense research. However, the (111) orientation often leads to the formation of rotational twins. Despite the potential negative effects on the optoelectronic properties of such devices, this growth defect is rarely taken into account so far. Recently, we demonstrated the importance of the twin suppression in GaP/Si(111) virtual substrates for the quality of VLS grown GaP nanowires (1). Besides the nucleation conditions (T_{nuc}, t_{nuc}, V/III ratio, etc.), the substrate misorientation has a decisive influence on the twin domain formation. For an atomistic understanding of the twinning process, DFT calculations on the GaP/Si(111):As interface, the twin boundary as well as nucleation at steps were performed. In addition to thermodynamic conditions, kinetic monte carlo simulations should also consider kinetic influences and confirm the experimentally determined trends.

(1) C. Koppka et al., Crystal Growth & Design (2016)

HL 84.10 Fri 12:15 POT 151

Ultrathin Magnetite in Fe_3O_4/MgO super-lattices – resolving the origin of an enhanced, thin film magnetic moment — Ozhet Mauit[1,2], •Karsten Fleischer[1], Cormac Ó Coileáin[1], Daniel S. Fox[1], Christopher M. Smith[1], Gulnar Sugurbekova[2], Hongzhou Zhang[1], and Igor V. Shvets[1] — [1]School of Physics and CRANN, Trinity College Dublin, The University of Dublin, Ireland — [2]National Laboratory Astana, Nazarbayev University, Astana, Kazakhstan

The electrical, crystallographic and magnetic properties of ultra-thin magnetite (Fe_3O_4) have been studied in detail, by employing superlattice structures of Fe_3O_4/$MgFe_2O_4$ and Fe_3O_4/MgO on a variety of substrates. By careful analysis of their properties, the influence of substrate stoichiometry, Fe_3O_4 thin film thickness, antiphase boundaries on the magnetic properties can be separated. In particular, the controversial enhanced magnetic moment in ultra-thin films (<5 nm) was found to be related to the substrate stoichiometry, specifically the migration of oxygen vacancies into the Fe_3O_4 thin films. The multilayer concept can be employed with many other such systems and offers new methods of tuning the properties of thin magnetic oxides.

HL 84.11 Fri 12:30 POT 151

Spilling of electronic states in Pb quantum wells on Si(111)-Au surface — Mieczysław Jałochowski[1], •Krisztián Palotás[2,3], and Mariusz Krawiec[1] — [1]Marie Curie-Skłodowska University, Lublin, Poland — [2]Budapest University of Technology and Economics, Budapest, Hungary — [3]Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia

Energy-dependent apparent step heights of two-dimensional ultrathin Pb islands grown on the Si(111)6x6-Au surface have been investigated by a combination of scanning tunneling microscopy, first-principles density-functional theory and particle-in-a-box model calculations [1]. The apparent step height shows thickness- and energy-dependent oscillatory behaviors, which are directly related to the spilling of electron states into the vacuum exhibiting a quantum size effect. This has been unambiguously proven by extensive first-principles scanning tunneling microscopy and spectroscopy simulations. An electronic contribution to the apparent step height is directly determined, which can reach values as high as the half of the atomic contribution at certain energies. The applicability of the particle-in-a-box model to the spilling of electron states is also discussed.

[1] M. Jałochowski et al., Phys. Rev. B 93, 035437 (2016)

HL 85: Topological Insulators III (joined session with TT)

Time: Friday 9:30–12:30 Location: POT 251

HL 85.1 Fri 9:30 POT 251

Time-dependent defects in photonic topological insulators — •Christina Jörg[1], Fabian Letscher[1,2], Michael Fleischhauer[1], and Georg von Freymann[1,3] — [1]Physics Department and Research Center OPTIMAS, University of Kaiserslautern, Germany — [2]Graduate School Materials Science in Mainz, Kaiserslautern, Germany — [3]Fraunhofer-Institute for Physical Measurement Techniques (IPM), Kaiserslautern, Germany

To model topological insulators by means of classical optics, we fabricate arrays of evanescently coupled waveguides. These waveguides are about 1 μm in diameter at an aspect ratio of 1:500, and helically curved. The inverse of the waveguide array is fabricated via direct laser writing in a negative-tone photoresist. Subsequently the sample is infiltrated with a material of higher refractive index, creating low-loss 3D waveguides. Arranging the waveguides on a honeycomb-lattice, a robust edge mode exists due to topological protection [1]. This means that light moves along the edge unidirectionally, and even walks around defects without backscattering. Here, we discuss defects with time-dependent coupling, i.e., one waveguide with a different helicity than the rest of the waveguides. We examine three kinds of time-dependent defects: a) a straight waveguide, b) a waveguide with opposite helicity, c) a waveguide with same helicity but shifted by half a helix pitch in the z-direction. In all three cases the edge mode moves along the edge regardless of the defect, going partially around the defect and partially through it.

[1] M. C. Rechtsman et al., Nature 496, 196-200 (2013).

HL 85.2 Fri 9:45 POT 251

Aharonov-Bohm-type oscillations in HgTe topological insulator nanowires — •Johannes Ziegler[1], Raphael Kozlovsky[2], Ming-Hao Liu[2], Dmitriy Kozlov[1,3,4], Hubert Maier[1], Ze Don Kvon[3,4], Nikolay Mikhailov[3], Sergey Dvoretsky[3], and Dieter Weiss[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]Institut für Theoretische Physik, Universität Regensburg, Germany — [3]A.V. Rzhanov Institue of Semiconductor Physics, Novosibirsk, Russia — [4]Novosibirsk State University, Russia

In topological insulator nanowires, the helical surface states form a conducting cylinder enclosing the bulk. These states give rise to Aharonov-Bohm-type oscillations when a magnetic field is applied along the wire axis [1]. These oscillations, periodic with the flux quantum Φ_0, are predicted to change their phase periodically as a function of the Fermi level E_f. We fabricate nanowires with typical cross sections of 80 x 150 nm using an optimized wet etching process to maintain the high mobility and mean free path. In our experiments, we found, as expected, h/e periodic oscillations as a function of magnetic flux Φ with alternating maxima and minima as a function of E_f for $\Phi/\Phi_0 = 1/2$ and $\Phi/\Phi_0 = 1$. We compare the resulting periodicity with a simple model and electrostatic simulations.

[1] J.H. Bardarson *et al.*, Phys. Rev. L **105**, 156803 (2010)

HL 85.3 Fri 10:00 POT 251

Correlation and current anomalies in helical quantum dots — •Christophe De Beule[1], Niccolò Traverso Ziani[2], Mohammad Zarenia[1], Bart Partoens[1], and Björn Trauzettel[2] — [1]Department of Physics, University of Antwerp, 2020 Antwerp, Belgium — [2]Institute of Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany

We investigate the ground-state properties of a quantum dot on the surface of a time-reversal invariant topological insulator. Confinement is realized by ferromagnetic barriers and Coulomb interaction is treated with exact diagonalization. The topological origin of the dot has several consequences: (i) spin polarization increases and the ground state exhibits quantum phase transitions as a function of interaction strength, (ii) the onset of Wigner correlations takes place mainly in one spin channel, and (iii) the ground state is characterized by a persistent current that changes direction as a function of the radius.

We also consider the effect of superconducting correlations on the properties of the quantum dot. This allows us to analyze the influence of perturbations that violate particle-number conservation on the formation of the Wigner molecule.

HL 85.4 Fri 10:15 POT 251

Double topological surface states in strained alpha-Sn — •Victor Rogalev[1], Tomáš Rauch[2], Markus Scholz[1], Felix Reis[1], Lenart Dudy[1], Andrzej Fleszar[3], Marius-Adrian Husanu[4], Vladimir Strocov[4], Jürgen Henk[2], Ingrid Mertig[2,5], Jörg Schäfer[1], and Ralph Claessen[1] — [1]Physikalisches Institut und Röntgen Center for Complex Materials Systems, Universität Würzburg, 97074 Würzburg, Germany — [2]Institute of Physics, Martin Luther University Halle-Wittenberg, 06099 Halle (Saale), Germany — [3]Institut für Theoretische Physik und Astronomie, Universität Würzburg, 97074 Würzburg, Germany — [4]Swiss Light Source, Paul Scherrer Institute, CH-5232 Villigen, Switzerland — [5]Max Planck Institute for Microstructure Physics, 06120 Halle (Saale), Germany

The low temperature phase of Sn, α-Sn, is a semimetal with two pairs of "inverted" bands and zero energy band gap, which can be increased by strain. Experimental works revealed so far only one topological surface state (TSS) that bridges one pair of inverted bands.

By means of a combined experimental and theoretical approach we show that the electronic structure of the compressively strained α-Sn (001) thin film hosts an additional TSS in the valence band due to the second band inversion. This sub-surface localized TSS is directly accessed by soft X-ray angle-resolved photoemission with high probing depth. The second TSS reveals a much stronger hybridization with bulk states, in contrast to the already known surface-localized TSS. We show that such difference is consistent with the analysis of orbital composition of bulk and surface states.

HL 85.5 Fri 10:30 POT 251

Stencil lithography of MBE grown superconductors on top of topological insulator thin films — •Michael Schleenvoigt, Peter Schüffelgen, Daniel Rosenbach, Tobias W. Schmitt, Martin Lanius, Benjamin Bennemann, Stefan Trellenkamp, Elmar Neumann, Gregor Mussler, Thomas Schäpers, and Detlev Grützmacher — Peter Grünberg Institute 9, Forschungszentrum Jülich & JARA-FIT, 52425 Jülich, Germany

A stack of the two binary 3D topological insulators Bi2Te3 (n-type doped) and Sb2Te3 (p-type) forms a PN-heterostructure. Growing those topological heterostructures by means of MBE offers the possibility to tune the Fermi level of the upper surface to the Dirac-point. To protect the delicate Dirac system from degradation and oxidation we cap our heterostructures with a thin Al layer, before taking the sample to ambient conditions. We further developed this process to allow for in-situ growth of two different Al layers, i.e. a thin 1-2 nm Al layer on the full wafer followed by a thick Al film on well-defined areas by means of stencil lithography. The thin Al layer will subsequently oxidize after exposure to air and protect the delicate topological surface, whereas the thick Al layer with spatial extent in the (sub-)micrometer range will serve as superconducting contacts. Superconductor-Topological Insulator-Superconductor junctions with lateral dimensions in the nm range have then been fabricated. Despite the in-situ deposition, transport measurements and transmission electron microscope analysis indicate a low transparency, due to an intermixed region at the interface between topological insulator thin film and metallic Al.

Coffee Break

HL 85.6 Fri 11:15 POT 251

Induced superconductivity in lateral topological Josephson junctions with $(Sb_{0.94}Bi_{0.06})_2Te_3$ interlayer — •Daniel Rosenbach[1], Peter Schüffelgen[1], Martin Lanius[1], Gregor Mussler[1], Stefan Trellenkamp[1], Martin P. Stehno[2], Alexander Brinkman[2], Detlev Grützmacher[1], and Thomas Schäpers[1] — [1]Peter Grünberg Institute 9, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]MESA+ Institute for Nanotechnology, University of Twente, 7500 AE Enschede, The Netherlands

The long sought Majorana fermion is predicted to arise in superconducting systems with p-wave pair correlation symmetry. Induced superconductivity in topological insulator thin films is expected to show partly p-wave pairing, such that Majorana zero modes (MZM) are thought to exist at the interface with a conventional s-wave superconductor. A current carried by these zero modes is supposed to show a doubled periodicity in the current-phase relation, compared to con-

ventional modes.
Molecular beam grown topological insulator ternary alloy thin films, of given composition, with a thin aluminum-oxide capping layer, have been prepared with lateral niobium superconducting contacts. Junctions of various geometries have been measured at low temperatures. The response to an externally applied magnetic field and to a radio-frequency signal is strongly dependent on the current-phase relation of the conductive modes. Characterization therefore includes an analysis of various Fraunhofer diffraction pattern as well as Shapiro step measurements at different frequencies.

HL 85.7 Fri 11:30 POT 251

Nontrivial topological phases in quantum mechanical many-body systems with gain and loss effects — •Marcel Klett, Holger Cartarius, and Guenter Wunner — 1. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart

Non-Hermitian $\mathcal{PT}$-symmetric potentials are capable of effectively describing quantum systems with balanced in- and outfluxes. They allow for the existence of a $\mathcal{PT}$-symmetric phase with purely real energy spectra of the non-Hermitian Hamiltonian. Recently a possible relation between the appearance of the $\mathcal{PT}$-symmetric phase and topologically nontrivial states were found in two studies of simple model systems. However, they came to opposite conclusions. In the Su-Schriefer-Heeger (SSH) model [1] the topological phase has a major influence. As soon as topologically nontrivial states appear $\mathcal{PT}$ symmetry gets broken. This is in contrast to the non-Hermitian Kitaev model [2], in which $\mathcal{PT}$ symmetry breaking does not depend on the topological phase. Our work is based on including different non-Hermitian potentials in the SSH model as well as the Kitaev model. We perform exact calculations of the eigenvalues and the eigenstates, clarify the relation between $\mathcal{PT}$ symmetry and topological phases, and explain why opposite results were found in the above mentioned systems.
[1] Baogang Zhu et al., Phys. Rev. A **89**, 062102 (2014)*
[2] Xiaohui Wang et al., Phys. Rev. A **92**, 012116 (2015)

HL 85.8 Fri 11:45 POT 251

Probing topological edge states in HgTe-based quantum wells by terahertz photogalvanic spectroscopy — •Kathrin-Maria Dantscher[1], Dimitry A. Kozlov[2], Maria-Theresia Scherr[1], Sebastian Gebert[1], Jan Bärenfänger[1], Mikhail Durnev[3], Sergey A. Tarasenko[3], Vasily V. Bel'kov[3], Nikolay N. Mikhailov[2], Sergey A. Dovertsky[2], Ze Dong Kvon[2], Dieter Weiss[1], and Sergey D. Ganichev[1] — [1]Terahertz Center, University of Regensburg, Regensburg, Germany — [2]A.V. Rzhanov Institute of Semiconductor Physics, Novosibirsk 630090, Russia — [3]Ioffe Institute, St.Petersburg, Russia

We report on the observation of a chiral photogalvanic current excited by terahertz laser radiation in the edge channels of HgTe-based 2D topological insulators (TI). The direction of the edge photocurrent reverses by switching the radiation polarization from the right- to left-handed one and, for fixed helicity, has opposite direction for opposite edges. The chiral edge photocurrent is detected in a wide range of gate voltages and reverse the sign twice upon variation of the gate voltage. We show that the data reveal that in the TI-regime the photocurrent is caused by photoionization of helical edge electrons to the conduction band, discuss the microscopic model of this phenomena and present the developed microscopic theory.

HL 85.9 Fri 12:00 POT 251

Topological phase space study of a generalized Kane-Mele spin-orbit Hamiltonian — •Tobias Frank, Petra Högl, Martin Gmitra, Denis Kochan, and Jaroslav Fabian — Theoretische Physik, Universität Regensburg

We study a generalized Kane-Mele [1] graphene spin-orbit coupling Hamiltonian, that is able to describe hybrid systems like graphene on transition metal dichalcogenides [2] or graphene - metal interfaces [3] with broken inversion symmetry. We identify the topological phase space in terms of its Z_2 invariant by variation of spin-orbit coupling parameters. We as well analyze the bulk-edge correspondence in terms of zigzag and armchair ribbons. We find that spin-orbit coupling proximitized graphene can exhibit helical edge states at the zigzag boundary even if it is in the trivial topological phase.

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] C. L. Kane and E. J. Mele, PRL 95 226801 (2005)
[2] M. Gmitra, D. Kochan, P. Högl, and J. Fabian, PRB 93 155104 (2016)
[3] T. Frank, M. Gmitra, and J. Fabian, PRB 93 155142 (2016)

HL 85.10 Fri 12:15 POT 251

HgTe shells on CdTe nanowires — •Jan Hajer, Maximilian Kessel, Christoph Brüne, Hartmut Buhmann, and Laurens W. Molenkamp — Physikalisches Institut, EP3, Am Hubland, 97074 Würzburg

Topological insulator nanowires in proximity to a superconductor are in research focus of condensed matter physics. Hosting Dirac-like surface states with high spin-orbit coupling, they are a possible platform for p-wave superconductivity and Majorana bound states.

In our work we investigate low temperature charge transport in quasi one-dimensional HgTe. Vapor-liquid-solid grown CdTe nanowires of high crystal quality serve as a substrate for epitaxial HgTe overgrowth. The core-shell heterostructures show residual strain, expected to transform the semi-metallic HgTe shell to a quasi one-dimensional topological insulator. Charge transport with proximitized superconductors indicates a high interface quality giving rise to the observation of multiple Andreev reflections and an induced supercurrent.

HL 86: New Materials

Time: Friday 9:30–12:45 Location: POT 112

HL 86.1 Fri 9:30 POT 112

Bulk-boundary correspondence from the inter-cellular zak phase — •Jun Won Rhim, Jan Behrends, and Jens H. Bardarson — Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany

The Zak phase γ, the generalization of the Berry phase to Bloch wave functions in solids, is often used to characterize inversion-symmetric 1D topological insulators; however, since its value can depend on the choice of real-space origin and unit cell, only the difference between the Zak phase of two regions is believed to be relevant. Here, we show that one can extract an origin-independent part of γ, the so-called inter-cellular Zak phase γ^{inter}, which can be used as a bulk quantity to predict the number of surface modes as follows: a neutral finite 1D tight-binding system has $n_s = \gamma^{\mathrm{inter}}/\pi \pmod 2$ number of in-gap surface modes below the Fermi level if there exists a commensurate bulk unit cell that respects inversion symmetry. We demonstrate this by first verifying that $\pm e\gamma^{\mathrm{inter}}/2\pi \pmod e$ is equal to the extra charge accumulation in the surface region for a general translationally invariant 1D insulator, while the remnant part of γ, the intra-cellular Zak phase γ^{intra}, corresponds to the electronic part of the dipole moment of the bulk's unit cell. Second, we show that the extra charge accumulation can be related to the number of surface modes when the unit cell is inversion symmetric.

HL 86.2 Fri 9:45 POT 112

Combined Control Mechanisms of the Interatomic Coulombic Electron Capture in Paired Quantum Dots — •Axel Molle[1], Essam Radwan[1], Sascha Bubeck[1], Federico Manuel Pont[2], and Annika Bande[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [2]Universidad Nacional de Córdoba, and IFEG-CONICET, Córdoba, Argentina

Ultrafast Interatomic Coulomb Electron Capture (ICEC) is a process in which a species A is capturing a free electron. This is mediated by long-range Coulomb-interaction with a bound electron in a neighbouring species B in such a way that the transferred energy releases the bound electron of species B into the continuum.

First predicted for atoms and molecules, ICEC has been established as an important energy-transfer process in paired-quantum-dot systems [1].

It was shown that semiconductor material variations signify one of the important control mechanisms for the ICEC process. Addition-

ally, a related energy transfer-process in quantum dots was found to be controllable by the geometries of both neighbouring quantum dots [2].

In this work, both effects are combined to understand the coupling of those two control mechanisms and predict advantageous experimental setups of the paired-quantum-dot system, underlining that ICEC proves to be a potential candidate for future energy-selective devices.

[1] F. M. Pont *et al.*, J. Phys. Condens. Matter **28**, 075301 (2016).
[2] P. Dolbundalchok *et al.*, J. Comput. Chem. **37**, 2249 (2016).

HL 86.3 Fri 10:00 POT 112

Molecular Self-Assembly of Organic-Inorganic Perovskite Nanocrystals — •Maximilian E. Löw[1,2], Verena A. Hintermayr[1,2], Theobald Lohmüller[1,2], Alexander S. Urban[1,2], and Jochen Feldmann[1,2] — [1]Chair of Photonics and Optoelectronics, Department of Physics and Center for Nanoscience (CeNS), Ludwig-Maximilians-Universität (LMU), Amalienstraße 54, 80799 Munich, Germany — [2]Nanosystems Initiative Munich (NIM), Schellingstraße 4, 80799 Munich, Germany

Having already shown great promise in the bulk form for optoelectronic applications, many researchers are now focusing on the synthesis of nanocrystals of organic-inorganic halide perovskites. Here, we present a straightforward method for producing highly ordered patterns of perovskite nanocrystals based on molecular self-assembly. With this new method, we are able to control structural parameters of the nanocrystal assembly, such as the particle size and interparticle distance over a large surface area. The optical properties of these nanocrystal arrays are investigated by UV-Vis and photoluminescence spectroscopy, while the spatial dimensions and lateral orientation of the nanocrystal assemblies are analyzed by electron microscopy. Overall, our approach represents a new and highly reproducible way of producing perovskite nanopatterns for photonics applications.

HL 86.4 Fri 10:15 POT 112

Characterization of electrochemically deposited MoS_x layers for thin film transistors — •Talha Nisar, Torsten Balster, Jonas Köhling, and Veit Wagner — Department of Physics and Earth Sciences, Jacobs University Bremen gGmbH, Campus Ring 1, 28759 Bremen, Germany

Molybdenum disulfide is a promising material for future electronics. MoS_2 thin layers can be deposited by several deposition methods. The current state of the art for large area deposition of thin layers is chemical vapor deposition.
In our study we used electrochemical deposition to grow large area thin films of MoS_x (x=2-3) onto a Au-substrate. Ammonium tetrathiomolydate (ATTM) has been used as precursor material in the cathodic regime (-0.35V) with respect to Ag/AgCl reference electrode. The obtained layers from aqueous electrolyte are amorphous MoS_3/MoO_3 as could be confirmed from Raman and XPS measurements. It is shown, that the use of organic solvents allow oxygen contamination to be significantly reduced. The characterization of obtained layers by XPS shows an almost ideal Mo:S ratio of 1:2.1. Furthermore, these layer are characterized by Raman, AFM and SEM measurements. Annealed layers are transferred to SiO_2/Si wafers to fabricate thin film transistors in top contact bottom gate geometry.

HL 86.5 Fri 10:30 POT 112

Investigation of dual-tone resists for low-temperature electron-beam lithography of deterministic quantum structures — •Sven Rodt, Arsenty Kaganskiy, Peter Schnauber, Tobias Heuser, Ronny Schmidt, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstrasse 36, D-10623 Berlin

The deterministic integration of light-emitting semiconductor nanostructures like e.g. single quantum dots is of large interest for novel quantum technologies that rely on the emission of single photons. For this we apply an approach that is based on cathodoluminescence spectroscopy in combination with in-situ electron-beam lithography (EBL) [1]. Due to the nature of light emission from quantum dots and its enhancement at low temperatures (LT), such processing is best carried out at liquid-helium temperature. Consequently, EBL resists are needed that perform well in this extreme temperature regime. Here we report on the resists PMMA and CSAR 62 and their applicability in the full range between room temperature and 4 K. They exhibit a dual-tone behavior as they operate in the positive-tone regime for small electron doses and enter the negative-tone regime for larger doses. Besides two-dimensional structuring also three-dimensional EBL is performed and evaluated. CSAR 62 is found to be superior to PMMA as the LT-EBL is more straightforward and results in a higher yield and quality of the processed structures [2].

[1] M. Gschrey et al., Appl. Phys. Lett. 102, 251113 (2013).
[2] A. Kaganskiy et al., J. Vac. Sci. Technol. B 34, 061603 (2016).

HL 86.6 Fri 10:45 POT 112

Transition from Jaynes-Cummings to Autler-Townes ladder in a quantum dot-microcavtity system — C. Hopfmann[1], A. Carmele[2], •A. Musiał[1,3], M. Strauss[4], M. Kamp[4], C. Schneider[4], S. Höfling[4,5], A. Knorr[2], and S. Reitzenstein[1] — [1]IFP, TU Berlin, Germany — [2]ITP, TU Berlin, Germany — [3]LOSN, Politechnika Wrocławska, Poland — [4]TEP, Universität Würzburg, Germany — [5]SUPA, University of St Andrews, UK

We report on experimental and theoretical study of resonantly-driven quantum dot exciton (X) strongly coupled to the microcavity mode (CM). Investigated system exhibits dramatically different character depending on the excitation strength from vacuum Rabi doublet when coupled X-CM is weakly probed to Mollow triplet-like behavior under strong coherent pump. Focus is on the unexplored intermediate regime, where the laser field dresses the polaritons and the coupling of the X to the confined CM and to the laser are equally important, as proven by observing injection pulling of the polariton branches. This regime is of particular interest since it connects the purely quantum mechanical Jaynes-Cummings and the semi-classical Autler-Townes ladder. In order to address underlying physics we excite the coupled system via the matter component of fermionic nature undergoing saturation - in contrast to commonly used cavity-mediated excitation which determines the evolution of the system at high occupations. Exploring the driving strength-dependence we establish robust fingerprint of the transition to be the maximum in the resonance fluorescence signal [1].

[1] C. Hopfmann et al., arXiv:1609.03462 (2016).

Coffee Break

HL 86.7 Fri 11:30 POT 112

Submicron scanning X-Ray diffraction imaging of strain in VO_2 microwires. — •Andreas Johannes[1], Jura Rensberg[2], Carsten Ronning[2], and Manfred Burghammer[1] — [1]ESRF - The European Synchrotron, 38043 Grenoble, France — [2]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

X-Ray diffraction remains the go-to method to identify and characterize the crystal structure of a given material. In general, the small brilliance of lab sources means that large volumes of single crystalline or powdered material have to be investigated, averaging over all localized effects. At the increasing number of synchrotron based, focused X-Ray beam-lines, however, it is becoming possible to perform scanning experiments that yield specially resolved diffraction data. The advantages of this method are highlighted in the scientific case of imaging the strain and multiple-phase-coexistence in VO_2 microwires.

HL 86.8 Fri 11:45 POT 112

EPR and DFT investigation of Fe and Fe-Ti doping in LiNbO3 — •Sara Arceiz Casas[1], Simone Sanna[1], Annamaria Zaltron[2], Giacomo Bettella[2], Gianluca Pozza[2], Cinzia Sada[2], and Siegmund Greulich-Weber[1] — [1]University of Paderborn, Warburger Str. 100, 33098 Paderborn, Germany — [2]University of Padova, Via Marzolo 8, 35131 Padova, Italy

The optical properties of Ti4+ indiffused LiNbO3 waveguides are heavily affected by extended and point defects. In particular, even small percentages of unintentional iron doping increase the photorefractive sensitivity of LiNbO3 considerably.

Ti4+ is known to stabilize Fe2+ impurities against oxidation[1], however, neither the defect complexes formed by Fe and Ti nor the mechanisms leading to the optical degrade are known. As a first step towards the understanding of the photorefractive properties of the waveguides, we investigate isolated Fe and Fe-Ti doped LiNbO3 [2,3] by electron paramagnetic resonance (EPR) and density functional theory (DFT).

Signals originating from different defect centers can be discriminated by EPR in Fe doped and Fe-Ti co-doped samples. Corresponding theoretical models are developed within DFT, showing the structural and electronic properties of the observed defects.

[1] V. Gericke, Appl. Phys. B 44, 155 (1987)
[2] O. F. Schirmer, J. Phys.: Cond. Matt. 21, 123201 (2009)
[3] O. F. Schirmer, Phys. Rev. B 83, 165106 (2011)

HL 86.9 Fri 12:00 POT 112

Hyperdoping silicon with tellurium by ion implantation and ultra-short annealing for optoelectronics — •Mao Wang[1,2], Fang Liu[1,2], Ye Yuan[1,2], Slawomir Prucnal[1], Berencen Yonder[1], Rebohle Lars[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 — [2]Technische Universität Dresden

Hyperdoping silicon with chalcogen atoms is a topic of increasing interest due to the strong sub-band gap absorption exhibited by the resulting materials, which can be exploited to develop infrared photodectectors and intermediate band solar cells [1-3]. In our work, tellurium-hyperdoped silicon layers have been fabricated by ion implantation followed by flash lamp annealing (FLA) or pulsed-laser melting (PLM). The Rutherford backscattering spectrometry / Channeling (RBS/C) results reveal the high-quality recrystallization of tellurium implanted silicon by both FLA and PLM. From the transport measurements, an insulator-to-metal transition is observed with increasing tellurium concentration. Moreover, the ellipsometry measurements show that the band gap narrows with increasing doping concentration. And the Fourier transform infrared (FTIR) spectroscopy show that tellurium hyperdoped Si has strong infrared absorption. All these results give us a signal that hyperdoped silicon with tellurium could enable silicon-based optoelectronics in the infrared band. [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 86.10 Fri 12:15 POT 112

Preparation and characterization of self-assembled monolayers on different semiconductive substrates for bio-sensing applications. — •Stefano Gremmo, Johannes Bartl, Martin Stutzmann, and Anna Cattani-Scholz — Walter Schottky Institut, Technische Universität München, München, Germany

Aim of the present work is to realize and characterize bio-interfaces based on self-assembled monolayers of phosphonic acids (SAMPs) stable under physiological conditions, to implement a label-free transduction mechanism for DNA detection. Such process is performed on different semiconductive substrates, such as ZnO and SiN, to investigate their characteristics and performance in detecting the target molecules.

SAMPs of (2-2-[2-hydroxy-ethoxy]-ethoxy-ethyl) phosphonic acid and 11-hydroxy-undecylphosphonic acid are generated on the substrates using a process based on tethering by aggregation and growth (T-BAG). By additional surface functionalization protocols, peptide nucleic acid (PNA) is covalently bound to biocompatible SAMPs interfaces.

Characterization of the electrochemical sensing ability of these new devices is achieved by cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS). Structural and morphological properties are investigated by several surface sensitive techniques such as contact angle (CA) measurements, atomic force microscopy (AFM) and X-ray photoelectron spectroscopy (XPS).

HL 86.11 Fri 12:30 POT 112

Photonic crystal fibers with disordered claddings — •Swaathi Upendar[1], Guangrui Li[2], Maxim L. Nesterov[1], Markus Schmidt[2], and Thomas Weiss[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [2]Leibniz Institute of Photonic Technology, Jena, Germany

Photonic crystal fibers use the photonic band gap effect to confine light in a central defect core with a periodic lattice as its cladding. When such photonic crystal fibers are fabricated, the cladding is never truly perfect as the fabrication process can result in different types of disorder such as diameter, position and shape disorder.

In this contribution, we present numerical investigations of the influence of disorder on the density of cladding states and the dispersion of the fundamental mode of the fiber. In particular, we investigate diameter disorder for an all solid fiber with high index strands in a silica background. We find that the response of the fiber is highly dependent on the range of diameter fluctuations. While fluctuations in the whole cladding region results in a narrowing of the band gap and hamper the light guidance, we observe that disorder in the core surround provides additional means to control the properties of the guided modes and to reduce the confinement loss.

HL 87: Carbon: Diamond and others

Time: Friday 9:30–12:30 Location: POT 06

HL 87.1 Fri 9:30 POT 06

Towards optical dynamical nuclear spin polarization of metabolites — •Samuel Müller[1], Jochen Scheuer[1], Christoph Müller[1], Ilai Schwarz[2], Mathen Markham[3], Pelayo Fernandez-Acebal[2], Martin Plenio[1], Boris Naydenov[1], and Fedor Jelezko[1] — [1]Institut für Quantenoptik, Universität Ulm, Germany — [2]Institut für Theoretische Physik, Universität Ulm, Germany — [3]Element Six, Ltd., Ascot, UK

^{13}C magnetic resonance spectroscopy allows a wide range of new applications in magnetic resonance imaging and in a first clinical study this technique already has been demonstrated for imaging prostate cancer [1]. However, due to its small gyromagnetic ratio and low abundance of ^{13}C spins, hyperpolarization of the nuclear spins is required for increasing the sensitivity. In contrast to conventional methods for hyperpolarization at low temperatures and high magnetic field dynamical nuclear polarization (DNP) via optically pumped Nitrogen-Vacancy centers (NV) in diamond allows a high degree of polarization to be reached even at room temperature and low magnetic field. Here we demonstrate DNP of ^{1}H nuclear spins in different molecules on the diamond surface using single shallow NV centers. This is an important step towards nuclear spin hyperpolarization of biomarkers such as ^{13}C in metabolites, e.g. pyruvate.

[1] Nelson, Sarah J., et al. Science translational medicine (2013)

HL 87.2 Fri 9:45 POT 06

Precision measurements of electric fields using NV centers in diamond — •Julia Michl[1], Philipp Neumann[1], Andrej Denisenko[1], Junichi Isoya[2], and Jörg Wrachtrup[1] — [1]3. Physikalisches Institut, Universität Stuttgart, Germany — [2]Research Center for Knowledge Communities, University of Tsukuba, Japan

As a quantum sensor, the nitrogen vacancy center in diamond can be used most prominently for magnetometry but also for thermometry, piezometry and electrometry.

Whereas the usage of single NV centers can lead to exciting applications for spatial resolution in field imaging, the measurement of an NV ensemble allows for precision measurements. In this fashion, a sensitivity for magnetic fields of under 1 pT/Hz$^{1/2}$ was shown to be possible with an NV ensemble[1].

Here, we show the combination of the precision measurement on NV ensembles with measurement techniques for electrometry already reported for single NVs[2].

Even though the coupling of the NV center electron spin in its ground state to electric fields is comparatively small, the high precision which can be achieved due to the long coherence times of the NV centers even at room temperature raise the prospect of its application as a quantum based electrometer.

[1] T. Wolf et al., PRX, 2015 [2] M. Doherty, NJP, 2014

HL 87.3 Fri 10:00 POT 06

Sub-millihertz magnetic spectroscopy with a nanoscale quantum sensor — •Simon Schmitt[1], Tuvia Gefen[2], Felix M. Stürner[1], Thomas Unden[1], Gerhard Wolff[1], Christoph Müller[1], Jochen Scheuer[1,3], Boris Naydenov[1,3], Matthew Markham[4], Sebastien Pezzagna[5], Jan Meijer[5], Ilai Schwarz[3,6], Martin Plenio[3,6], Alex Retzker[2], Liam P. McGuinness[1], and Fedor Jelezko[1,3] — [1]Institute of Quantum Optics, Ulm University, 89081 Ulm, Germany — [2]Racah Institute of Physics, Hebrew University of Jerusalem, 91904 Jerusalem, Israel — [3]Center for Integrated Quantum Science and Technology (IQST), Ulm University, 89081 Ulm, Germany — [4]Element Six, Harwell Campus, Fermi Avenue, Didcot,

OX11 0QR, United Kingdom — [5]Institut für Experimentelle Physik II, Universität Leipzig, 04103 Leipzig, Germany — [6]Institute for Theoretical Physics, Ulm University, 89081 Ulm, Germany

A general limit on the performance of quantum sensors is their coherence time since this sets the maximum time for coherent signal accumulation. Here we discuss a novel quantum sensing technique which allows a frequency resolution beyond the sensor coherence limit to be obtained. The technique also demonstrates an enhanced precision scaling not previously seen in quantum sensing scenarios. Using single nitrogen vacancy centres in diamond we apply this high resolution magnetometry technique to nanoscale NMR spectroscopy.

HL 87.4 Fri 10:15 POT 06

Efficient electrical spin readout of NV$^-$ centers in diamond — •Florian M. Hrubesch, Georg Braunbeck, Felix N. Hartz, Martin Stutzmann, Friedemann Reinhard, and Martin S. Brandt — Walter Schottky Institut and Physik-Department, Technische Universität München

Using pulsed photoionization the coherent spin manipulation and echo formation of ensembles of NV$^-$ centers in diamond are detected electrically realizing contrasts of up to 17 %. The underlying spin-dependent ionization dynamics are investigated experimentally and compared to Monte-Carlo simulations. This allows the identification of the conditions optimizing contrast and sensitivity which compare favorably with respect to optical detection [1].

[1] F. M. Hrubesch, G. Braunbeck, M. Stutzmann, F. Reinhard and M. S. Brandt, arXiv:1608.02459 (2016)

Coffee Break

HL 87.5 Fri 11:00 POT 06

Enhancement of the zero-phonon emission rate of an NV centre in minimally processed diamond — •Daniel Riedel, Patrick Maletinsky, and Richard J. Warburton — Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland

The precise optical control of the coherent spin associated with the nitrogen vacancy (NV) centre in diamond enables both solid-state-based quantum information experiments and ultra-precise sensing. For future applications it is crucial to improve the interrogation frequency by engineering the photonic modes, for instance by embedding the NV centres into nanophotonic structures. A key challenge is to maintain a stable environment in the diamond in order to preserve the long optical and spin coherence times.

Here, for the first time, we report cavity-assisted Purcell enhancement of the zero-phonon line (ZPL) of a single NV centre in a minimally processed diamond membrane. The membrane is incorporated into a fully tunable Fabry-Perot microcavity, where photons are deterministically coupled to the TEM_{00} mode rendering them suitable for long distance communication. We find a 20-fold enhancement of the ZPL emission photon flux, which corresponds to an overall change in the radiative lifetime from 11 ns out of resonance to 7 ns on resonance.

Our approach constitutes a promising route towards a scalable quantum-network based on solid-state emitters.

HL 87.6 Fri 11:15 POT 06

Wigner crystallization in graphene nanoribbons with zigzag edges — •Alev Devrim Guclu — Izmir Institute of Technology, Izmir, Turkey

We investigate the Wigner crystallization of electrons and holes at the zigzag edges of graphene nanoribbons using many-body configuration interaction method. We show that Wigner crystallization occurs at a surprisingly high electronic density of ~ 0.8 nm^{-1}. In contrast with one-dimensional electron gas, the flat-band structure of the edge states makes the system interaction dominated, facilitating the electronic localization. The Wigner localization is found to affect strongly the magnetic coupling between the nearest neighbor electrons, causing an antiferromagnetic-ferromagnetic phase transition. As the width of the ribbon is decreased to 11 Å, interedge coupling becomes important, hence increased kinetic energy overcomes the long-range Coulomb repulsion and suppresses the Wigner crystallization. Finally, we show that Wigner crystallization can also occurs for holes, albeit weaker than for electrons. This work was supported by The Scientific and Technological Research Council of Turkey (TUBITAK) under the 1001 Grant Project Number 114F331.

HL 87.7 Fri 11:30 POT 06

Voltage-dependent photocurrent spectroscopy in surface-conductive diamond devices — •Philipp Beck[1], Patrick Simon[1], Ankit Rathi[1], Jose A. Garrido[2], and Martin Stutzmann[1] — [1]Walter Schottky Institut und Physik-Department, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany — [2]Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and The Barcelona Institute of Science and Technology, Campus UAB, Bellaterra, 08193 Barcelona, Spain

For many applications of nitrogen-vacancy (NV) centers in diamond especially in the field of quantum technology the understanding of their electronic addressability is highly desirable. Based on hydrogen-terminated and thus surface-conductive diamond enriched with NV centers, we fabricate an all diamond device based on selective surface oxidation for the creation of highly insulating potential barriers for surface-conducting holes with widths in the range of 50nm-500nm. Across these hydrogenated-oxidized lateral heterostructures we measure spectrally resolved photocurrent as a function of temperature and illumination intensity and examine the influence of nitrogen-related defects and other defect states on the observed photocurrents. Additionally, we explain a nonlinear I-U characteristics of the photocurrent in these devices by its specific electronic band structure and examine the potential of such structures for an electrical control of the spectral energy of selected defect states.

HL 87.8 Fri 11:45 POT 06

Ballistic and resonant negative photocurrents in single carbon nanotubes — •Carolina Duque Sierra, Christoph Karnetzky, Lukas Sponfeldner, Max Engl, and Alexander W. Holleitner — Walter Schottky Institute and Physics Department, Technical University of Munich, Am Coulombwall 4a, 85748 Garching, Germany

We present ultrafast photocurrent experiments on semiconducting, single-walled carbon nanotubes under a resonant optical excitation of their subbands. We demonstrate that a ballistic transport of the photogenerated charge carriers can be achieved. Moreover, thermionic emission processes to the contacts dominate the photocurrent. In contrast, the charge current without laser excitation is well described by a Fowler-Nordheim tunneling. The time-averaged photocurrent changes polarity as soon as sufficient charge carriers are injected from the contacts, which can be explained by an effective population inversion in the optically pumped subbands. We acknowledge the ERC via the project NanoREAL.

HL 87.9 Fri 12:00 POT 06

Fabrication of Dense Arrays of Nanocrystalline Diamond Nanopillars — •Alexander Schmidt, Johann Peter Reithmaier, and Cyril Popov — Institute of Nanostructure Technologies and Analytics, Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

One-dimensional diamond nanostructures, namely diamond nanopillars, have been prepared using nanocrystalline diamond (NCD) films as starting material. The fabrication process of arrays of nanopillars consisted of their definition by electron beam lithography (EBL) applying gold as a hard mask material and subsequent inductively coupled plasma reactive ion etching (ICP-RIE) with oxygen. Three different pillar diameters were investigated, namely 200, 100 and 50 nm, with different lateral distances ranging from 100 nm to 400 nm in order to determine the minimal resolution, which could be defined depending on the variation of a major process parameter in the EBL process – namely the exposure dose. Furthermore, its influence on the resulting shape of the pillars was investigated. The integration of NV centers within the fabricated diamond nanopillars either during the film growth or by follow-up ion implantation can be used to develop quantum memories.

HL 87.10 Fri 12:15 POT 06

Physics — •Dennis Oing — Uni Due

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HL 88: Organic Electronics and Photovoltaics V: OPV

Time: Friday 10:15–13:15 Location: ZEU 255

HL 88.1 Fri 10:15 ZEU 255

Non-Radiative Voltage Losses Reduce the Upper Limit of the Power Conversion Efficiency in Fullerene-Based Organic Solar Cells — •Johannes Benduhn[1], Kristofer Tvingstedt[2], Fortunato Piersimoni[3], Sascha Ullbrich[1], Dieter Neher[3], Donato Spoltore[1], and Koen Vandewal[1] — [1]IAP, TU Dresden — [2]EP VI, University of Würzburg — [3]University of Potsdam

The open-circuit voltage of organic solar cells (OSCs) is low as compared to the optical gap of the absorber molecules, indicating high energy losses per absorbed photon. These voltage losses arise only partly due to necessity of an electron transfer event to dissociate the excitons. A large part of these voltage losses is due to recombination of photo-generated charge carriers, including inevitable radiative recombination. In this work, we study the non-radiative recombination losses and we find that they increase when the energy difference between charge transfer (CT) state and ground state decreases. This behavior is in agreement with the energy-gap law for non-radiative transitions, which implies that internal conversion from CT state to ground state is facilitated by skeletal molecular vibrations. This intrinsic loss mechanism, which until now has not been thoroughly considered for OSCs, is different in its nature as compared to the commonly considered inorganic photovoltaic loss mechanisms of defect, surface, and Auger recombination. As a consequence, the theoretical upper limit for the power conversion efficiency of a single junction OSC reduces by 25% as compared to the Shockley-Queisser limit for an optimal optical gap of the main absorber between (1.45-1.65) eV.

HL 88.2 Fri 10:30 ZEU 255

Quantifying Coupling Rate Constants of Bound Charges to the Ground State and Free Charges in Organic Semiconductors — •Safa Shoaee[1], Martin Stolterfoht[1], and Ardalan Armin[2] — [1]Institute for Physics and Astronomy, University of Potsdam, Potsdam, Germany — [2]School of Mathematics and Physics, University of Queensland, Australia

Bimolecular recombination of the free charges in the donor/acceptor organic solar cells has been considered as the main loss mechanism. For very few donor/acceptor systems the bimolecular recombination rate constant is shown to be lower than what predicted by the classic Langevin model. We and others have recently shown that this suppression may originate from weaker coupling rate of the so called interfacial charge transfer states to the ground state [Burk et al. AEM 2015, Armin et al. AEM 2016]. In Particular we have shown that recombination can be 150 times less than that predicted by Langevin model, resulting in efficiencies as high as 9%, at junction $>$ 300 nm. These studies show the importance of the kinetic constants of the charge transfer states. Recently we have developed methodology to quantify these kinetic rates as well as charge generation efficiency in organic photovoltaic systems [Stolterfoht, Shoaee et al. Nature Comm 2016, Shoaee et al. Unpublished results], as well as determining the kinetic rate constants of the charge transfer states. These are pathway towards better understanding donor acceptor solar cells and optimise their photovoltaic performance for better efficiencies.

HL 88.3 Fri 10:45 ZEU 255

Energy losses in organic small molecule photovoltaics — •Theresa Linderl, Alexander Hofmann, Thomas Zechel, and Wolfgang Brütting — Universität Augsburg, 86135 Augsburg, Germany

One of the most important factors that limits the efficiency of organic photovoltaics is the relatively large energy loss between the optical gaps of the neat materials and the open-circuit voltage V_{OC}. Partly, this can be explained by the energetic offset between the energy levels of the donor and acceptor material, which is often called the driving force to form the charge transfer complex. The energy of this charge transfer complex is regarded as the upper limit for V_{OC} at 0 K. In contrast, at room temperature V_{OC} is further reduced by radiative and non-radiative recombination losses.
By combining different donors with fullerene and non-fullerene acceptor materials, we have investigated the influence of interface energetics, molecular orientation and morphology on the total energy loss in organic small molecule solar cells. We find, that for proper non-fullerene acceptor materials the overall loss can be significantly reduced to about 0.6 eV, which is comparable to the best polymer solar cells.

HL 88.4 Fri 11:00 ZEU 255

Sensitive charge transfer state spectroscopy in organic solar cells — •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 the former determine both photocurrent and open circuit voltage. In order to investigate the influence of interface structure on charge transfer state recombination, we use confocal emission and excitation spectroscopy which we developed and applied to study the reorganisation energy of single molecules [1]. Sensitive measurements of both emission and excitation spectra on the timescale of seconds enable the characterisation of environmental and molecular conformational influences on dynamic spectral properties. Using this technique, we investigate the donor–acceptor charge transfer state in diluted bulk heterojunction systems. We discuss the impact of reorganisation energy and energetic disorder on the charge transfer state distribution in systems directly relevant for organic solar cells.

[1] M. Streiter, S. Krause, C. von Borczyskowski, C. Deibel, J. Phys. Chem. Lett., 7, 4281 (2016).

Invited Talk HL 88.5 Fri 11:15 ZEU 255

Charge transfer states for organic opto-electronics — •Koen Vandewal — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, George-Bähr-Strasse 1, 01062, Dresden, Germany

Intermolecular charge transfer (CT) states at the interface between electron-donating and electron-accepting (A) materials in organic thin films are characterized by absorption and emission bands within the optical gap of the interfacing materials. Depending on the used donor and acceptor materials, CT states can be very emissive, or generate free carriers at high yield. The former can result in rather efficient organic light emitting diodes, via thermally activated delayed fluorescence, while the latter property is exploited in organic photovoltaic devices and photodetectors. In this contribution, we will discuss the fundamental properties of CT states and link them to organic opto-electronic device performance. Furthermore, we introduce a new device concept, using an optical cavity resonance effect to boost CT absorption at photon energies below the optical gap of both donor and acceptor, enabling narrow-band, near infrared (NIR) photo-detection.

15 min break

HL 88.6 Fri 12:00 ZEU 255

Interfacial Energetics in Organic Multi-Heterojunctions by Charge-Transfer Emission — •Christian Kästner[1], Koen Vandewal[2], Daniel A. M. Egbe[3], and Harald Hoppe[4] — [1]Institute of Thermodynamics and Fluid Mechanics, Technische Universität Ilmenau, Am Helmholtzring 1, 98693 Ilmenau, Germany — [2]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), George-Bähr-Str. 1, 01069 Dresden, Germany — [3]Linz Institute for Organic Solar Cells, Johannes Kepler University Linz, Altenbergerstr. 69, 4040 Linz, Austria — [4]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosphenweg 7a, 07743 Jena, Germany

Charge generation via exciton dissociation in organic solar cells requires donor-acceptor interfaces. Semi-crystalline phases of polymer and fullerene domains result in smaller energy gaps between the highest occupied molecular orbital and the lowest unoccupied molecular orbital as compared to the situation for amorphous phases. These molecular energy level shifts result in different interfacial charge transfer (CT) transitions depending on the disordered or ordered character of interfacing domains. In this work, a systematic variation of the order at the donor-acceptor interface was obtained via ternary blending of semi-crystalline and amorphous model polymers with a fullerene acceptor (PCBM). Using photo- and electroluminescence spectroscopy, various transition energies due to recombination across different donor-acceptor interfaces could be detected.

HL 88.7 Fri 12:15 ZEU 255

Charge transfer recombination at planar hybrid inorganic/organic interfaces — •Ulrich Hörmann[1], Fortunato Piersimoni[1], Stefan Zeiske[1], Lukas Hoffmann[2], Thomas Riedl[2], and Dieter Neher[1] — [1]Universität Potsdam, Potsdam, Germany — [2]Bergische Universität Wuppertal, Wuppertal, Germany

The role of the intermolecular energy gap in all-organic donor/acceptor heterojunction (HJ) solar cells is well established. In the case of hybrid inorganic/organic HJs the situation is less clear. Recently, Piersimoni et al. have shown that the energy of the hybrid charge transfer (HCT) emission in electroluminescence experiments correlates with the interface energetics determined by UPS and with the open circuit voltage (V_{oc}) of hybrid solar cells [1]. Here we focus on photovoltaic characterization of planar HJs between ZnO or SnO_x acceptor layers and different organic donor materials. Tools well established for all-organic solar cells are carefully transferred to these hybrid systems and their validity is confirmed. Reconstruction of the dark jV-curve from light intensity dependent measurement of V_{oc} and the short circuit current gets rid of the otherwise drastic influence of the series resistance in these devices and allows access to the ideality factor associated with the hybrid interface. Temperature dependent characterization in a carefully chosen operation regime allows the extraction of an effective energy gap, whose origin is – opposed to all-organic HJs – not completely clear, yet. With our combined analysis, we shed light on the nature of HCT states and their role for recombination at metal oxide/organic interfaces.

[1] Piersimoni et al. / Phys. Chem. Lett. 6, 500 (2015)

HL 88.8 Fri 12:30 ZEU 255

Overcoming interfacial losses in solution-processed organic multi-junction solar cells — •Xiaoyan Du[1], Ole Lytken[1], Hans-Peter Steinrück[1], Rainer H. Fink[1], Ning Li[2], and Christoph Brabec[2] — [1]Physical Chemistry 2 and ICMM Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) Egerlandstr. 3, 91058 Erlangen, Germany — [2]Institute of Materials for Electronics and Energy Technology (i-MEET) Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) Martensstraße 7, 91058 Erlangen, Germany

We report on a systematic study of interface losses in both single- and multi-junction solar cells based on representative polymer donors and hole transporting layers (HTLs). It is found that a facile mixed HTL containing PEDOT:PSS and MoOx nanoparticles successfully overcomes the interfacial losses in both single- and multi-junction solar cells based on various active layers by reducing interface protonation, promoting better energy-level alignment, and forming a dense and smooth layer. Multi-junction solar cells with different polymers containing nitrogen atoms as the first layer and the mixed PEDOT:PSS and MoOx nanoparticles as HTL reach fill factor (FF) of over 60%, and power conversion efficiency (PCE) of over 8% [1], while the identical stack with pristine PEDOT:PSS or MoOx nanoparticles show significantly lower performance. This work is funded by the DFG within GRK 1896. [1] X. Du, et.al, Adv. Energy Mater. 2016, DOI:10.1002/aenm.201601959

HL 88.9 Fri 12:45 ZEU 255

Following the Formation of Metal Electrodes for Organic Photovoltaics — •Franziska Löhrer[1], Volker Körstgens[1], Matthias Schwartzkopf[2], Alexander Hinz[3], Oleksandr Polonskyi[3], Thomas Strunskus[3], Franz Faupel[3], Stephan Roth[2,4], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, D-85748 Garching — [2]Deutsches Elektronensynchrotron DESY, D-22607 Hamburg — [3]CAU zu Kiel, Institut für Materialwissenschaft, D-24143 Kiel — [4]KTH, Teknikringen 56-58, SE-100 44 Stockholm

With their easy processability, high flexibility and tunable optical properties, organic photovoltaics offer a wide range of potential applications. Although based on organic materials, photovoltaic devices typically contain metal contacts due to their unrivaled electronic conductivity. These contacts have a major influence on the solar cell performance. Our work focuses on the nanostructure evolution of metal-polymer interfaces inherent in organic solar cells. We follow the morphological changes during the sputter deposition of metal electrodes onto photoactive layers using in-situ GISAXS and GIWAXS. This technique allows us to investigate the deposition process with a high spatial as well as temporal resolution. Comparing the deposition behavior of typical electrode materials (such as Au or Al) on thin films of photoactive organic materials (e.g. PTB7) helps to understand their influence on the respective photovoltaic performance.

HL 88.10 Fri 13:00 ZEU 255

Procedures and Practices for Evaluating Thin-Film Solar Cell Stability — •Roland Rösch[1], Tobias Faber[1], Monica Lira-Cantu[2], Elizabeth von Hauff[3], Thomas Brown[4], and Harald Hoppe[1] — [1]CEEC Jena, FSU Jena — [2]ICN2, Barcelona — [3]Vrije Universiteit Amsterdam — [4]University of Rome "Tor Vergata"

Novel thin film PV technologies require an attestation of their stability in order to get ready for their qualification. In order to improve the understanding of degradation effects and how they can be prevented, stress testing under different conditions is commonly applied. By careful combination of stress factors and thorough analysis of photovoltaic parameter decaying curves, an understanding of the underlying degradation pathways can be gained. With the help of standardized and accelerated stress tests, as described in the ISOS-protocols [1], statements concerning application lifetimes can finally be made and compared among different labs. Once a photovoltaic technology has proven long lasting durability, the ultimate barrier for entering the commercial market are the IEC tests, taking a deeper look on overall safety and reliability, not only on durability. Here, the most prominent stress tests are reviewed, discussed and extended with respect to learning the most about photovoltaic device stability [2]. The most prominent outcome of this discussion an analytical determination of the *burn-in* time (tS) and furthermore the operational lifetime (tS80) and the lifetime energy yield (LEY), a newly introduced figure of merit as a measure for the energy a solar cell can produce during its lifetime. [1] Reese, SOLMAT, 95 (2011) 1253-1267 [2] Roesch, AEM, 5 (2015) 1501407

HL 89: Frontiers of Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond

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

Invited Talk HL 89.1 Fri 10:30 HSZ 02

Going Beyond Conventional Functionals with Scaling Corrections and Pairing Fluctuations — •Weitao Yang — Duke University

Fractional fractional charges and fractional spins provide a clear analysis of the errors of commonly used functionals. We developed a scaling correction scheme by imposing the Perdew-Parr-Levy- Balduz linearity condition. Our novel scheme leads to the significantly improved description of dissociating molecules, transition-state species, and charge-transfer systems. Within many-electron theory, we have formulated the ground-state exchange-correlation energy in terms of pairing matrix linear fluctuations, opening new a channel for density functional approximations. This method has many highly desirable properties. It has minimal delocalization error with a nearly linear energy behavior for systems with fractional charges, describes van der Waals interactions similarly and thermodynamic properties significantly better than the conventional RPA, and captures the energy derivative discontinuity in strongly correlated systems. We also adopted pp-RPA to approximate the pairing matrix fluctuation and then determine excitation energies by the differences of two-electron addition/removal energies. This approach captures all types of interesting excitations: single and double excitations are described accurately, Rydberg excitations are in good agreement with experimental data and CT excitations display correct 1/R dependence.

Invited Talk HL 89.2 Fri 11:00 HSZ 02

Multi-reference density functional theory — •Andreas Savin — Laboratoire de Chimie Théorique, CNRS and UPMC, Univ. Paris VI, Sorbonne University, Paris, France

It is sometimes said that there is no multi-reference density functional theory. The talk presents a personal viewpoint, and will focus on the following points. 1) There are many ways to introduce multi-determinant wave functions into density functional theory. 2) Several variants have been successfully explored. 3) Difficulties inherent to ap-

proximations (both for wave functions and density functionals) persist, but can be attenuated.

Invited Talk HL 89.3 Fri 11:30 HSZ 02

Density functionals from machine learning — •Kieron Burke — UC Irvine

Machine learning is spreading to all aspects of our lives. A particular method, kernel ridge regression, has proven very useful for fitting and interpolating in high-dimensional spaces.

Several years ago, in collaboration with the group of Klaus-Robert Muller in computer science at TU Berlin, we demonstrated how to construct a machine-learned density functional on a simple toy problem, non-interacting fermions in a box. We showed both its successes and limitations. We have continued to develop this method (PRL, 2012).

I will report on two recent works. In the first (arXiv:1609.02815), we construct the non-interacting kinetic energy functional for small molecules in 3D using a basis. We avoid the challenge of finding functional derivatives by learning the potential to density map directly, thereby bypassing the need to solve the Kohn-Sham equations.

In the second, we learn the interacting functional directly for the first time. In 1D, we model chains of H atoms of different length, and learn F[n] itself, from highly accurate DMRG calculations. With a novel choice of basis for the densities, we are able to learn the functional to chemical accuracy in the thermodynamic limit (arXiv:1609.03705).

Invited Talk HL 89.4 Fri 12:00 HSZ 02

Taming Memory-Dependence in Time-Dependent Density Functional Theory — •Neepa Maitra — Hunter College of the City University of New York

The exact exchange-correlation functional of time-dependent density functional theory (TDDFT) is known to depend on the history of the densities and the initial states, a dependence which is ignored in almost all of the calculations today that use an adiabatic approximation. The lack of this dependence can sometimes lead to drastically incorrect predictions of the dynamics, as has been shown in several examples recently. We present here a new approach to developing functional approximations that breaks free of the adiabatic approximation, and test the resulting approximations on a number of model systems.

Invited Talk HL 89.5 Fri 12:30 HSZ 02

Quantum Embedding Theories — •Fred Manby — School of Chemistry, University of Bristol, Cantock's Close, Bristol, BS8 1TS, UK

Issues of accuracy in density functional theory can be addressed by making more accurate methods (like coupled-cluster theory) more efficient; or by making density functional approximations more accurate. Efforts in both directions are underway in our group, but in this talk I will focus on a third possibility, namely the development of quantum-mechnical multiscale models that enable the use of a high-accuracy method in a small, physically important region coupled to density-functional theory (or other low-cost methods) to describe the molecular environment.

HL 90: Inhomogeneous Materials for Solar Cells

Time: Friday 11:30–13:00 Location: POT 81

HL 90.1 Fri 11:30 POT 81

Tailoring the electronic properties of semiconducting nanocrystal-solids: InAs embedded in SnS_x matrices — •Emilio Scalise[1], Stefan Wippermann[1], Giulia Galli[2], and Dmitri Talapin[2] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]The University of Chicago, Chicago, Illinois, USA

Recent advances in wet chemical techniques enable the facile synthesis of nanocrystals (NCs) and their assembly into complex solid structures (NC-solids), offering exciting prospects for solar energy conversion, light emission and electronic applications. The properties of these composites are strongly determined by structural details at the NC/matrix interface and the composition of the embedding matrix. We carried out a systematic study of the interaction between InAs NCs and SnS_x matrices using a grand canonical *ab initio* thermodynamics approach to identify general trends for the stability of structural motifs possibly occurring at the NC/matrix interface. The resulting models have been used as a basis for *ab initio* molecular dynamics calculations to investigate the impact of different mass densities and stoichiometries on the internal matrix structure and the NC-solids' electronic properties. We demonstrate that both the NC-matrix interface and the internal regions of the matrix show complex structural features, depending on specific synthesis conditions. Thus to obtain a detailed understanding of experimental data it is necessary to take into account such complex interfacial and matrix-internal structures beyond simplified NC-solid models. S. W. acknowledges BMBF NanoMatFutur grant 13N12972.

HL 90.2 Fri 11:45 POT 81

Formation process of the CIGSe absorber layers in a sequential process — •Sven Schönherr, Philipp Schöppe, Michael Oertel, Udo Reislöhner, and Carsten Ronning — Institut für Festkörperphysik, Friedrich Schiller Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

$Cu(In,Ga)Se_2$ (CIGSe) solar cells processed in a sequential process lead to high efficiencies of light conversion. However, the formation of the CIGSe absorber layer in such a process is still not completely clarified. In our process, the metallic precursor on top of a molybdenum back contact was reactively annealed in two steps in a selenium vapour atmosphere where it is typically converted to a CIGSe absorber layer. For a better understanding of the CIGSe formation process we varied the substrate temperature in the first step and aborted the selenization prematurely. X-ray diffraction measurements at the partly selenized layers were taken to indicate binary and chalcopyrite phases. For a detailed characterization, 200 nm thick lamellas were prepared with a focused ion beam. The thin cross sections lead to a high spatial resolution which is mainly limited by the diameter of the electron beam. Energy dispersive X-ray spectroscopy measurements were taken to measure the local element composition. Additionally, cathodoluminescence measurements at the lamellas were used to locate CIGSe chalcopyrite phases and to show where these phases arise during the selenization.

HL 90.3 Fri 12:00 POT 81

Band gap changes in $Cu_2ZnSn(S,Se)_4$ solar cell absorbers with varying Cu concentration — •Mario Lang[1], Tobias Renz[1], Niklas Mathes[1], Markus Neuwirth[1], Thomas Schnabel[2], Simon Woska[1], Heinz Kalt[1], and Michael Hetterich[1,3] — [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, KIT, 76131 Karlsruhe, Germany

The efficiency of $Cu_2ZnSn(S,Se)_4$ solar cells highly depends on the composition of the absorber layer. A Cu-poor and Zn-rich composition is crucial for highly efficient devices. This is due to the fact that unwanted and harmful secondary phases and defects are reduced in this case. The effect of the Cu content is not only relevant for the efficiency but also for certain optical device parameters as, e.g., the band gap. In this contribution we analyse the influence of the Cu content of Cu-poor $Cu_2ZnSn(S,Se)_4$ solar cell absorbers on several optical properties and device parameters. We find an increase in band gap with decreasing Cu content whereas the band tailing does not change. Furthermore, the defect luminescence shifts in parallel to the band gap but does also not change its nature.

HL 90.4 Fri 12:15 POT 81

Effect of buffer layer cations on absorber dopant profiles of Cu(In,Ga)Se2 thin film solar cells — •Florian Werner, Michele Melchiorre, Hossam Elanzeery, and Susanne Siebentritt — Laboratory for Photovoltaics, Physics and Materials Science Research Unit, University of Luxembourg, 41 rue du Brill, L-4422 Belvaux, Luxembourg

The correct interpretation of apparent dopant profiles obtained by capacitance-based techniques on chalcopyrite thin film solar cell absorbers is still debated. We have recently shown that Cd in-diffusion into the absorber might in part explain the observed dopant pro-

files. We expand on this study by comparing frequency-dependent capacitance-voltage measurements of different buffer/window stacks, e.g. CdS/ZnO, Zn(O,S)/ZnO, and MgF2, on the same absorber. Deconvolution of the measured impedance spectra allows to separate the capacitance of the main junction from parasitic elements. We find parasitic capacitances which agree reasonably well with the geometric capacitance of the respective buffer layer. Dopant profiles constructed from the extracted voltage-dependent junction capacitance exhibit significant differences between different buffer/window configurations and are consistent with cation in-diffusion reducing the surface-near acceptor concentration. This in-diffusion gives rise to a depth-dependent dopant profile and is more pronounced for Cd than for Zn. The MgF2 layer in contrast appears to be stable and we obtain depth-independent dopant concentrations close to 1017 cm-3, comparable to the free hole concentration obtained by Hall measurements on similar absorbers.

HL 90.5 Fri 12:30 POT 81

Charge Carriers Dynamics in Kesterite Band Tails: From Ultra-fast Trapping via Hopping Transport to Cryogenic Microsecond Recombination — •Hannes Hempel[1], Rainer Eichberger[2], and Thomas Unold[1] — [1]Department structure and dynamics of energy materials, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109, Berlin, Germany — [2]Institute for solar fuels, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Kesterite solar cells are known to exhibit band tails originating from atomic disorder. We investigate how these tails affect the dynamics of photo-excited charge carrier by applying transient absorption, time resolved THz spectroscopy and photoluminescence spectroscopy to co-evaporated $Cu_2ZnSnSe_4$ thin film. 100 fs after excitation with 1.5 eV photons the carriers form a hot (>1100 K) Boltzmann distribution in the band states. Within 2 ps they thermalize to lattice temperature and reach simultaneously band edge and tail states. After 10 ps up to 10^{17} cm^{-3} carriers are additionally captured into deeper defect states. Then the carriers are distributed in bands, tails and defects and exhibit in average a localized AC-mobility with a DC-value of 100 cm^2/Vs. Their transport can be described by a sequence of trapping and detrapping between extended band and localized tail states. At low temperatures the carriers further localize into these tail states which slows down their hopping transport to the recombination sites and increases the measured lifetime from nano to microseconds.

HL 90.6 Fri 12:45 POT 81

Intermediate gap states in core/shell nanoparticles for solar energy conversion — •Musa Alaydrus[1], Marton Vörös[2], Gergely Zimanyi[3], and Stefan Wippermann[1] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [2]Argonne National Lab, Chicago, USA — [3]University of California, Davis, USA

Multi-exciton generation (MEG) and intermediate band (IB) transitions in semiconducting nanoparticles (NPs) are promising paths towards surpassing the Shockley-Queisser limit in solar energy conversion devices. Recent studies demonstrate MEG to be more efficient in NPs than in the bulk. However, quantum confinement effects believed to be responsible for efficient MEG in NPs, also increase their optical gap, swiftly shifting the MEG threshold beyond the solar spectrum. We propose to introduce intermediate states inside the gap to lower the optical absorption threshold and possibly provide additional pathways for multi-exciton processes at energies lower than the fundamental NP gap. We investigate the formation of such intermediate states in core/shell NPs from first principles.