Semiconductor Physics Division
Fachverband Halbleiterphysik (HL)

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Overview of Invited Talks and Sessions

(Lecture rooms: ER 164, ER 270, EW 54, EW 201, EW 202, and EW 203; Posters: B and F)

Invited Talks

HL 1.1	Sun	16:00–16:45	H 1058	**Challenges in the theoretical description of structures and processes at electrochemical interfaces** — •Axel Gross
HL 1.2	Sun	16:50–17:35	H 1058	**Raman under water - Of photons, phonons and the fun of tuning the Fermi level** — •Katrin F. Domke
HL 1.3	Sun	17:40–18:25	H 1058	**Scanning probe microscopies for electrochemical problems** — •Gunther Wittstock
HL 4.1	Mon	9:30–10:00	EW 201	**Exploring the optical properties of 1D nanomaterials at sub-nanometer scale with a direct correlation to its structure at atomic scale** — •Jordi Arbiol
HL 4.7	Mon	11:30–12:00	EW 201	**Studying single semiconductor nanowires using a hard X-ray nanoprobe** — •Gema Martinez-Criado
HL 13.1	Mon	15:00–15:30	EW 201	**Light-matter interaction in wire cavities - from Purcell effect to Bose-Einstein condensates** — •Rüdiger Schmidt-Grund
HL 13.7	Mon	17:00–17:30	EW 201	**Quantum Transport in Core/Shell Semiconductor Nanowires** — •Thomas Schäpers, Fabian Haas, Patrick Zellekens, Torsten Rieger, Tobias Wenz, Yusuf Günel, Önder Gül, Natalia Demarina, Mihail Lepsa, Hans Lüth, Detlev Grützmacher
HL 15.1	Mon	15:00–15:30	EW 203	**Semiconductor-based plasmonics** — •Fritz Henneberger, Sascha Kalusniak, Sergey Sadofev
HL 22.1	Tue	9:30–10:00	ER 164	**Ultrastrong coupling regime of excitons interacting with microcavity photons or localized surface plasmons** — •Salvatore Savasta
HL 31.1	Tue	10:30–11:00	EW 201	**Bruno K. Meyer: Excitons, defects and impurities in nitrides and oxides** — •Axel Hoffmann
HL 40.1	Wed	9:30–10:00	ER 164	**Boon and bane of polarization induced effects in group III-nitride based heterostructures** — •Oliver Ambacher
HL 40.5	Wed	10:45–11:15	ER 164	**Overview of theoretical aspects of semi-polar and non-polar nitride surfaces** — •John Northrup
HL 48.1	Wed	11:00–11:30	EW 201	**Transformation Optics: From Fundamentals to Applications for Energy Harvesting** — •Martin Wegener, Martin Schumann
HL 48.2	Wed	11:30–12:00	EW 201	**Nanostructures and materials for intermediate band solar cells** — •Antonio Martí
HL 51.3	Wed	15:30–16:00	ER 164	**Impact of reduced polarization fields on the optical properties of semipolar nitride quantum wells** — •Mitsuru Funato, Yoichi Kawakami
HL 54.1	Wed	15:00–15:30	EW 201	**Nanophotonic light harvesting concepts from the visible to the mid-infrared** — •Stefan A Maier
HL 54.2	Wed	15:30–16:00	EW 201	**Material Design of Luminescent Glasses and Glass Ceramics for White-LED Applications** — •Stefan Schweizer, Franziska Steudel, Sebastian Loos, Bernd Ahrens, Peter Nolte, Florian Wagner
HL 62.1	Thu	9:30–10:00	ER 270	**Folded Graphene - Solid State Physics in a Nutshell** — •Rolf J. Haug, Johannes C. Rode, Hennrik Schmidt, Dmitri Smirnov
HL 64.1	Thu	9:30–10:00	EW 202	**Energy efficient optical interconnects for datacom and HPCs** — •Dieter Bimberg

HL 64.2	Thu	10:00–10:30	EW 202	**Plasmonic and Metallic Cavity Semiconductor Nanolasers for Ultimate Miniaturization** — •C.Z. Ning
HL 64.3	Thu	10:30–11:00	EW 202	**Polymer waveguides for electro-optical integration in data centers** — •Roger Dangel, Jens Hofrichter, Folkert Horst, Daniel Jubin, Antonio La Porta, Norbert Meier, Jonas Weiss, Bert Jan Offrein
HL 64.4	Thu	11:15–11:45	EW 202	**Silicon Photonics for Optical Interconnects** — •Roel Baets
HL 64.5	Thu	11:45–12:15	EW 202	**Long wavelength VCSELs for optical interconnects** — •Markus Amann
HL 78.1	Thu	12:30–13:00	ER 164	**Electrical spin injection into high mobility 2DEG systems** — Martin Oltscher, •Mariusz Ciorga, Josef Loher, Dieter Schuh, Dominique Bougeard, Dieter Weiss
HL 82.1	Thu	15:00–15:30	EW 202	**Group IV GeSn alloys - a viable solution for Si-based light emitters** — •Dan Buca, Stephan Wirths, Siegfried Mantl, Detlev Grützmacher
HL 99.1	Fri	9:30–10:00	EW 202	**Fractional quantum Hall effect states in ultrahigh mobility two-dimensional electron systems** — •Werner Wegscheider, Christian Reichl, Jun Chen, Werner Dietsche, Stephan Baer, Lars Tiemann, Szymon Hennel, Clemens Rössler, Thomas Ihn, Klaus Ensslin

Invited talks of the joint symposium SYOP

See SYOP for the full program of the symposium.

SYOP 1.1	Mon	15:00–15:30	H 0105	**Formation mechanisms of covalent nanostructures** — •Jonas Björk
SYOP 1.2	Mon	15:30–16:00	H 0105	**Selective C-H Activation and C-C coupling on Metal Surfaces** — •Lifeng Chi
SYOP 1.3	Mon	16:00–16:30	H 0105	**On-Surface Synthesis on Insulating Substrates** — •Angelika Kuehnle
SYOP 1.4	Mon	16:45–17:15	H 0105	**On-surface polymerization - a synthetic route to 2D polymers** — •Markus Lackinger
SYOP 1.5	Mon	17:15–17:45	H 0105	**On-surface azide-alkyne click chemistry and a novel metal-organic network based on Cu adatom trimers** — •Trolle Linderoth

Invited talks of the joint symposium SYNP

See SYNP for the full program of the symposium.

SYNP 1.1	Tue	9:30–10:00	H 0105	**Connectomics: The dense reconstruction of neuronal circuits** — •Moritz Helmstädter
SYNP 1.2	Tue	10:00–10:30	H 0105	**Whole-brain imaging and analysis of network activity in behaving zebrafish** — •Misha Ahrens
SYNP 1.3	Tue	10:30–11:00	H 0105	**Circuit neurophysics: Theory and biophysics of information-flow through large-scale neuronal systems** — •Fred Wolf
SYNP 1.4	Tue	11:15–11:45	H 0105	**Cognitive devices based on ion currents in oxide thin films** — •Stuart Parkin
SYNP 1.5	Tue	11:45–12:15	H 0105	**Distributed neuro-physical interfaces: technology and "exciting" biophysics** — •Shy Shoham

Invited talks of the joint symposium SYMM

See SYMM for the full program of the symposium.

SYMM 1.1	Thu	9:30–10:15	H 0105	**From MAX to MXene - From 3D to 2D** — •Michel Barsoum
SYMM 1.2	Thu	10:15–10:45	H 0105	**Structure evolution during low temperature growth of nanolaminate thin films** — •J.M. Schneider, L. Shang, H. Bolvardi, Y. Jiang, A. Al Gaban, D. Music, M. to Baben
SYMM 1.3	Thu	11:00–11:30	H 0105	**Autonomous healing of crack damage in MAX phase ceramics** — •Willem G. Sloof
SYMM 1.4	Thu	11:30–12:00	H 0105	**Magnetic MAX phases from first principles and thin film synthesis** — •Johanna Rosen
SYMM 1.5	Thu	12:00–12:30	H 0105	**Weak Field Magneto-Transport Properties of Mn+1AXn Phases** — •Thierry Ouisse, Lu Shi, Benoit Hackens, Benjamin Piot, Didier Chaussende

Invited talks of the joint symposium SYME

See SYME for the full program of the symposium.

SYME 1.1	Fri	9:30–10:00	H 0105	**Excitations and charge transfer phenomena in C based systems** — •Elisa Molinari
SYME 1.2	Fri	10:00–10:30	H 0105	**Towards optimal correlation factors for many-electron perturbation theories** — •Andreas Grüneis
SYME 1.3	Fri	10:30–11:00	H 0105	**Towards an ab-initio description of high temperature superconductivity** — •Garnet Chan
SYME 1.4	Fri	11:15–11:45	H 0105	**Correlation effects in unconventional superconductors: from micro- to nano- and macroscales.** — •Roser Valenti
SYME 1.5	Fri	11:45–12:15	H 0105	**Stochastic density functional and GW theories scaling linearly with system size** — •Roi Baer, Daniel Neuhauser, Eran Rabani

Sessions

HL 1.1–1.3	Sun	16:00–18:25	H 1058	**Tutorial: Electro chemistry 4 condensed matter physicists**
HL 2.1–2.6	Mon	9:30–11:00	ER 164	**Organic-inorganic perovskite semiconductors (with O)**
HL 3.1–3.8	Mon	9:30–11:30	ER 270	**Graphene: THz, NIR and transport properties (with O/TT)**
HL 4.1–4.12	Mon	9:30–13:15	EW 201	**Focus Session (with TT): Functional semiconductor nanowires I**
HL 5.1–5.9	Mon	9:30–11:45	EW 202	**Photovoltaics: CIGS and related compounds**
HL 6.1–6.14	Mon	9:30–13:00	H 2032	**Organic electronics and photovoltaics (DS with HL/CPP)**
HL 7.1–7.13	Mon	9:30–13:00	H 3005	**Transport: Quantum coherence and quantum information systems - Theory (TT with HL)**
HL 8.1–8.9	Mon	9:30–12:00	A 053	**Transport: Spintronics and magnetotransport (TT with HL)**
HL 9.1–9.11	Mon	10:00–13:00	EW 203	**Quantum dots: Optical properties**
HL 10.1–10.7	Mon	11:15–13:00	ER 164	**Photovoltaics: Kesterites and less widely used materials (with DF)**
HL 11.1–11.5	Mon	11:45–13:00	ER 270	**Transition-metal dichalcogenides and boron nitride (with O)**
HL 12.1–12.9	Mon	15:00–17:15	ER 164	**Graphene: mostly Theory (with O/TT)**
HL 13.1–13.12	Mon	15:00–18:45	EW 201	**Focus Session (with TT): Functional semiconductor nanowires II**
HL 14.1–14.7	Mon	15:00–16:45	EW 202	**Organic photovoltaics and electronics - mostly cell design (with DS)**
HL 15.1–15.1	Mon	15:00–15:30	EW 203	**Invited Talk Fritz Henneberger**
HL 16.1–16.9	Mon	15:00–17:15	H 0110	**Transport: Quantum coherence and quantum information systems - Experiments (TT with HL)**
HL 17.1–17.9	Mon	15:00–17:45	A 053	**Transport: Topological insulators 1 (TT with DS/HL)**
HL 18.1–18.6	Mon	15:45–17:15	EW 203	**Plasmons, plasmonic laser, and spaser**
HL 19.1–19.8	Mon	17:00–19:00	EW 202	**Organic photovoltaics and electronics - mostly properties of the absorber (with DS)**
HL 20.1–20.22	Mon	15:00–20:00	Poster B	**Poster IA (Ultrafast phenomena; Optical properties; Transport; Theory)**
HL 21.1–21.33	Mon	15:00–20:00	Poster B	**Poster IB (Oxide semiconductors; II-VI and group IV semiconductors; Nanotubes and Buckyballs)**
HL 22.1–22.1	Tue	9:30–10:00	ER 164	**Invited Talk Salvatore Savasta**
HL 23.1–23.8	Tue	9:30–11:30	ER 270	**Spintronics: Excitons and local spins (with MA/TT)**
HL 24.1–24.13	Tue	9:30–13:00	EW 202	**Thermoelectricity**
HL 25.1–25.6	Tue	9:30–11:00	EW 203	**Quantum dots: Microcavities and microlaser**
HL 26.1–26.13	Tue	9:30–13:00	C 130	**Organic electronics and photovoltaics: Transport of charges - from molecules to devices (CPP with HL/TT)**
HL 27.1–27.7	Tue	9:30–13:00	H 2032	**Doped Si nanostructures (DS with HL/TT)**
HL 28.1–28.12	Tue	9:30–13:00	H 3005	**Transport: Topological insulators 2 (TT with HL/DS)**
HL 29.1–29.10	Tue	9:30–12:15	A 053	**Transport: Graphene (TT with CPP/DS/DY/HL/O)**
HL 30.1–30.6	Tue	10:15–11:45	ER 164	**Photovoltaics: Nanostructured materials**
HL 31.1–31.1	Tue	10:30–11:00	EW 201	**Invited Talk in honor of Bruno K. Meyer: Axel Hoffman**
HL 32.1–32.10	Tue	10:30–13:00	MA 041	**Graphene: Growth & intercalation (O with HL/TT)**
HL 33.1–33.11	Tue	10:30–13:30	MA 004	**Frontiers of Electronic Structure Theory: Nuclear Dynamics, Methods**
HL 34.1–34.7	Tue	11:15–13:00	EW 201	**Nitrides: Dots, rods, and structures**

HL 35.1–35.6	Tue	11:15–12:45	EW 203	**Semiconductor laser**
HL 36.1–36.7	Tue	14:00–16:00	C 130	**Organic electronics and photovoltaics: OPV I (CPP with HL/TT)**
HL 37.1–37.8	Tue	14:00–16:00	H 0110	**Transport: Topological insulators 3 (TT with HL/DS)**
HL 38.1–38.6	Tue	14:00–15:45	MA 004	**Frontiers of electronic structure theory: Charge and spin dynamics**
HL 39.1–39.38	Tue	14:00–20:00	Poster F	**Posters II (Topological insulators; Graphene; Spintronics and spin physics; Quantum information science)**
HL 40.1–40.5	Wed	9:30–11:15	ER 164	**Focus Session: Role of polarization fields in nitride devices I**
HL 41.1–41.8	Wed	9:30–11:30	ER 270	**Topological insulators: Theory (with DS/MA/O/TT)**
HL 42.1–42.9	Wed	9:30–12:00	EW 015	**Devices**
HL 43.1–43.5	Wed	9:30–10:45	EW 202	**Ultra-fast phenomena**
HL 44.1–44.13	Wed	9:30–13:00	EW 203	**Quantum dots: Preparation and characterization**
HL 45.1–45.13	Wed	9:30–13:00	C 130	**Organic electronics and photovoltaics: OPV II (CPP with HL/TT)**
HL 46.1–46.9	Wed	10:30–13:00	MA 041	**Graphene: Dynamics (O with HL/TT)**
HL 47.1–47.11	Wed	10:30–13:30	MA 004	**Frontiers of electronic structure theory: Organics and materials**
HL 48.1–48.6	Wed	11:00–13:00	EW 201	**Focus Session (with O): Nanophotonic concepts and materials for energy harvesting - Plasmonics, transformation optics, upconversion, and beyond I**
HL 49.1–49.8	Wed	11:00–13:00	EW 202	**Quantum information systems: mostly concepts (with TT)**
HL 50.1–50.5	Wed	11:45–13:00	ER 270	**Topological insulators: Transport (with MA/O/TT)**
HL 51.1–51.6	Wed	15:00–16:45	ER 164	**Focus Session: Role of polarization fields in nitride devices II**
HL 52.1–52.6	Wed	15:00–16:30	ER 270	**Topological insulators: Structure and electronic structure (with DS/MA/O/TT)**
HL 53.1–53.4	Wed	15:00–16:00	EW 015	**Photonic crystals**
HL 54.1–54.4	Wed	15:00–16:30	EW 201	**Focus Session: Nanophotonic concepts and materials for energy harvesting - Plasmonics, transformation optics, upconversion, and beyond II**
HL 55.1–55.7	Wed	15:00–16:45	EW 203	**Quantum dots: Interaction with environment**
HL 56.1–56.13	Wed	15:00–18:30	MA 004	**Frontiers of electronic structure theory: Optical excitations**
HL 57.1–57.7	Wed	16:15–18:00	EW 015	**Optical properties of bulk semiconductors**
HL 58.1–58.9	Wed	16:30–18:45	EW 202	**OFETs, OLEDs, and organic optoelectronics**
HL 59.1–59.8	Wed	16:45–18:45	ER 270	**Graphene: Applications, luminescence and spin relaxation (HL with O/TT)**
HL 60.1–60.6	Wed	17:15–18:45	EW 203	**Quantum dots: Transport**
HL 61.1–61.42	Wed	15:00–20:00	Poster F	**Posters III (Organic-inorganic perovskite semiconductors; Organic photovoltaics and electronics; Photovoltaics; Energy science; New materials and concepts)**
HL 62.1–62.1	Thu	9:30–10:00	ER 270	**Invited Talk Rolf Haug**
HL 63.1–63.8	Thu	9:30–11:30	EW 015	**Group IV elements and compounds**
HL 64.1–64.7	Thu	9:30–12:45	EW 202	**Focus Session: Optical interconnects - Materials, devices, and integration**
HL 65.1–65.9	Thu	9:30–12:45	H 2032	**Focus Session (DS with HL): Oxide semiconductors I**
HL 66.1–66.11	Thu	9:30–13:00	C 130	**Focus Session (CPP with HL): Hybrid photovoltaics and perovskites I**
HL 67.1–67.10	Thu	9:30–12:00	EB 202	**Topological insulators I (MA with HL/TT)**
HL 68.1–68.6	Thu	9:30–11:00	H 3010	**Low-dimensional systems: Molecular conductors (TT with CPP/HL/MA/O)**
HL 69.1–69.8	Thu	9:30–13:00	EB 407	**GHz Dielectrics - Materials for mobile communication I (DF with HL/MM)**
HL 70.1–70.9	Thu	10:00–12:30	ER 164	**Spintronics: Mobile electrons and holes (with MA/TT)**
HL 71.1–71.9	Thu	10:15–12:30	EW 201	**New concepts and new materials**
HL 72.1–72.6	Thu	10:15–11:45	EW 203	**Quantum wires**
HL 73.1–73.10	Thu	10:30–13:00	MA 041	**Graphene: Structure (O with HL/TT)**
HL 74.1–74.10	Thu	10:30–13:15	MA 004	**Frontiers of electronic structure theory: 2D TMDC and excitonic effects**

HL 75.1–75.8	Thu	11:00–13:00	A 053	**Transport: Quantum dots, quantum wires, point contacts 1 (TT with HL)**
HL 76.1–76.6	Thu	11:30–13:00	EW 015	**Carbon nanotubes**
HL 77.1–77.6	Thu	11:30–13:00	H 3010	**Low-dimensional systems: Topological order 1 (TT with HL)**
HL 78.1–78.1	Thu	12:30–13:00	ER 164	**Invited Talk Mariusz Ciorga**
HL 79.1–79.8	Thu	15:00–17:00	ER 164	**Quantum information systems: Si vacancies and NV centers (with TT)**
HL 80.1–80.9	Thu	15:00–17:15	EW 015	**Challenges in semiconductor theory**
HL 81.1–81.12	Thu	15:00–18:15	EW 201	**Heterostructures and interfaces**
HL 82.1–82.1	Thu	15:00–15:30	EW 202	**Invited Talk Dan Buca**
HL 83.1–83.12	Thu	15:00–19:00	H 2032	**Focus Session: Oxide semiconductors II (DS with HL)**
HL 84.1–84.10	Thu	15:00–18:15	C 130	**Focus Session (CPP with HL): Hybrid photovoltaics and perovskites II**
HL 85.1–85.11	Thu	15:00–17:45	EB 202	**Topological Insulators 2 (MA with HL/TT)**
HL 86.1–86.12	Thu	15:00–18:30	A 053	**Transport: Quantum dots, quantum wires, point contacts 2 (TT with HL)**
HL 87.1–87.13	Thu	15:00–18:30	H 3010	**Low-dimensional systems: Topological order 2 (TT with DS/HL/MA/O)**
HL 88.1–88.5	Thu	15:00–17:00	EB 407	**GHz Dielectrics - Materials for mobile communication II (DF with DY/HL/MM)**
HL 89.1–89.13	Thu	15:00–18:15	MA 041	**Graphene: Electronic structure (O with HL/TT)**
HL 90.1–90.14	Thu	15:00–18:45	H 0111	**Phase change / resistive switching (DS with HL)**
HL 91.1–91.13	Thu	15:00–18:30	MA 004	**Frontiers of electronic structure theory: Many-body effects, methods**
HL 92.1–92.8	Thu	15:45–17:45	EW 202	**VCSELs, optical interconnects and Si photonics**
HL 93.1–93.8	Thu	15:45–17:45	EW 203	**III-V semiconductors (other than nitrides)**
HL 94.1–94.13	Thu	14:00–20:00	Poster B	**Poster IV A (Laser; Devices; Heterostructures; Surfaces, interfaces and defects)**
HL 95.1–95.31	Thu	14:00–20:00	Poster B	**Poster IV B (Quantum dots and wires: Prepration, characterization, optical properties, and transport)**
HL 96.1–96.23	Thu	14:00–20:00	Poster B	**Poster III C (III-V Semiconductors incl. Nitrides)**
HL 97.1–97.6	Fri	9:30–11:00	ER 164	**Quantum dots and wires: Pillars and cavities**
HL 98.1–98.11	Fri	9:30–12:30	EW 201	**Nitrides: Bulk material, films, surfaces and quantum wells**
HL 99.1–99.1	Fri	9:30–10:00	EW 202	**Invited Talk Werner Wegscheider**
HL 100.1–100.10	Fri	9:30–12:15	EW 203	**ZnO and its relatives**
HL 101.1–101.5	Fri	9:30–12:15	H 0105	**Frontiers of electronic structure theory: Many-body effects on the nano-scale**
HL 102.1–102.7	Fri	9:30–12:00	C 130	**Organic electronics and photovoltaics: Devices (CPP with HL/TT)**
HL 103.1–103.9	Fri	9:30–12:00	EB 202	**Spintronics incl. quantum dynamics (MA with HL/TT)**
HL 104.1–104.10	Fri	9:30–12:15	H 0110	**Transport: Molecular electronics (TT with CPP/HL/MA/O)**
HL 105.1–105.10	Fri	9:30–12:15	H 0104	**Transport: Majorana fermions (TT with DS/HL/MA/O)**
HL 106.1–106.11	Fri	10:00–13:00	EW 202	**Transport, magnetotransport and quantum Hall physics**
HL 107.1–107.10	Fri	10:15–13:00	EW 015	**Microcavities, polaritons and condensates**
HL 108.1–108.9	Fri	10:30–12:45	MA 041	**Graphene: Intercalation (O with HL/TT)**
HL 109.1–109.8	Fri	11:15–13:15	ER 164	**Quantum dots and wires: Quantum communication and quantum information science**

Annual General Meeting of the Semiconductor Physics Division

Donnertag 18:00–19:00 EW 015

- Bericht
- Wahl
- Verschiedenes

HL 1: Tutorial: Electro chemistry 4 condensed matter physicists

Organized by Erich Runge and Jörg Neugebauer on behalf of the Semiconductor Physics Division (HL) and the Metal and Material Physics Division (MM), respectively.

Time: Sunday 16:00–18:25 Location: H 1058

Invited Talk HL 1.1 Sun 16:00 H 1058

Challenges in the theoretical description of structures and processes at electrochemical interfaces — •Axel Gross — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany — Helmholtz Institut Ulm, 89069 Ulm, Germany

In spite of its technological relevance in the energy conversion and storage, our knowledge about the microscopic structure of electrochemical electrode-electrolyte interfaces is still rather limited. The theoretical description of these interfaces is hampered by three challenges [1]. i) In electrochemistry, structures and properties of the electrode-electrolyte interfaces are governed by the electrode potential which adds considerable complexity to the theoretical treatment since charged surfaces have to be considered. ii) The theoretical treatment of processes at solid-liquid interfaces includes a proper description of the liquid which requires to determine free energies instead of just total energies. This means that computationally expensive statistical averages have to be performed. iii) Electronic structure methods based on density functional theory (DFT) combine numerical efficiency with a satisfactory accuracy which makes them appropriate for electrochemical systems. However, there are severe shortcomings of the DFT description of liquids, in particular water, using current functionals.

In this tutorial talk, I will give an overview over concepts and theoretical methods for the realistic description of electrochemical interfaces. Examples of insights gained from theoretical studies will be presented but open challenges will be identified as well.

[1] N.G. Hörmann *et al.*, J. Power Sources **275**, 531 (2015).

Short break

Invited Talk HL 1.2 Sun 16:50 H 1058

Raman under water - Of photons, phonons and the fun of tuning the Fermi level — •Katrin F. Domke — MPI for Polymer Research, Ackermannweg 10, D-55128 Mainz

t.b.a.

Short break

Invited Talk HL 1.3 Sun 17:40 H 1058

Scanning probe microscopies for electrochemical problems — •Gunther Wittstock — Carl v. Ossietzky University of Oldenburg, School of Mathematics and Science, Department of Chemistry, D-26111 Oldenburg

Electrified solid-liquid interfaces are characterized by a vertical and horizontal inhomogeneity in structure. Even well prepared single crystal electrodes show, adatoms, steps kinks and other defects. The investigation of such structures by STM has dramatically enhanced our understanding of such interfacial structures. However, the experiments were mostly performed in the absence of a Faradayic reaction (.i.e. electrolysis). With a few exceptions, electrodes are designed for controlling Faradayic reactions. High current densities are requested for efficient energy conversion devices; very low current densities are a requirement for materials that shall resist corrosion under harsh environments. Such materials (polycrystalline, multiphase or composites) show a large variation of local current densities that are neither accessible by I-V-curves nor by STM. Scanning electrochemical microscopy (SECM) provides this information. It uses the electrolysis current of a dissolved redox-active compound at a probe microelectrode to generate the signal. The electrolysis at the probe is coupled to local reaction at the sample by diffusion of reactants in the probe-sample gap. Different working modes and examples will be explained with the aim to differentiate between fundamental barriers and current instrumental limitations that might be overcome by the impact of well trained physicist.

HL 2: Organic-inorganic perovskite semiconductors (with O)

Time: Monday 9:30–11:00 Location: ER 164

HL 2.1 Mon 9:30 ER 164

Tunable ferroelectric polarization and its interplay with spin-orbit coupling in tin iodide perovskites — •Silvia Picozzi[1], Alessandro Stroppa[1], Domenico Di sante[1], Paolo Barone[1], Menno Bodkam[2], Georg Kresse[2], Cesare Franchini[2], and Myung-hwan Whangbo[3] — [1]CNR SPIN L'Aquila (IT) — [2]Univ. Vienna, Fac. Physics Wien (AT) — [3]North Carolina State Univ. Raleigh (USA)

Ferroelectricity is a potentially crucial issue in halide perovskites, breakthrough materials in photovoltaic research. Using density functional theory simulations and symmetry analysis, we show [1] that the lead-free perovskite iodide (FA)SnI3, containing the planar formamidinium cation FA, (NH2CHNH2)+, is ferroelectric (FE). In fact, the perpendicular arrangement of FA planes, leading to a "weak" polarization, is energetically more stable than parallel arrangements of FA planes. Moreover, we show that the "weak" and "strong" FE states with polar axis along different crystallographic directions are energetically competing. Therefore, at least at low temperatures, an electric field could stabilize different states with the polarization rotated by 45 degrees, resulting in a highly tunable ferroelectricity appealing for multi-state logic. Intriguingly, the relatively strong spin-orbit coupling in non-centrosymmetric (FA)SnI3 gives rise to a coexistence of Rashba and Dresselhaus effects and to a spin-texture that can be induced, tuned and switched by an electric field.

[1] A.Stroppa, D.Di Sante, P.Barone, M.Bodkam, G.Kresse, C.Franchini and S.Picozzi, Nature Comms. (in press)

HL 2.2 Mon 9:45 ER 164

In situ XRD monitoring of phases formed during growth of co-evaporated perovskite thin films — •Juliane Borchert[1], Paul Pistor[1], Wolfgang Fränzel[1], René Csuk[2], and Roland Scheer[1] — [1]Martin-Luther-University Halle-Wittenberg, Physics Department, Halle, Germany — [2]Martin-Luther-University Halle-Wittenberg, Organic Chemistry Department, Halle, Germany

Currently, information on the phases and crystal structures, which form during the growth and annealing of $(CH_3NH_3)Pb(I,Cl)_3$ perovskite films is scarce. To gain an insight into these, we studied thin films during their growth. Films were grown through co-evaporation of $(CH_3NH_3)I$ and $PbCl_2$ or PbI_2. In situ x-ray diffraction (XRD) was utilized to study phase formation in real time. Films grown by evaporation of $PbCl_2$ and MAI exhibited a cubic crystal structure and two different $(CH_3NH_3)Pb(I_xCl_{(1-x)})_3$ phases could be distinguished for varying $(CH_3NH_3)I$ to $PbCl_2$ flux ratios. They differed in their crystal structure observed by XRD, optical absorption properties and I/I+Cl ratio (either above 0.95 or below 0.5). For films grown with PbI_2 and MAI a tetragonal structure was observed. To monitor thermally induced changes and decomposition, we studied the films during heating. Below $200°C$, recrystallization was observed. The chlorine free films additionally showed a transition from tetragonal to cubic structure. Above $200°C$ decomposition was observed. These results show the strong dependence of the phase formation on varying growth conditions. The formed structures can be monitored and adjusted in real time with the help of in situ XRD.

HL 2.3 Mon 10:00 ER 164

Electroabsorption spectroscopy investigation and hysteresis study of perovskite solar cells — •Cheng Li[1], Steffen Tscheuschner[2], Tanaji Gujar[1], Johannes Kiessling[1], Anna Köhler[2], Mukundan Thelakkat[1], and Sven Hüttner[1] — [1]Macromolecular Chemistry I, University of Bayreuth, 95440

Bayreuth, Germany — [2]Experimental Physics II, University of Bayreuth, 95440 Bayreuth, Germany

Solution-processed organic-inorganic perovskite solar cells (e.g. $CH_3NH_3PbI_{3-x}Cl_x$ and $CH_3NH_3PbI_3$) currently show the highest and most promising performances. However, the hysteresis in the J-V curve, i.e. the history dependence of the applied voltage, is still not sufficiently understood. This hysteresis is related to the way how perovskite solar cells are processed. This process exhibits significant influence on the electronic properties of these photovoltaic devices. In this respect, we study the temperature dependent dynamic processes in these pervoskite solar cells by characterizing their current-voltage behaviour. Through this method, we can elucidate the migration of ions and the origin of the hysteresis behaviour. Furthermore, we also use electroabsorption (EA) spectroscopy, a unique non-invasive characterization approach, to investigate the built-in potential in the working device. In this way, we can understand the interaction at the interface between the perovskite active layer and electrodes, providing guideline to optimize the device architecture.

HL 2.4 Mon 10:15 ER 164

Rutherford Backscattering Spectroscopy of Mass Transport by Transformation of PbI_2 into $CH_3NH_3PbI_3$ within np-TiO_2 — •Felix Lang[1], Albert Juma[1,2], Voranuch Somsongkul[1,3], Thomas Dittrich[1], and Marisa Arunchaiya[3] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Tallinn University of Technology, Department of Materials Science, Ehitajate tee 5, Tallinn 19086, Estonia — [3]Department of Materials Science, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand

A key technique in methylammonium lead iodide ($CH_3NH_3PbI_3$) thin film preparation is the sequential transformation of an inorganic precursor layer such as PbI_2, infiltrated in nanoporous TiO_2 to the final $CH_3NH_3PbI_3$ by dipping into an organic precursor solution containing CH_3NH_3I. Here, we present an investigation on the mass transport during transformation by Rutherford backscattering spectroscopy (RBS). Energy dispersive X-Ray (EDX) spectroscopy mapping of cross sections first, revealed a homogenious PbI_2 infiltration in nanoporous TiO_2 before transformation and second, an accumulation of Pb and I at the surface after transformation. Quantitative depth profiles of Pb and I were obtained from RBS analysis. An instant degradation of $CH_3NH_3PbI_3$ upon $^4He^+$ ion radiation was found. The concentration profiles of Pb could be simulated with a one dimensional diffusion model taking into account an effective diffusion coefficient of Pb in the nanocomposite (about $1.5 \cdot 10^{-11}$ cm^2/s) as well as a parameter considering frazzling at the surface due to formation of crystallites.

HL 2.5 Mon 10:30 ER 164

Fluorescence studies on organometal halide perovskite nanoparticles — •Niklas Mutz[1,2], Carlos Cárdenas-Daw[1,2], Ming Fu[1,2], Verena Hintermayr[1,2], Mathias Vollmer[1,2], Jacek Stolarczyk[1,2], Alexander Urban[1,2], and Jochen Feldmann[1,2] — [1]Photonics and Optoelectronics Group, Ludwig-Maximilians-Universität München, Amalienstr. 54 80799 München, Germany — [2]Nanosystems Initiative Munich Schellingstraße 4 80799 München, Germany

During recent years organometal halide perovskite based solar cells have shown a significant rise in power conversion efficiency. Despite this improvement in fabricating efficient perovskite solar cells, the underlying photophysical properties are not yet fully understood. An important insight into processes such as charge generation and separation can be obtained by studying single particles instead of disordered films. In this project we investigate the morphology and photoluminescence properties of individual lead halide perovskite particles by varying the chemical synthesis procedure. In particular we investigate their temperature dependent photoluminescence signal and in addition have performed electric field-dependent studies to get insight into the charge separation process.

HL 2.6 Mon 10:45 ER 164

Band structure and optical absorption of halide organometal perovskites from first principles — •Menno Bokdam, Tobias Sander, Cesare Franchini, and Georg Kresse — University of Vienna, Faculty of Physics, Sensengasse 8, A-1090 Vienna, Austria

The high efficiency of lead halide organic perovskite solar cells has raised many questions on the mechanisms at work here. An accurate description of the macroscopic dielectric properties is essential for understanding the origin of the materials ability to convert light to electricity. In this talk, we present an accurate account of the electronic, optical and excitonic properties of twelve halide organometal perovskites ABX_3 ($A = CH_3NH_3^+, HC(NH_2)_2^+$; $B = Pb, Sn$; $X = Cl, Br, I$) by means of many-body first principles methods. We use optimized structures obtained at room temperature using parallel tempering molecular dynamics. Quasi particle band structures and absorption spectra are calculated at the GW_0 level. Electron-hole interactions have been included in the dielectric function by solving a Bethe-Salpeter equation for the polarizability. We demonstrate that a description beyond independent particles is necessary to describe the onset of the optical absorption. The calculated degree of localization of the excitons in k-space indicates Wannier-Mott type excitons with binding energies ranging from 30 meV (ABI_3) and 100-200 meV ($ABCl_3$). To validate our predictions, we compare the results with available experimental data (band gap and optical absorption).

HL 3: Graphene: THz, NIR and transport properties (with O/TT)

Time: Monday 9:30–11:30 Location: ER 270

HL 3.1 Mon 9:30 ER 270

Ratchet effects in graphene with a lateral periodic potential — •P. Olbrich[1], J. Kamann[1], J. Munzert[1], M. König[1], L.E. Golub[2], L. Tutsch[1], J. Eroms[1], F. Fromm[3], Th. Seyller[3], D. Weiss[1], and S.D. Ganichev[1] — [1]University of Regensburg, Regensburg, Germany — [2]Ioffe Institute, St. Petersburg, Russia — [3]Technical University of Chemnitz, Germany

We report on the observation of terahertz (THz) radiation induced photocurrents in (a) epitaxially grown and (b) exfoliated graphene with a lateral periodic potential. The samples were covered with an insolating layer and a sequence of asymmetrically spaced thin/thick metallic stripes. While in the reference of sample (a) under normal incidence of THz radiation no photosignal was observed, the illumination of the lateral periodic potential resulted in pronounced photosignals, consisting of polarization dependent and independent contributions. In case of sample (b) the thin/thick metallic stripes act as a dual top gate structure to vary the potential profile and a back gate allows to change the carrier type and density of the sample. Here, the photocurrent reflects the degree of asymmetry induced by different top gate potentials and even vanished for a symmetric profile. Moreover, around the Dirac point the photocurrent shows strong oscillation. We discuss the experimental data, taking into account the calculated potential profile, near field effects of light scattering and the theoretical model [1, 2].

[1] E. L. Ivchenko and S. D. Ganichev, JETP Lett. 93, 673 (2011).
[2] P. Olbrich et al., Phys. Rev. B 83, 165320 (2011).

HL 3.2 Mon 9:45 ER 270

Mechanically Modulated Graphene for THz-Nanoelectronics. — •Jonas Sichau[1], Timothy Lyon[1], August Dorn[1], Amaia Zurutuza[2], Amaia Pesquera[2], Alba Centeno[2], and Robert Blick[1] — [1]Center for Hybrid Nanostructures, Institutes of Nanostructure and Solid State Physics, University of Hamburg, Jungiusstrasse 11c, 20355 Hamburg, Germany. — [2]Graphenea S.A., 76 Tolosa Hiribidea, Donostia-San Sebastian, E-20018, Spain.

Graphene offers very high charge carrier mobility and a mean free path of several microns at room temperature. Consequently, it is a promising material for THz electronics [1]. For flat monolayer graphene, studies on microwave-photo excited transport have found spin resonance and zero-field pseudo-spin splitting [2]. The aim of our work is to investigate spatially modulated graphene under microwave excitation. Once carriers are propagating ballistically through the undulated graphene sheet, it is predicted that THz-radiation should be emitted [1].

We fabricated extremely large graphene membranes of up to 1 mm side lengths and transferred these onto a SiO_2-substrate. The pitch

and height of the mechanical modulation are of the order of 200 nm and 50 nm, respectively. The measurements are performed with a variable temperature insert (VTI) at magnetic fields up to 12T. The microwave signal is coupled to the sample via a micro inductor forming a resonator with the graphene sheet. With this configuration we are able to probe magnetotransport and the interaction with electromagnetic radiation.

[1] Tantiwanichapan et al., Nanotechnology 24, 375205 (2013)
[2] Mani, R.G. et al., Nat. Commun., 3:996 (2012)

HL 3.3 Mon 10:00 ER 270

Investigations on the polarization dependent carrier excitation in graphene with low energetic photons — •Jacob Otto[1,2], Martin Mittendorff[1,2], Torben Winzer[3], Ermin Malic[3], Andreas Knorr[3], Harald Schneider[1], Manfred Helm[1,2], and Stephan Winnerl[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]Technische Universität Dresden, 01062 Dresden, Germany — [3]Technische Universität Berlin, 10623 Berlin, Germany

We demonstrate that in graphene a nonequelibrium charge carrier distribution retains its anisotropic nature on a 10 ps timescale if the photon energy is below the optical phonon energy. Recently evidence for an anisotropic carrier distribution has been found in near-infrared pump-probe experiments with varied angle between the orientation of pump and probe polarization [1]. This anisotropy vanishes after 150 fs due to electron optical-phonon scattering. Extending this study to the mid-infrared range (E_{Photon} = 74 meV), i.e. to energies below the optical phonon energy, allows to strongly suppress this scattering mechanism. In accord with microscopic theory, traces of an anisotropic distribution on a 10 ps timescale are found. Note that carrier-carrier scattering, acting on a 10 fs timescale, is mainly colinear and therefor preserves the anisotropic distribution on rather long timsecales.

[1] M. Mittendorff, T. Winzer, E. Malic, A. Knorr, C. Berger, W. A. de Heer, H. Schneider, M. Helm and S. Winnerl *Nano Lett.* 2014, 14, 1504-1507

HL 3.4 Mon 10:15 ER 270

Magnetotransport in small angle twisted bilayers of folded graphene — •Johannes Rode[1], Hennrik Schmidt[1,2], Dmitri Smirnov[1], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover — [2]Centre for Advanced 2D Materials and Graphene Research Centre, National University of Singapore

Naturally occurring double-layer graphene consists of two hexagonal lattices in Bernal-stacking, described by a translational displacement between layers. While this type of bilayer is most commonly studied, the introduction of a rotational mismatch opens up a whole new field of rich physics, especially at small interlayer twist[1,2]. We investigate magnetotransport measurements on twisted graphene bilayers, prepared by folding of single layers. These reveal a strong dependence on the twist angle, which can be estimated by means of sample geometry. At small rotation, superlattices with a wavelength in the order of 10 nm arise and are observed by friction atomic force microscopy. Magnetotransport measurements in this small-angle regime show the formation of satellite Landau fans, which are attributed to additional Dirac singularities in the band structure[3].

[1] Lopes dos Santos, J. M. B., Peres, N. M. R. & Castro Neto, A. H. *Phys. Rev. Lett.* **99**, 256802.
[2] Mele, E. J. *Phys. Rev. B* **84**, 235439.
[3] Schmidt, H., Rode, J. C., Smirnov, D. & Haug, R. J. *Nat. Commun.* (accepted, Nov. 2014).

HL 3.5 Mon 10:30 ER 270

Carrier dynamics in Landau-quantized graphene — •Florian Wendler[1], Martin Mittendorff[2], Stephan Winnerl[2], Manfred Helm[2], Andreas Knorr[1], and Ermin Malic[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

We investigate the carrier dynamics in Landau-quantized graphene after an optical excitation using microscopic time-resolved calculations as well as differential transmission measurements. The calculations are performed within the density matrix theory accounting for the carrier-light, carrier-carrier, and carrier-phonon interaction which allows for a microscopic explanation of the experimental spectra.

The energy spectrum of Landau-quantized graphene is characterized by non-equidistant Landau levels where the optical selection rules enable a selective excitation of specific transitions. This is exploited to investigate the carrier dynamics in the energetically lowest Landau levels where an unexpected sign reversal in pump-probe spectra, observed in experiment and theory, provides an evidence for strong Auger scattering [1]. Based on our calculations we predict a substantial carrier multiplication [2]. Furthermore, the theory reveals the occurrence of population inversion in Landau-quantized graphene, suggesting its application as gain medium for a widely tunable Landau level laser[3].

[1] M. Mittendorff et al., Nat. Phys., DOI:10.1038/nphys3164.
[2] F. Wendler et al., Nat. Commun. 5:3703 (2014).
[3] F. Wendler, and E. Malic, arXiv:1410.2080v1.

HL 3.6 Mon 10:45 ER 270

Giant magnetophotoelectric effect in suspended graphene — •Jens Sonntag, Annika Kurzmann, Martin Geller, Ralf Schützhold, and Axel Lorke — Faculty of Physics and CeNIDE, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

Due to the broad absorption bandwidth and the possibility for carrier multiplication, graphene is a promising candidate for optoelectric applications.

In this context, we performed photocurrent measurements on a suspended graphene field-effect transistor structure in a magnetic field in the quantum Hall regime. Using an illumination power of only 3 μW, our device generates a current of up to 400 nA without an applied bias, which corresponds to a photoresponsivity of 0.14 A/W. To the best of our knowledge, this is one of the highest values ever measured for single layer graphene. Furthermore, the high current suggests that every absorbed photon creates more than 8 charge carriers, so that carrier multiplication is apparent.

We discuss these photocurrents in the framework of magnetothermoelectric effects and recent calculations of photocurrent generation in edge channels [1]. Taking into account the observed gate voltage, magnetic field and polarization dependence, we develop a quasi-ballistic model for the measured photocurrent. It includes edge channel transport and charge carrier multiplication and is in good agreement with the experimental results.

[1] Queisser et al. Phys. Rev. Let. **111**, 046601 (2013)

HL 3.7 Mon 11:00 ER 270

Ballistic transport in graphene antidot arrays — •Andreas Sandner[1], Tobias Preis[1], Christian Schell[1], Paula Giudici[1], Kenji Watanabe[2], Takashi Taniguchi[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan

We report on the observation of antidot peaks in ρ_{xx} in monolayer-graphene (MLG), encapsulated between hexagonal boron nitride (hBN). The hBN-MLG-hBN heterostructures were fabricated with a dry transfer pick-up technique; subsequently mesas were etched in Hall bar geometry and contacted with 1-dimensional side contacts. The periodic antidot lattice was defined in a following step by additional electron-beam lithography and reactive ion etching.

We performed measurements on stacks with different antidot lattice periods down to 100 nm. Several peaks in magnetoresistance can be identified and assigned to orbits around one and several antidots. This proves ballistic transport in our graphene heterostructures, in spite of the critical etching step for small lattice periods. We show measurements at different temperatures and can study antidots peaks down to very low carrier densities ($n = 2 \cdot 10^{11}$ cm^{-2}) and magnetic fields (B = 0.5 T). At higher magnetic fields, well defined quantum Hall plateaus with filling factors down to $\nu = 1$ are observed, even at an antidot period of 100 nm.

HL 3.8 Mon 11:15 ER 270

Ballistic supercurrents in suspended graphene — •Markus Weiss and Christian Schönenberger — Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel

Since the discovery of graphene there have been numerous efforts to use this material as a Josephson weak link between two superconductors. Devices based on oxidized silicon substrates have been produced a few years ago, and have shown bipolar, gate-tuneable supercurrents. The observation of effects are that unique to the Dirac semimetal graphene however has been prevented up to now by the large disorder modulation of the electric potential in graphene on silicon based substrates. For the direct observation of e. g. specular Andreev reflection, the disorder modulation of the Dirac point would have to be smaller that the proximity induced superconducting gap, a regime that cannot be reached in conventional devices. The road to cleaner graphene might go via deposition onto commensurate substrates like hexagonal boron

nitride, or the removal of the silicon oxide substrate and suspension of graphene. The latter technique has been perfected in the recent years for devices with normal metal contacts, but turned out to be difficult to realize for superconducting contacts due to incompatibilities of superconducting materials with the fabrication process.

We have developed a device architecture that allows the realization of suspended graphene devices with superconducting contacts, and will show first experimental results, like the ballistic Josephson current through a graphene weak link.

HL 4: Focus Session (with TT): Functional semiconductor nanowires I

The growth of nearly any kind of semiconductor in the form of nanowires as well as its properties have been intensely investigated in the past 15 years, because nanowires often offer superior properties compared to their bulk or thin-film counterparts. To fully exploit their unique properties, the challenging step is the integration of semiconductor nanowires into specific functional environments and devices. In this focus session, we present and offer a platform to discuss recent developments in exactly this area with applications in electronics, photonics and optoelectronics.

Organization: Carsten Ronning (FSU Jena), Martin Eickhoff (JLU Giessen), Tobias Voss (TU Braunschweig)

Time: Monday 9:30–13:15 Location: EW 201

Invited Talk HL 4.1 Mon 9:30 EW 201

Exploring the optical properties of 1D nanomaterials at sub-nanometer scale with a direct correlation to its structure at atomic scale — •Jordi Arbiol — Institució Catalana de Recerca i Estudis Avançats (ICREA), 08010 Barcelona, CAT, Spain — Institut de Ciència de Materials de Barcelona, ICMAB-CSIC, E-08193 Bellaterra, CAT, Spain

Technology at the nanoscale has become one of the main challenges in science as new physical effects appear and can be modulated at will. New generations of functionalized materials are taking advantage of the low dimensionality, improving their properties and opening a new range of applications. As developments in materials science are pushing to the size limits of physics and chemistry, there is a critical need for understanding the origin of these unique physical properties (optical and electronic) and relate them to the changes originated at the atomic scale, e.g.: linked to changes in (electronic) structure of the material. Combining advanced electron microscopy imaging with electron spectroscopy, as well as cathodoluminescence in a STEM will allow us to probe the elemental composition and electronic structure simultaneously with the optical properties in unprecedented spatial detail. The seminar will focus on several examples in advanced nanomaterials for optical and plasmonic applications. In this way the latest results obtained by my group on direct correlation between optical properties at sub-nanometer scale and structure at atomic scale will be presented.

HL 4.2 Mon 10:00 EW 201

Selective Area Growth of GaN Nanowires and Nanotubes — •Martin Hetzl[1], Fabian Schuster[1], Saskia Weiszer[1], Jose A. Garrido[1], María de la Mata[2], Jordi Arbiol[2], and Martin Stutzmann[1] — [1]Walter Schottky Institut and Physics Department, Technische Universität München, Garching, Germany — [2]Institut de Ciència de Materials de Barcelona, ICMAB-CSIC, Bellaterra, Spain

Selective area growth (SAG) of GaN nanowires (NWs) by molecular beam epitaxy has been investigated in a systematic way. A high uniformity of SAG NWs and a complete suppression of unintentional growth has been achieved. The nucleation sites were predefined by a titanium mask structured by e-beam lithography. The underlying growth kinetics will be addressed by varying the substrate temperature, the III/V-ratio, the growth time and the NW arrangement. For that, diamond (111) substrates have been used as a model material. However, successful transfer of SAG on Si (111), c-plane sapphire and other substrates confirms the general validity of the presented growth mechanism. Scanning transmission electron microscopy has been performed to investigate the structural quality of the NWs and to determine the polarity of the wurtzite lattice. At lower temperatures, so called "tripods" instead of NWs can occur, which result from large GaN zinc blende nuclei. The exact NW arrangement changes the local III/V-ratio. This has been used to force a transition from GaN NW to nanotube growth, leading to a much higher effective surface-to-volume ratio. The controllability of SAG GaN NWs represents an important step towards NW-based devices, e.g. for optoelectronics, sensing or catalysis.

HL 4.3 Mon 10:15 EW 201

Stability of heteroepitaxial coherent growth modes on nanowire radial surfaces — •Thomas Riedl[1,2] and Jörg Lindner[1,2] — [1]University of Paderborn, Department of Physics, Warburger Straße 100, 33098 Paderborn, Germany — [2]Center for Optoelectronics and Photonics Paderborn (CeOPP), Warburger Straße 100, 33098 Paderborn, Germany

Semiconductor nanowires (NWs) exhibit a large surface-to-volume ratio and are therefore interesting as a substrate for the growth of nanoscale heteroepitaxial islands as well as core-shell structures for use in optoelectronic applications. Compared to planar substrates the NW curvature leads to a modified thermodynamic stability of the coherent Frank-van-der-Merwe and Stranski-Krastanov (SK) heteroepitaxial growth modes. In the present contribution we investigate the stability of these growth modes on cylindrical NWs by means of continuum theory. In contrast to previous studies (i) the exact geometrical shape of pyramidal islands and (ii) the impact of the island contact angle on the elastic relaxation energy are considered. Maps of the growth mode stability are derived for the Si core / Ge shell structure, which display the favoured mode as a function of deposited volume, wetting layer thickness and NW radius. When using a Ge surface energy of 1.3 J/m^2 for both the shell and the pyramid surfaces the SK mode becomes stable only for large contact angles and NW radii larger than 40 nm. However, if the reduced surface energy of low-index Ge facets is taken into account, the transition between the two growth modes is shifted to smaller NW radii, as observed in experiments.

HL 4.4 Mon 10:30 EW 201

Cd_3As_2 Nanowires by Chemical Vapour Deposition — •Piet Schönherr and Thorsten Hesjedal — Department of Physics, Clarendon Laboratory, University of Oxford, Oxford OX1 3PU, United Kingdom

Cd_3As_2 has been well known for its very high mobility. Recently, it was discovered that the material displays two Dirac points with linearly dispersing states that are stabilized by crystal symmetry (three-dimensional Dirac semimetal). The Dirac cones live in three-dimensional k-space unlike topological insulators that only have two-dimensional Dirac cones on their surface. This makes Cd_3As_2 a three-dimensional analogue of graphene.

We present the growth and characterisation of Cd_3As_2 nanowires including results from electric transport measurements. Nanowires with a diameter as small as 10 nm were grown in a self-catalysed vapour-liquid-solid process using chemical vapour deposition. We analyse the growth mechanism and compare the vibrational modes of Cd_3As_2 nanostructures with bulk samples.

HL 4.5 Mon 10:45 EW 201

MOCVD Growth and Characterization of InGaN/GaN Nanowire-based core/shell Heterostructures — Bartosz Foltynski, Christoph Giesen, and •Michael Heuken — AIXTRON SE, Dornkaulstr. 2, 52134 Herzogenrath, Germany

GaN based nanostructures have stimulated great interest in their applications for fabricating next-generation light emitting diodes (LEDs) for solid state lighting (SSL). Nanowires, benefiting from their geom-

etry and offer a set of extraordinary properties like increase of light emission by utilizing the nanostructure side walls, limitation of negative effect of polarization fields and reduction of dislocation density. In our studies we present the optical and structural characterization of InGaN/GaN core/shell nanowires grown on Si(111) substrates by MOCVD. SEM,Photoluminescence and cathodoluminescence were used as characterization techniques. All growth experiments were performed in an AIXTRON CCS (Close Coupled Showerhead) reactor. The self-organized GaN nanowires were grown on Si(111) substrates using AlN buffer and in-situ SiNx masking layer. The growth conditions were optimized to achieve maximum density of vertical GaN microrods perpendicularly aligned to the substrate. Detailed results on growth optimization and structure characterization will be presented and discussed.

HL 4.6 Mon 11:00 EW 201

Modulation doped GaAs-AlGaAs core-shell nanowires — •Dominik Irber[1], Stefanie Morkötter[1], Jonathan Becker[1], Nari Jeon[2], Daniel Rudolph[1], Bernhard Loitsch[1], Markus Döblinger[3], Max Bichler[1], Jonathan J. Finley[1], Lincoln J. Lauhon[2], Gerhard Abstreiter[1,4], and Gregor Koblmüller[1] — [1]Walter Schottky Institut and Physik Department, Technische Universität München, Garching, Germany — [2]Department of Materials Science and Engineering, Northwestern University, Evanston, U.S.A. — [3]Department of Chemistry, Ludwig-Maximilians-Universität München, Munich, Germany — [4]Institute for Advanced Study, Technische Universität München, Garching, Germany

In this work we will present electrical and structural properties of GaAs-AlGaAs core-shell nanowire (NW) MODFETs. The GaAs core was grown on Si (111) substrates via [111]-oriented self-catalyzed growth using MBE, followed by a Si δ-doped radial <110>-oriented AlGaAs shell. Using HRTEM and atom probe tomography (APT), the structure and elemental composition of the NWs were analyzed. The APT analysis revealed the position of the δ-doped layer and the Si dopant concentration, allowing to calculate the expected 2DEG carrier density. Electrical measurements using a top gate geometry verified the expected 2DEG density and further showed very steep switching behavior (SS=70mV/dec) with on/off-ratios $>10^4$ at 300K. The device geometry allowed to measure mobility at different sites of the NW. In combination with the APT data the influence of structural parameters on mobility can be studied.

Coffee break

Invited Talk HL 4.7 Mon 11:30 EW 201

Studying single semiconductor nanowires using a hard X-ray nanoprobe — •Gema Martinez-Criado — European Synchrotron Radiation Facility, Grenoble, France

Semiconductor nanowires present great advantages for optoelectronic and spintronic nanodevices. Their applications are basically controlled by multiple property-function relationships taking place at the nanoscale in the spatial and time regimes. Only a combination of high-resolution methods offer a comprehensive characterization of their complex nature. Here we present how a multimodal hard X-ray nanoprobe addresses fundamental questions in nanowire research. Selected topics ranging from cluster formation, dopant segregation, and phase separations to quantum confinement effects are examined with sub-100 nm spatial resolution and sub-50 ps temporal resolution. This scheme opens new opportunities for structural, composition and optical investigations with large potential in materials science.

HL 4.8 Mon 12:00 EW 201

Influence of surface depletion on electrical conductivity of freestnding GaAs nanowires investigated by a multi-tip STM — •Weihong Zhao[1], Matthias Steidl[1], Stefan Korte[2], Hubertus Junker[2], Werner Prost[3], Peter Kleinschmidt[1], and Thomas Hannapel[1] — [1]Photovoltaics Group, Institute for Physics, Technische Universität Ilmenau, D-98684 Ilmenau — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, D-52425 — [3]CeNIDE and Center for Semiconductor Technology and Optoelectronics, University of Duisburg-Essen, D-47057 Duisburg

P-type Zn-doped GaAs-Nanowires were prepared by the Au-assisted vapor-liquid-solid growth mode in a metal-organic vapor phase apparatus. Electrical investigation was carried out by a multi-tip scanning tunneling microscope as nano-prober on free-standing p-GaAs nanowires. As an approach to understand the doping process through the growing process, Zn-doped GaAs nanowires with different diameter were prepared. The electrical measurements and analysis on the nanowires deliver the key-information about process related dopant incorporation along the nanowires, which is responsible for the varying charge carrier depletion thickness.

HL 4.9 Mon 12:15 EW 201

Antimony doped ZnO nanowires — •Thomas Kure[1], Alexander Franke[1], Sarah Schlichting[1], Emanuele Poliani[1], Felix Nippert[1], Markus R. Wagner[1], Marcus Müller[2], Peter Veit[2], Sebastian Metzner[2], Frank Bertram[2], Eswaran S. Kumar[3], Faezeh Mohammadbeigi[3], Jürgen Christen[2], Janina Maultzsch[1], Simon Watkins[3], and Axel Hoffmann[1] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Berlin, Germany — [2]Otto-von-Guericke-University, Institut für Experimentalphysik, Germany — [3]Simon Fraser University, Department of Physics, Burnaby, Canada

We investigated the morphology of metalorganic vapor phase epitaxy (MOVPE) grown c-axis aligned Sb doped ZnO NWs as well as the doping distribution and structural defects of single NWs. Cathodoluminescence spectroscopy (CL) along several single NWs reveal that the luminescence stems predominately from the tip and decreases towards the bottom of the NW. Raman measurements on ensemble NWs show additional vibrational modes, where some appear exclusively in Sb doped ZnO. Tip-enhanced Raman spectroscopy (TERS) was performed to investigate the local doping concentration. The significant increase of Sb-related Raman modes towards the apex confirms the increase of Sb along the NW.

HL 4.10 Mon 12:30 EW 201

Hard X-ray detection in a single 100 nm-diameter nanowire — •Jesper Wallentin[1], Markus Osterhoff[1], Robin Wilke[1], Karl-Magnus Persson[2], Lars-Erik Wernersson[2], Michael Sprung[3], and Tim Salditt[1] — [1]Institute for X-Ray Physics, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Department of Electrical and Information Technologies, Lund University, Lund S-221 00, Sweden — [3]DESY, Notkestrasse 85, 22607 Hamburg, Germany

While hard X-rays can now be focused below 10 nm, current semiconductor-based X-ray detectors have pixel sizes of tens of micron. It is desirable to shrink the detector pixel size in order to improve the resolution in imaging, spectroscopy and crystallography, but smaller detector volumes are expected to lead to a weak electrical signal. We investigated the electrical response of a 100 nm-diameter InP nanowire exposed to a hard X-ray nanofocus. A fixed bias voltage was used, and the current was measured with a picoammeter. The conductance increased about 4 orders of magnitude under full X-ray flux. Dynamic measurements revealed very slow processes, with lifetimes at the order of seconds. Such long lifetimes, possibly related to surface states, could explain the strong X-ray induced current. As a demonstration of the potential of nanowires as X-ray detectors, we imaged the X-ray nanofocus by making a 2D raster with the device. The spatial resolution was less than 1 micron, and could be improved by making devices with the nanowire oriented along the optical axis. These results show that nanostructures can have much stronger X-ray response than expected from a simple scaling of bulk parameters.

HL 4.11 Mon 12:45 EW 201

synchrotron X-ray photoelectron spectroscopy study of GaAs/InAs core/shell nanowires grown by MBE — •behnam khanbabaee[1], torsten rieger[2], nataliya demarina[2], detlev grützmacher[2], mihail Ion lepsa[2], rainer timm[3], and ullrich pietsch[1] — [1]Solid State Physics, Dept. of Physics, University of Siegen, Siegen, Germany — [2]Peter Grünberg Institute and JARA-FIT, Forschungszentrum Jülich GmbH, Jülich, Germany — [3]Synchrotron Radiation Research and The Nanometer Structure Consortium, Dept. of Physics, Lund University, Lund, Sweden

Semiconductor nanowire (NW) heterostructures are promising building blocks for future electronic devices. In particular, GaAs/InAs radial NWs heterostructures are candidates for nano-electronics, where a lower band gap semiconductor, e.g. InAs, is grown on a semiconductor with a higher band gap, e.g. GaAs, providing band bending at the interface. For effective band confinement it is necessary to control the radial thickness, and the local defect structure at the hetero-interface and its relation to the electronic properties. Here we report on X-ray photoelectron spectroscopy of GaAs/InAs core/shell NWs grown by molecular beam epitaxy. After cleaning under atomic hydrogen the As-oxides on top of the NWs were considerably reduced while the Ga-

and In-oxides were slightly reduced. The binding energy of the As 3d core levels was shifted about 1 eV towards lower energies. These results show that the As component of the native oxide turns the NWs surface strongly n-type. Our findings show that the shelling of GaAs NWs with InAs may leads to band bending of 0.2 to 0.3 eV at hetero-interface.

HL 4.12 Mon 13:00 EW 201

Seebeck effect measurements on single InAs and GaAs nanowires — •Alexander Hirler[1], Vanessa Schaller[1], Jonathan Becker[1], Bernhard Loitsch[1], Stefanie Morkötter[1], Julian Treu[1], Gerhard Abstreiter[1,2], Jonathan Finley[1], and Gregor Koblmüller[1] — [1]Walter Schottky Institut and Physik Department, TU München, Garching, Germany — [2]TUM Institute of Advanced Study, Garching, Germany

We present recent results on measurements of the Seebeck coefficient of intrinsic n-type InAs and carbon doped p-type GaAs nanowires (NWs) grown on Si(111) substrates via catalyst free molecular beam epitaxy. To measure the Seebeck effect on single NWs, a temperature gradient is applied via lithographically fabricated heating coils and measured by two resistance thermometers each in a four-point measurement geometry, which also act as electric contacts to the NW. Equipped with another heating resistor the temperature dependent Seebeck-coefficient can be measured as well. Compared to field effect transistor (FET) measurements, the carrier density can be conducted independent of the gate geometry. In addition, the carrier type can be determined from the sign of the Seebeck voltage. Seebeck measurements presented here, demonstrate successful p-type doping of GaAs NWs via carbon. P-type doping and the quantitative measurement of the doping concentration via Seebeck measurements are important steps towards future heterojunction NW devices.

HL 5: Photovoltaics: CIGS and related compounds

Time: Monday 9:30–11:45 Location: EW 202

HL 5.1 Mon 9:30 EW 202

Investigation of Defect Levels in Al/Cu(In,Ga)Se_2 Schottky Contacts and ZnO:Al/CdS/Cu(In,Ga)Se_2 Heterojunctions via Temperature-Dependent Admittance Spectroscopy — •Sara L. Gadeberg, Maria S. Hammer, and Ingo Riedel — Energy and Semiconductor Research Laboratory, Chair: Jürgen Parisi, Department of Physics, University of Oldenburg

Regardless their broad application and investigation, many properties of the Cu(In,Ga)Se_2 compound semiconductors (CIGSe) have still not been sufficiently explained. For instance, the nature of certain defect signatures (interface or bulk) is still under discussion. In this study different Schottky contacts (Al/CIGSe/$MoSe_2$/Mo) were prepared from CIGSe solar cells (ZnO:Al/CdS /CIGSe/$MoSe_2$/Mo) via etching removal of the ZnO:Al/CdS window layer, surface treatment of the remaining CIGSe layer, and subsequent metal deposition. In order to differentiate between bulk and heterojunction interface defects, we recorded temperature-dependent admittance spectra (TAS) (T=30 - 310 K). The TAS data were evaluated in two ways: i) by applying the common method using the derivative of the capacitance and ii) by direct analysis of the phase shift of the impedance, which does not require particular assumptions on the electrical device equivalent circuit. The defect signatures found in the Schottky devices were compared to those found in the original CIGSe solar cells. Based on our results we will discuss the spatial origin of the different defect levels and comment on the reliability of the direct evaluation method for TAS data as proposed in this work.

HL 5.2 Mon 9:45 EW 202

Influence of metastable defect characteristics on the carrier collection in Cu(In,Ga)Se_2 thin film solar cells — •Maria S. Hammer[1], Viktor Gerliz[1], Stephan J. Heise[1], Jörg Ohland[1], Janet Neerken[1], Jan Keller[2], and Ingo Riedel[1] — [1]Energy and Semiconductor Research Laboratory, Chair: Jürgen Parisi, Department of Physics, University of Oldenburg — [2]Currently: Department of Engineering Sciences, Solid State Electronics, Uppsala Universitet

Despite the current progress of Cu(In,Ga)Se_2 thin film photovoltaics, the relation between the metastable defect characteristics and key parameters of the solar cells has not yet been fully explained. In this work we discuss the correlation between metastable defect densities and short-circuit current J_{SC} of solar cells conditioned via white-light soaking (LS) and dark air-annealing (DA), respectively. The J_{SC} of DA-treated devices was found to decrease by 0.8 $mAcm^{-2}$ upon LS treatment, which suggests a conditioning-induced change of the carrier collection. Partly, this phenomenon can be attributed to a change of the metastable net doping density. However, device simulations and cross-section EBIC measurements suggest that this explanation is not sufficient to describe the observed J_{SC} difference. Moreover, time-resolved photoluminescence revealed a significant decrease of the decay lifetime upon LS along with an increase of the N1 defect concentration by $9.5{\cdot}10^{14}$ cm^{-3}, as evaluated from temperature dependent admittance spectra. In conclusion, we propose, that the observed J_{SC} metastability originates from both, treatment-induced changes of the net doping concentration and defect-related transport properties.

HL 5.3 Mon 10:00 EW 202

Kinetics of phase separation and coarsening in Cu-In-Ga precursor thin films for sequentially processed Cu(In,Ga)Se_2 solar cells — •Jan-Peter Bäcker[1], Humberto Rodriguez-Alvarez[1], Manuel Hartig[3], Christian A. Kaufmann[1], Jaison Kavalakkatt[2], Roland Mainz[2], Saoussen Merdes[1], Sebastian S. Schmidt[1], Christian Wolf[1], Florian Ziem[1], and Rutger Schlatmann[1] — [1]PVcomB, Helmholtz-Zentrum Berlin, Germany — [2]Helmholtz-Zentrum Berlin, Germany — [3]Technische Universität Berlin, Germany

Obtaining smooth and homogenous Cu(In,Ga)Se_2 films by fast selinzation of metallic precursors is a major challenge. Separation and coarsening of metallic phases in Cu-In-Ga precursor films can lead to solar cells with low shunt resistance due to pinhole formation, and to reduced open circuit voltages due to locally varying Ga concentration. In this study we attempt to establish a general model for the kinetics of the phase separation and coarsening of sputtered Cu-Ga-In metallic films as used for Cu(In,Ga)Se_2 fabrication. For this we measure the roughness with atomic force microscopy and the Ga spatial distribution by energy dispersive X-ray spectroscopy. We study four different metallic precursor stacks heated to 170°C, 350°C and 580°C, at rates between 0.01K/s and 1K/s. Finally, we present a statistical analysis of the effect of our optimized multilayered precursors on the fill factor of the solar cells prepared in our atmospheric-pressure in-line and fast selenization baseline, that has led to power conversion efficiencies of up to 15.5% (active area).

HL 5.4 Mon 10:15 EW 202

A Real-Time XRD Investigation of $Cu(In,Ga)Se_2$ by Three-Stage Thermal Co-Evaporation — •Setareh Zahedi-Azad, Paul Pistor, Enrico Jarzembowski, Stefan Hartnauer, Leonard Wägele, Wolfgang Fränzel, and Roland Scheer — Institute of Physics, Martin-Luther-University Halle-Wittenberg

Solar cells based on $Cu(In,Ga)Se_2$ (CIGS) thin films have achieved efficiencies of up to 21.7%, which makes this technology comparable to Si-based Solar cells. Further improvement requires a detailed understanding of the crystal phase evolution during preparation. Therefore, the phase evolution of $Cu(In_{1-x},Ga_x)Se_2$ thin films prepared by multi-stage co-evaporation and with x (= Ga/Ga+In) ranging from 0 to 1, was investigated during the deposition process via time resolved in situ X-ray diffractometry (in situ XRD). Dependent on x, films exhibit different crystalline phases during the different stages of the growth. The phases monitored during the growth of $CuInSe_2$ (x=0) are in agreement with the $In_2Se_3 - Cu_2Se$ pseudo-binary phase diagram. In this case and in the case of x = 0.33, ordered vacancy phases of $Cu(In,Ga)_5Se_8$ and $Cu(In,Ga)_3Se_5$ are observed, while for higher Gallium contents (x>=0.55), no such phases were detected. The formation of Cu_2Se phases was observed at the beginning of the Cu-rich growth regime for all processes. The Cu_2Se diffraction peaks disappear again in the third stage when the samples become Cu-poor again. The XRD peak width is analyzed quantitatively and interpreted in terms of crystallite size, crystalline quality and compositional gradients within the layer.

HL 5.5 Mon 10:30 EW 202

Composition-dependent atomic-scale structure of the Cu-

(In,Ga)-Se system — •Erik Haubold[1], Philipp Schöppe[1], Stefanie Eckner[1], Susan Schorr[2], Francesco di Benedetto[3], Ivan Colantoni[4], Francesco d'Acapito[4], 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 & Institut für Geologische Wissenschaften, Freie Universität Berlin, Malteserstr. 74-100, 12249 Berlin, Germany — [3]Dipartimento di Scienze della Terra, Università degli Studi di Firenze, Via La Pira 4, 50121 Firenze, Italy — [4]European Synchrotron Radiation Facility, 6 rue Jules Horowitz, BP 220, 38043 Grenoble Cedex, France

$Cu(In,Ga)Se_2$ shows the highest conversion efficiencies of all thin film solar cells with more than 20%. It is believed that the formation of copper poor surface regions within the absorber is important for reaching these high efficiencies. The properties of the material, including the bandgap energy, are determined not only by the material composition and crystal structure but also by the local arrangement of atoms. Therefore, we studied the atomic-scale structure of $Cu(In,Ga)Se_2$ and the two copper poor phases $Cu(In,Ga)_3Se_5$ and $Cu(In,Ga)_5Se_8$ as a function of the In/Ga ratio using extended X-ray absorption fine structure spectroscopy. This yields the element-specific average bond lengths and bond length variations as a function of In/Ga ratio and Cu content thus providing a comprehensive picture of the relationship between local structural parameters and material composition.

HL 5.6 Mon 10:45 EW 202

First Principle Calculation on the Energetics of Na and K Incorporation in CuInSe2 and CuIn5Se8 — Elaheh Ghorbani[1,2], •Janos Kiss[3], Hossein Mirhosseini[3], Thomas Kuehne[4], and Claudia Felser[3] — [1]Johannes Gutenberg univesity, Mainz, Germany — [2]IBM, Mainz, Germany — [3]MPI for Chemical Physics of Solids, Dresden, Germany — [4]University of Paderborn, Paderborn, Germany

In the present work we study sodium and potassium extrinsic defects incorporating into several substitutional and interstitial positions in CuInSe2 and CuIn5Se8 by means of theoretical density functional theory calculations (including some fraction of exact Hartree-Fock exchange). Our research reveals the most and least favorable sites for Na and K in the light absorber layer of CIGS-based thin film solar cells. We have also studied the energetics of dumbbells. Our calculations show: (i) Among substitutional positions, occupying a Cu position (by Na or K) takes much less energy than occupying an In or a Se position. (ii) Interstitial positions which are tetrahedrally coordinated by 2 Na and 2 In are more favourable for both Na and K than interstitial positions which are tetrahedrally coordinated by 4 Se atoms. (iii) All (Na-Na), (Na-K) and (K-K) dumbbells can form in CuInSe2 and CuIn5Se8. Among dumbbells (Na-Na) and (K-K) have the lowest and highest formation energies respectively. (iv) Dumbbells can occupy the pristine vacant copper position of CuIn5Se8, without creating new Cu-defects. (v)Our band structure results show which defects will cause the appearance of new defects states in the gap of absorber.

HL 5.7 Mon 11:00 EW 202

Local versus global electronic properties of chalcopyrite alloys — Rafael Sarmiento-Pérez[1], Silvana Botti[1], •Claudia S. Schnohr[2], Iver Lauermann[3], Angel Rubio[4,5], and Benjamin Johnson[5] — [1]Institut Lumière Matière, Université Lyon 1-CNRS, 69622 Villeurbanne Cedex, France — [2]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [4]Departamento de Física de Materiales, Universidad del País Vasco UPV/EHU, Avenida de Tolosa 72, 20018 San Sebastián, Spain — [5]Fritz Haber Institute, Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany

Among the materials used for thin film solar cells, $Cu(In,Ga)(S,Se)_2$ has reached the highest conversion efficiencies with record values well above 20%. The bandgap energy of the material can be tailored by adjusting the In/Ga ratio which mostly affects the position of the conduction band minimum. Therefore, we have studied the element-specific unoccupied electronic states of $Cu(In,Ga)S_2$ as a function of the In/Ga ratio by combining X-ray absorption spectroscopy with ab initio calculations. The S absorption edge shifts with changing composition as expected from the variation of the band gap. In contrast, the cation edge positions are largely independent of composition. This unexpected behavior is well reproduced by our calculations and originates from the dependence of the electronic states on the local atomic environment. The variation of the bandgap arises from a changing spatial average of these localized states with changing alloy composition.

HL 5.8 Mon 11:15 EW 202

Photoreflectance and photoluminescence of Cu(In,Ga)S2 thin film solar cells — •Sergiu Levcenko, Joachim Klaer, Steffen Kretzschmar, and Thomas Unold — Helmholtz Zentrum Berlin für Materialien und Energie, Berlin, Germany

An increased open-circuit voltage and an improved photocurrent collection have been recently achieved in Cu(In1-x,Gax)S2 (CIGS)- thin film based cell due to properly designed gallium alloying in the absorber layer. Nevertheless, the open-circuit voltage deficiency in CIGS devices is still larger than in selenide chalcogenide-based solar cells. It is believed that recombination at CdS/CIGS interface strongly reduces the device performances.

In our study we employ the nondestructive and contactless photoreflectance (PR) and photoluminescence (PR) techniques for characterizing CIGS devices. The CIGS absorbers with Ga/Ga+In ratio of 0.27 were fabricated under copper-rich conditions by a rapid thermal process with subsequent removal of segregated CuS by KCN etching. The effect of sulfurization temperature and post deposition treatments (KCN etching, NaF, In2S3 and In thin layer extra depositions) of the absorber in CIGS devices was revealed by PR and PL measurements at a room temperature. In the near band edge region the PR spectra show distinct structures at 1.5 and 1.55eV, while the PL signal consist of a broad band at 1.5eV with full width at half maximum of 100meV. The structures in PL and PR spectra are found to be influenced by the absorber preparation parameters.

HL 5.9 Mon 11:30 EW 202

Simulation of interference-related lineshape distortions in electroreflectance spectra of $Cu(In,Ga)Se_2$ thin-film solar cells — •Christian Huber[1], Christoph Krämmer[1], David Sperber[1], Heinz Kalt[1], Michael Powalla[2], and Michael Hetterich[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Light Technology Institute, KIT and Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg, 70565 Stuttgart, Germany

Modulation spectroscopy techniques like electroreflectance (ER) have proven to be powerful methods to determine the energetic positions of critical points (CPs) in a semiconductor's band structure. In the low-field regime the sharp, derivative-like features at the CPs can easily be evaluated by fitting a third-derivative functional form (TDFF) lineshape to the measured spectra.

However, when applied to thin-film solar cells to determine the absorber band gap, deviations from the TDFF approach have to be considered. One important aspect is that the layer stack of the solar cell introduces layer thickness interferences in the reflection signal, which can strongly distort the ER spectra.

In this contribution a transfer matrix approach will be presented in order to model the ER spectra of $Cu(In,Ga)Se_2$ thin-film solar cells. It shows that interference effects introduce lineshape distortions whenever interference minima lie energetically close to a CP. These distortions can easily be misinterpreted as contributions from several CPs and will therefore lead to wrong results in a TDFF-evaluation.

HL 6: Organic electronics and photovoltaics (DS with HL/CPP)

Time: Monday 9:30–13:00 Location: H 2032

HL 6.1 Mon 9:30 H 2032

Metal-organic interfaces: from molecular self-assembly to electronic transport through ultrathin functional monolayers — •Florian von Wrochem — Sony Deutschland GmbH, Stuttgart

The continuous development of organic electronic devices, combined with the advances in spectroscopy and electrical characterization, dramatically extended our understanding of the physical and chemical processes occurring at metal/organic interfaces. Here, an overview of experimental and theoretical efforts aiming towards the selective modification of interfaces is given. Various anchor groups designed to connect organic materials to metal electrodes are presented (e.g. thiolates, dithiocarbamates, mercuryls and stannyls) and their potential for optimizing the charge injection as well as the morphological, chemical, and electronic nature at the contact is illustrated. On this basis, functional molecular building blocks are grafted to the surface by self-assembly, providing rectification, switching, or chemical selectivity. Once the key parameters for interface formation and fabrication are under control, a huge number of potential applications emerge, ranging from optoelectronics to organic printed circuits. As one example, electrostatic dipole layers for tuning the injection barrier between metals and organic semiconductors are presented, which may find applications in organic light emitting diodes, field effect transistors, and solar cells. When further reducing device dimensions towards the nanoscale, organic monolayers might foster the development of molecular electronics, as illustrated here by highly robust metal-molecule-metal junctions based on FeII-terpyridine molecular wires or by optically switchable protein layers.

HL 6.2 Mon 9:45 H 2032

Grain boundaries in $CuInSe_2$ and $CuGaSe_2$ solar cell materials: New insights from hybrid functional calculations — Hossein Mirhosseini, •Janos Kiss, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany.

Polycrystalline thin-film solar cells based on $CuIn_{1-x}Ga_xSe$ (CIGSe) are an economically viable alternative to the Si based technology. During the deposition of the polycrystalline light absorber layer grain boundaries (GBs) are formed in the CIGSe material, and the effect of these GBs upon the structural and electronic properties of the thin-film solar cells are not yet fully understood. Different atomic structures of the GBs in CIGSe have been reported experimentally. The outcomes of the theretical calculations, however, are diverse and sometimes inconsistent due to the limitation of the functionals, which fail to properly describe the band gap of thin film solar cell materials. Employing a state of the art method using the HSE hybrid functional, which is known to predict the atomic and electronic structure of solar cell materials rather well, we have looked at the behavior and properties of GBs in $CuInSe_2$ and $CuGaSe_2$. In the framework of our investigation, we have studied the atomic relaxation and electronic structure of various GBs and also considered the effect of the impurity segregation close to the GBs.

HL 6.3 Mon 10:00 H 2032

Relationship between the chemical structure of low band gap polymers and self-organization properties — •Milutin Ivanovic[1], Umut Aygül[1], Ulf Dettinger[1], Aurelien Tournebize[1], David Batchelor[2], Stefan Mangold[2], Heiko Peisert[1], and Thomas Chassé[1] — [1]) University of Tuebingen, Institute of Physical and Theoretical Chemistry, 72076 Tuebingen, Germany — [2]Karlsruhe Institute of Technology (KIT), ANKA Synchrotron Radiation Facility, 76344 Eggenstein-Leopoldshafen, Germany

A possible approach to improve the efficiency of donor-acceptor based bulk heterojunction (BHJ) of OPV cells is the use of low band gap (LBG) polymers as donor materials. Basic electronic processes in OPV cells are however strongly influenced by the morphology and the ability for self-organization of the polymers in the thin-films. We utilize NEXAFS spectroscopy to study the molecular orientation of novel LBG polymers (PCPDTTBBTT, PCPDTTBTT and PCPDTzTBTT) for OPVs in thin films. The influence of post-processing annealing as well as of blending with Phenyl-C61-butyric acid methyl ester (PCBM) on the orientation is investigated. The studied LBG polymers are characterized by a variation of (hexyl-) thiophene groups compared to related LBG polymers recently studied.[1,2]. Acknowledgments: This research is funded by the European Union Seventh Framework Programme (FP7/2011 under grant agreement ESTABLIS n° 290022). References: 1.*Aygül, U. et al. J. Phys. Chem. C 2012, 116, 4870-4874. 2.*Aygül, U. et al. Sol. Energ. Mat. Sol. Cells 2014, 128, 119-125.

HL 6.4 Mon 10:15 H 2032

Organic ambipolar field-effect transistors: *In situ* electrical investigation of MnPC-OFETs — •Franziska Lüttich, Ovidiu D. Gordan, and Dietrich R. T. Zahn — Semiconductor Physics, Technische Universität Chemnitz, Chemnitz, Germany

On the way to low-cost and flexible applications organic semiconducting materials are promising. Devices like organic light-emitting diodes, organic solar cells, and organic field-effect transistors (OFETs) can be produced *e.g.* on flexible and elastic substrates and with chemical variation of side groups or substitution of metal centers their properties like optical absorption and charge carrier mobilities can be influenced.

Here we present a temperature dependent study on Manganese Phthalocyanine (MnPc)-OFETs, which reveal an ambipolar behaviour. In order to investigate the electrical properties of MnPc we used OFET "'end-of-line"' substrates from Fraunhofer IPMS with a 100 nm thick thermal silicon dioxide layer as dielectric. The investigated bottom-contact OFETs were fabricated under high vacuum conditions ($p < 4 \cdot 10^{-7}$ mbar) by evaporating MnPc on top of the pre-structured substrates. The electrical DC characteristics were measured *in situ* as a function of temperature. This procedure enables us to determine the activation energies for the hole and electron transport. The influence of ambient atmosphere was also investigated and revealed strong impact on the electrical performance. The topography was determined using an Atomic Force Microscope (AFM).

HL 6.5 Mon 10:30 H 2032

Photoelectron spectroscopy studies on efficient air-stable molecular n-dopants — •Martin Schwarze[1], Max L. Tietze[1], Paul Pahner[1], Ben Naab[2], Zhenan Bao[2], Björn Lüssem[1], Daniel Kasemann[1], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Department of Chemical Engineering, Stanford University, Stanford, California 94305, United States

Understanding the working mechanism of electrical doping in organic semiconductors is essential for the optimization of organic semiconductor devices such as organic light emitting diodes or organic solar cells. A defined doping concentration allows for the control of the Fermi-level position as well as the adjustment of the conductivity of transport layers. In comparison to molecular p-doping of organic semiconductors, n-doping creates the additional problem of air instability. To successfully transfer an electron to the lowest unoccupied molecular orbital (LUMO) of the matrix material, dopants exhibiting shallow highest molecular orbitals (HOMO) are necessary, rendering them prone to reactions with e.g. oxygen. In this study, three different types of n-dopants are compared: air stable cationic DMBI dopants, halogen-free DMBI dimers, and the established but air sensitive Cr2(hpp)4. Fermi-level shift and conductivity of co-evaporated Bis-HFl-NTCDI layers at different doping concentrations as well as stability during air exposure are investigated by UPS and electrical measurements.

HL 6.6 Mon 10:45 H 2032

Mode-selective vibrational manipulation of charge transport in π-conjugated molecular materials — •Robert Lovrincic[1,2], Artem A. Bakulin[3,4], Yu Xi[1], Oleg Selig[3], Huib J. Bakker[3], Yves L. A. Rezus[3], Pabitra K. Nayak[1], Alexandr Fonari[5], Veaceslav Coropceanu[5], Jean-Luc Bredas[5,6], and David Cahen[1] — [1]Department of Materials & Interfaces, Weizmann Institute of Science, Israel — [2]IHF, TU Braunschweig & Innovationlab, Germany — [3]FOM Institute AMOLF, The Netherlands — [4]Cavendish Laboratory, University of Cambridge, UK — [5]School of Chemistry and Biochemistry , Georgia Institute of Technology, USA — [6]Solar & Photovoltaics Center, King Abdullah University, Saudi Arabia

The soft character of organic materials leads to strong coupling between molecular nuclear and electronic dynamics. This coupling opens the way to control charge transport in organic electronic devices by directing molecular vibrational motions. However, despite encouraging

theoretical predictions, experimental realization of such control has remained elusive. Here we demonstrate experimentally that photoconductivity in a model organic optoelectronic device can be controlled by the selective excitation of molecular vibrations. Using an ultrafast infrared laser source to create a coherent superposition of vibrational motions in a pentacene/C60 photoresistor, we observe that excitation of certain modes in the $1500-1700\,\mathrm{cm}^{-1}$ region leads to photocurrent enhancement. The effect depends on the nature of the vibration and its mode-specific character can be well described by the vibrational modulation of intermolecular electronic couplings.

HL 6.7 Mon 11:00 H 2032

Investigation of charge transfer in organic semiconductors using infrared spectroscopy — •Tobias Glaser[1,2], Sebastian Beck[1,2], and Annemarie Pucci[1,2,3] — [1]Universität Heidelberg, Kirchhoff-Institut für Physik — [2]InnovationLab GmbH, 69115 Heidelberg — [3]Universität Heidelberg, Centre for Advanced Materials

Charge transfer in organic semiconductors is used in various ways to increase the performance of organic electronic devices. For example electrochemical doping is used to increase the conductivity in charge transport layers. Additionally, charge injection layers are used to decrease injection barriers between electrodes and organic transport layers. In both cases molecular charge transfer plays an important role, but the basic mechanisms are still subject of heated debate. Due to strong relaxation effects upon molecular charging, infrared (IR) spectroscopy is very well suited to investigate charge transfer in organic semiconductors. Neutral and charged molecules can be distinguished by their different specific vibrational features in spectra of doped layers as well as for interfaces. In this study we investigated charge transfer in thin layers of commonly known transport materials such as 4,4*-bis(N-carbazolyl)-1,1*-biphenyl (CBP) doped with inorganic and organic dopants such as MoO3 or F4TCNQ and at interfaces of organic semiconductors. By quantitative analysis of the experimental spectra the doping efficiency and the degree of charge transfer can be determined for the doped layers. Whereas, for interfacial charge transfer, the formation of a space charge region can be mapped. Financial support by BMBF (project MESOMERIE) is gratefully acknowledged.

HL 6.8 Mon 11:15 H 2032

Structure and Photovoltaic Performance of Chiral Anilino Squaraines — •Manuela Schiek[1], Matthias Schulz[2], Stefanie Brück[1], Martin Silies[3], Heiko Kollmann[3], Christoph Lienau[3], Arne Lützen[2], and Jürgen Parisi[1] — [1]Energy and Semiconductor Research Laboratory, University of Oldenburg, Germany — [2]Kekule-Institute for Organic Chemistry and Biochemistry, University of Bonn, Germany — [3]Ultrafast Nano-Optics, University of Oldenburg, Germany

Small molecular semiconductors such as squaraines are advantageous compared to polymeric materials because they allow a more direct control of the structure on the molecular level and consequently solid state properties. Especially the implementation of chiral side chains introduces new functionalities such as circular dichroism. Different 1,3-bis(N,N-substituted-2,6-dihydroxy-anilino)squaraines with varying terminal N-substitution, in some cases including a stereogenic center, are investigated as single crystals, in thin films and blended with a fullerene acceptor as active layer in bulk heterojunction organic solar cells.

HL 6.9 Mon 11:30 H 2032

Charge separation and C_{60} crystallinity in bulk heterojunction solar cells: the decisive role of device architecture — •Felix Schell[1,2], Michael Scherer[1,3], Diana Nanova[1,2,3], Anne Katrin Kast[2,4], Wolfgang Kowalsky[1,2,3], Rasmus R. Schröder[1,4,5], and Robert Lovrincic[1,3] — [1]InnovationLab GmbH, Heidelberg — [2]Kirchhoff-Institute for Physics, Heidelberg University — [3]Institute for High-Frequency Technology, TU Braunschweig — [4]CellNetworks, BioQuant, Heidelberg University — [5]Center for Advanced Materials, Heidelberg University

The crucial influence of C_{60} crystallinity on the charge separation in organic solar cells (OSC) has been realized very recently. Here, we show the importance of the device architecture on C_{60} crystallisation in the bulk-heterojunction (BHJ). Active layer morphology of small molecule BHJ OSC and its influence on device performance are studied by means of energy-filtered transmission electron microscopy (EFTEM) and electrical characterization. The influence of substrate temperature during deposition and of pure sublayers is assessed. BHJs fabricated at room temperature are found to be finely mixed and amorphous, whereas the corresponding films deposited onto heated substrates show pronounced phase separation. Despite these clear morphological changes, substrate heating does not increase efficiency of OSCs in a non-inverted device architecture. Improvements found in literature for inverted cells can be attributed to stronger acceptor crystallization, present, if deposited onto a pure C_{60} layer but not with an F_4ZnPc substrate, leading to more efficient exciton dissociation.

HL 6.10 Mon 11:45 H 2032

Influence of DMSO-treatment on morphology, composition and performance of PEDOT:PSS layers in organic photovoltaic cells — Sidhant Bom, •Torsten Balster, Marlis Ortel, and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

PEDOT:PSS layers in organic solar cells are used as hole transport (HTL) and electron blocking layers. Therefore the morphology and composition of the layer and the interface have a great influence on the performance of organic photovoltaic devices.

Additional post-deposition treatment of the PEDOT:PSS layers (HTL) in P3HT/PCBM solar cells were studied in this work. For this purpose, pristine PEDOT:PSS layers were spin coated with dimethyl sulfoxide (DMSO) after annealing. Pristine and treated layers were characterized by means of electrical characterization, atomic force microscopy (AFM) and x-ray photoelectron spectroscopy (XPS).

The additional post-deposition DMSO treatment induces an increase in power conversion efficiency by more than 50%. In addition, the open circuit voltage and the short-circuit current were enhanced, whereas the fill factor remained constant. This behavior is explained by modification of the PEDOT:PSS-semiconductor interface. On the one hand smoothening of the interface by reduction of large PSS particles visible in AFM occurs. On the other hand XPS data show a reduction of PSS-sulphur species. Less PSS at the interface should improve the charge carrier injection properties, as observed experimentally.

HL 6.11 Mon 12:00 H 2032

Charge transfer, optical and transport properties in pure organic heterostructures — •Liebing Simon, Hahn Torsten, and Kortus Jens — Institute of Theoretical Physics, TU Bergakademie Freiberg, Leipziger Strasse 23, 09599 Freiberg

We will present theoretical investigation on pure charge transfer materials within the density functional theory framework (DFT). Starting from the recently fabricated picene-F_4TCNQ [1] we explore the electronic and optical properties of novel representatives of this new class of materials. These representatives are formed of polycyclic hydrocarbons and TCNQ derivatives and we compare our results with experimental spectroscopic data.

The picene-F_4TCNQ system shown pronounced diode transistor behavior [2]. By means of DFT/NEGF (non equilibrium green function formalism) [3,4] we obtain the IV-characteristics of selected model devices for these systems. The formation of hybrid orbitals together with intrinsic charge transfer seems to be the origin of the novel electronic and transport properties [5].

[1] Mahns, B. et. al. Crystal Growth & Design (2014). [2] Hahn T., Liebing S., and Kortus J., Nanoscale 6, 14508 (2014). [3] Pederson, M. et. al. Phys. Status Solidi b 217, 197. (2000) [4] Enkovaara, J. et al. Journal of Physics: Condensed Matter 22, 253202 (2010). [5] Lindner S. et. al. Phys. Rev. Lett. 109, 027601 (2012).

HL 6.12 Mon 12:15 H 2032

Single molecule circuits with N-heterocyclic carbene linkers — •Hector Vazquez — Inst. of Physics, Academy of Sciences of the Czech Rep., CZ

In single molecule circuits, where an electrical current flows through a molecule, conducting molecules often have terminal linker groups which bind to the metallic electrodes [1]. These chemical link groups strongly influence the conducting properties, often acting as bottlenecks for electron transmission and result in low-transmission resonances localized at the interface. Therefore, identifying adequate chemical linker groups is essential for achieving ideal mechanical and conducting properties in molecular circuits.

Recently, SAMs of N-heterocyclic carbenes on gold were shown to have very high thermal and oxidative stability [2], making N-heterocyclic carbenes potentially very useful linkers for single molecule transport. In this talk, I will present results from first-principles simulations based on DFT-NEGF for the electronic and conducting properties of carbene-terminated molecules. I will show results for the adsorption properties of N-heterocyclic carbenes on gold. I will also

present transmission calculations of carbene-terminated molecules and discuss these results in the context of other metal-molecule links with Au-C bonds [3].

[1] F. Schwarz and E. Loertscher, J. Phys. Condens. Matter 26 474201 (2014).
[2] C.M. Crudden et al., Nature Chemistry 6 409 (2014).
[3] W. Chen et al., J. Am. Chem. Soc. 133 17160 (2011).

HL 6.13 Mon 12:30 H 2032

Charge and spin transfer materials for molecular electronic and spintronic applications — •Torsten Hahn, Simon Liebing, and Jens Kortus — TU Freiberg, Institut für Theoretische Physik, Leipziger Str. 23, 09599 Freiberg

The combination of different functionalized metal phthalocyanines was found to lead to novel charge- and spin transfer compounds [1,2]. The recently synthesized picene / F4TCNQ charge transfer salt [3] also shows promising physical properties and the theoretical modeling predicts the material to act as a molecular diode with high rectification ratio [4]. Based on density-functional theory calculations we show that in case of the metal phthalocyanines as well as for the picene / F4TCNQ system hybrid states formed by the donor / acceptor system are playing the key role to determine the spectroscopic and quantum transport properties. We further conclude that the tuning of quantum transport properties through hybrid states is a general concept which opens a new route towards functional materials for molecular electronics.

[1] R. Friedrich et al., Phys. Rev. B 87, 115423 (2013). [2] R. Friedrich, B. Kersting, and J. Kortus, Phys. Rev. B 88, 155327 (2013). [3] Mahns, B. et. al., Cryst. Growth and Design 14, 1338-1346 (2014). [4] T. Hahn, S. Liebing, and J. Kortus, Nanoscale 6, 14508 (2014).

HL 6.14 Mon 12:45 H 2032

Device-like calcium corrosion test for ultra-barrier materials — •Frederik Nehm[1], Hannes Klumbies[1], John Fahlteich[2], Felix Dollinger[1], Karl Leo[1], and Lars Müller-Meskamp[1] — [1]Institut für Angewandte Photophysik, TU Dresden, Dresden, Deutschland — [2]Fraunhofer FEP, Dresden, Deutschland

The continuous progress of organic electronics demands for flexible moisture barriers with water vapor transmission rates (WVTRs) below $10^{-4}\ \frac{g(H_2O)}{m^2 d}$ and quick, reliable measurement techniques for such WVTRs. The electrical calcium corrosion test is an extremely sensitive technique used widely in research groups. However, setups differ strongly as do their accuracy and background rates. We report on common issues and show how we manage them in our setup. Barrier corrosion because of direct water condensation on its surface is prevented by a glued-on PET film and Ca-induced stress is mitigated by organic decoupling layers. We demonstrate the effectiveness of our approach with studies on sputtered Zinc-Tin-Oxide and atomic layer deposited (ALD) alumina moisture barriers in different aging climates. Single barriers show a linear WVTR increase with rising absolute humidity at given temperature. Below $40°C$, this is even valid independent of temperature. A divergence at higher temperatures probably originates from the actual barrier layer, since this effect cannot be observed for the pure substrate. Also, nanolaminates using ALD alumina, titania and alkoxide, and multilayer barriers with polymer interlayers with WVTRs down to at least $2 \cdot 10^{-5}\ \frac{g(H_2O)}{m^2 d}$ in $38°C$, 90% relative humidity environments are investigated.

HL 7: Transport: Quantum coherence and quantum information systems - Theory (TT with HL)

Time: Monday 9:30–13:00 Location: H 3005

HL 7.1 Mon 9:30 H 3005

Collective modes in the fluxonium qubit — •Gianluigi Catelani[1] and Giovanni Viola[2] — [1]Forschungszentrum Jülich, PGI-2 — [2]RWTH Aachen, IQI

In the fluxonium qubit, an array comprising a large number of identical Josephson junctions form a so-called superinductance. The superinductance is connected to a junction – the phase slip element – with a smaller Josephson energy and a different charging energy. We investigate the effects of unavoidable capacitive couplings to ground as well as non-linearities of the superinductance: they both introduce interactions between the low-energy qubit degree of freedom and higher-energy collective modes of the circuit. We also consider the role of the additional capacitances that are used to couple the qubit to a resonator for driving and read-out. We show that the interactions with the collective modes can affect not only the spectrum of the qubit but also its coherence.

Work supported in part by the EU under REA grant agreement CIG-618258

HL 7.2 Mon 9:45 H 3005

Optimal Control of Quantum Measurement — Daniel Egger and •Frank Wilhelm — Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany

Pulses to steer the time evolution of quantum systems can be designed with optimal control theory. In most cases it is the coherent processes that can be controlled and one optimizes the time evolution towards a target unitary process, sometimes also in the presence of non-controllable incoherent processes. Here we show how to extend the GRAPE algorithm in the case where the incoherent processes are controllable and the target time evolution is a non-unitary quantum channel. We perform a gradient search on a fidelity measure based on Choi matrices. We illustrate our algorithm by optimizing a measurement pulse for superconducting phase qubits. We show how this technique can lead to large measurement contrast close to 99%. We also show, within the validity of our model, that this algorithm can produce short 1.4 ns pulses with 98.2% contrast.

HL 7.3 Mon 10:00 H 3005

Optimal control of single flux quantum pulses — •Per Liebermann, Daniel Egger, and Frank Wilhelm — Universität des Saarlandes, Saarbrücken

Rapid single flux quantum pulses are a natural candidate for on-chip control of superconducting qubits [1]. We apply trains of single flux quantum pulses to perform single qubit gates. Under the constraint of constant amplitudes and gate times we use genetic algorithms for optimising the pulse sequence to decrease the gate error by two orders of magnitude. We consider leakage transitions into a third energy level as well as timing jitter of the pulses, exploring the robustness of our optimized sequence. This takes us one step further to on-chip qubit controls.

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

HL 7.4 Mon 10:15 H 3005

Adaptive characterization of coherent states — •Markku P. V. Stenberg, Kevin Pack, and Frank K. Wilhelm — Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany

We present a method for efficient characterization of an optical coherent state $|\alpha\rangle$. We choose measurement setups adaptively based on the data while it is collected. Our algorithm divides the estimation in three different steps with different measurement strategies: (i) searching a crude estimate, (ii) rapidly improving the accuracy, and (iii) the phase where the improvement of the accuracy slows down due to the quantum nature of the coherent state. Our algorithm significantly outperforms nonadaptive schemes. While our standard strategy is robust against measurement errors we also present strategies optimized for the presence of such errors.

HL 7.5 Mon 10:30 H 3005

Qubit dephasing due to Quasiparticle Tunneling — •Sebastian Zanker, Michael Marthaler, and Gerd Schön — Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany

We study dephasing of a superconducting qubit due to quasiparticle tunneling through a Josephson junction. While qubit decay due to tunneling processes is well understood within a golden rule approximation, pure dephasing due to BCS quasiparticles gives rise to a divergent golden rule rate. We calculate qubit dephasing due to quasiparti-

cle tunneling beyond lowest order approximation in coupling between qubit and quasiparticles. Summing up a certain class of diagrams we show that qubit dephasing due to purely longitudinal coupling to quasiparticles leads to dephasing $\sim \exp(-x(t))$ where $x(t) \propto t^{3/2}$ for short time scales and $x(t) \propto t \log(t)$ for long time scales.

HL 7.6 Mon 10:45 H 3005

Detecting nonlocal Cooper pair entanglement by optical Bell inequality violation — Simon E. Nigg, Rakesh P. Tiwari, Stefan Walter, and •Thomas L. Schmidt — Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland

Based on the Bardeen Cooper Schrieffer (BCS) theory of superconductivity, the coherent splitting of Cooper pairs from a superconductor to two spatially separated quantum dots has been predicted to generate nonlocal pairs of entangled electrons. In order to test this hypothesis, we propose a scheme to transfer the spin state of a split Cooper pair onto the polarization state of a pair of optical photons. We show that the produced photon pairs can be used to violate a Bell inequality, unambiguously demonstrating the entanglement of the split Cooper pairs.

[1] Nigg et al., arXiv:1411.3945 [cond-mat.mes-hall]

HL 7.7 Mon 11:00 H 3005

Detection of non-local spin-entanglement by light emission from a superconducting pn-junction — •Alexander Schroer and Patrik Recher — Institut für Mathematische Physik, Technische Universität Braunschweig, D-38106 Braunschweig, Germany

We model a superconducting pn-junction in which the n- and the p-site are contacted through two optical quantum dots, each embedded into a photonic nanocavity. Whenever a Cooper pair is transported from the n-site to the p-site, two photons are emitted. When the two electrons of a Cooper pair are transported through different quantum dots, polarization entangled photons are created, provided that the Cooper pairs retain their spin-singlet character although being spatially separated on the two quantum dots. We show that a CHSH Bell-type measurement is able to detect the entanglement of the photons over a broad range of microscopic parameters, even in the presence of parasitic processes and imperfections. Observing this signature is a direct proof of crossed Andreev reflection, or, equivalently, Cooper pair splitting, retaining the spin-singlet wave function.

15 min. break.

HL 7.8 Mon 11:30 H 3005

Scattering of two photons from two distant qubits: exact solution — Matti Laakso and •Mikhail Pletyukhov — Institute for Theory of Statistical Physics, RWTH Aachen, 52056 Aachen

We consider the inelastic scattering of two photons from two qubits separated by an arbitrary distance and coupled to a one-dimensional transmission line. We present an exact, analytical solution to the problem, and use it to explore a particular configuration of qubits which is transparent to single-photon scattering, thus highlighting non-Markovian effects of inelastic two-photon scattering: Strong two-photon interference and momentum dependent photon (anti)bunching. This latter effect can be seen as an inelastic generalization of the Hong-Ou-Mandel effect.

HL 7.9 Mon 11:45 H 3005

Robust entanglement under multipartite correlated dephasing — •Edoardo Carnio[1,2], Manuel Gessner[2], and Andreas Buchleitner[2,3] — [1]Department of Physics, University of Warwick, Coventry, CV4 7AL, United Kingdom — [2]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Straße 3, 79104 Freiburg, Germany — [3]Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität Freiburg, Albertstraße 19, 79104 Freiburg, Germany

We derive an analytical description for the dephasing process undergone by a system on non-interacting atomic qubits, immersed in a uniform, fluctuating magnetic field. The dephasing process is correlated, as the noise source is common to all the particles and induces an effective atom-atom interaction on them. This correlated nature allows to specify field orientations that preserve any degree of atomic entanglement for all times, and families of states with entanglement properties that are time-invariant for arbitrary field orientations. Our formalism applies to arbitrary spectral distributions of the fluctuations.

HL 7.10 Mon 12:00 H 3005

Bell inequalities and waiting times — •Christina Pöltl and Michele Governale — School of Chemical and Physical Sciences and MacDiarmid Institute for Advanced Materials and Nanotechnology, Victoria University of Wellington, PO Box 600, Wellington 6140, New Zealand

We propose a Bell test based on waiting time distributions for spin entangled electron pairs, which are generated and split in mesoscopic Coulomb blockade structures, denoted as entanglers. These systems have the advantage that quantum point contacts enable a time resolved observation of the electrons occupying the system, which gives access to quantities such as full counting statistics and waiting time distributions. We use the partial waiting times to define a CHSH-Bell test, which is a purely electronic analogue of the test used in quantum optics. After the introduction of the Bell inequality we discuss the findings on the two examples of a double quantum dot and a triple quantum dot. This Bell test allows the exclusion of irrelevant tunnel processes from the statistics normally used for the Bell correlations. This can improve the parameter range for which a violation of the Bell inequality can be measured significantly.

HL 7.11 Mon 12:15 H 3005

Quantum dynamics of a strongly driven Josephson Junction — •Jennifer Gosner, Björn Kubala, and Joachim Ankerhold — Institute for Complex Quantum Systems, University of Ulm, Germany

A Josephson Junction embedded in a dissipative circuit can be driven to exhibit non-linear oscillations.

Classically the non-linear oscillator shows under sufficient strong driving and weak damping dynamical bifurcations and a bistable region similar to the conventional Duffing-oscillator. These features depend sensitively on initial conditions and parameters. The sensitivity of this circuit, called Josephson Bifurcation Amplifier, can be used to amplify an incoming signal, to form a sensing device or even for measuring a quantum system.

The *quantum* dynamics can be described by a dissipative Lindblad master equation. Signatures of the classical bifurcation phenomena appear in the Wigner representation, used to characterize and visualize the resulting behaviour. In order to compare this quantum dynamics to that of the conventional Duffing-oscillator, the complete cosine-nonlinearity of the Josephson Junction is kept for the quantum description while going into a rotating frame.

HL 7.12 Mon 12:30 H 3005

Dissipation-induced first order decoherence phase transition in a non-interacting fermionic system — •Mihailo Cubrovic — Institute for Theoretical Physics, Universität zu Köln, Zülpicher Str. 77, D-50937, Köln, Germany

We consider a dissipative tight-binding fermionic chain as a model for a nanowire with current leakage due to imperfect isolation. The dissipation manifests as tunneling into/out of the chain from/to the environment. The evolution of the system is described by the Lindblad equation, generalized to incorporate the memory effects in the bath. Already infinitesimally small dissipation along the chain induces a quantum phase transition (QPT). This is a decoherence QPT: the reduced density matrix of a subsystem (far from the ends of the chain) can be represented as the tensor product of single-site density matrices. We analyze the QPT in the thermodynamic limit by looking at the entropy and the response function in the bulk, and compare in detail the results with and without memory in the bath. To gain a better intuitive understanding we also contruct the analogous classical model (a correlated random walk process) and compare its behavior to the QPT of the quantum chain.

HL 7.13 Mon 12:45 H 3005

Spin dynamics using the Majorana representation: validity, path integral and higher correlators — •Pablo Schad[1], Boris N. Narozhny[1,2], Gerd Schön[3], Yuriy Makhlin[4,5], and Alexander Shnirman[1] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany — [2]National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe shosse 31, 115409 Moscow, Russia — [3]Institut für Theoretische Festkörperphysik und Institut für Nanotechnologie, Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany — [4]Landau Institute for Theoretical Physics, acad. Semyonov av., 1a, 142432, Chernogolovka, Russia — [5]Moscow Institute of Physics and Technology, 141700, Dolgoprudny, Russia

We present a method to calculate higher spin correlators via the Majorana fermion representation of spin operators. We show explicitly that the Majorana representation does not require any projection procedure. Previously found identities [1,2] between spin and Majorana fermion correlation functions are extended. As an example we consider a spin-1/2 coupled to an isotropic, ohmic bath. We formulate a path-integral approach, which is valid at B=0 in contrast to perturbation theory, find the saddle-point solution and discuss fluctuations. We demonstrate that spin correlators in the high-temperature regime can be obtained using saddle-point Green's functions.

[1] A. Shnirman and Y. Makhlin,
Phys. Rev. Lett. 91, 207204 (2003).
[2] W. Mao, P. Coleman, C. Hooley, and D. Langreth,
Phys. Rev. Lett. 91, 207203 (2003).

HL 8: Transport: Spintronics and magnetotransport (TT with HL)

Time: Monday 9:30–12:00 Location: A 053

HL 8.1 Mon 9:30 A 053

Low Temperature THz Spectroscopy and Transport in Nanostructures — •Julian Braun, Sergej Andreev, Elke Scheer, and Torsten Pietsch — Universität Konstanz, Konstanz, Germany

Theoretical predictions [1] suggest a new source for THz radiation, based on a spin relaxation in metallic heterocontacts. In a dilute ferromagnet a spin imbalance can be created by a spin polarized current originating in a ferromagnet of opposite magnetization. Relaxation in the energetically more favorable spin distribution should occur by emission of a photon with an energy in the THz range.

We constructed a compact cw-THz spectrometer working at temperatures down to 4 K and a frequency range from 0.1 GHz to 2000 GHz. Installed in a vector magnet we can thereby correlate magnetotransport measurements with the spectroscopic analysis to investigate the spin imbalance in metallic heterocontacts. Additionally characterization measurement on different metallic and superconducting samples will be presented.

[1] A.M. Kadigrobov et al., Europhys. Lett. 67, 948-954 (2004).

HL 8.2 Mon 9:45 A 053

Room-Temperature Spin Thermoelectrics in Metallic Films — •Sebastian Tölle[1], Cosimo Gorini[2], and Ulrich Eckern[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Faculty of Physics, University of Regensburg, 93040 Regensburg, Germany

Efficient heat-to-spin conversion is the central goal of spin caloritronics. When considering metallic systems, two interesting phenomena stand out in this field: the spin Nernst effect and thermally-induced spin polarizations. They consist in the generation of, respectively, a spin current or a spin polarization transverse to an applied temperature gradient, i.e., they are the thermal counterparts of the well known spin Hall effect and current-induced spin polarization (Edelstein effect). We study these phenomena considering dynamical spin-orbit coupling, namely the spin-orbit coupling with phonons and vibrating impurities, which give rise to a dynamical side-jump mechanism and dynamical Elliott-Yafet spin relaxation. Such processes, which have not been considered before in this context, dominate at temperatures $T > T_D$, with T_D the Debye temperature. This condition is met in typical spin injection/extraction experiments performed at room temperature in transition metals such as Pt, Au, and Ta. Our results show a nonlinear T-dependence of the spin Nernst and spin Hall conductivities due to an interplay between intrinsic (Bychkov-Rashba type) and extrinsic (dynamical) spin-orbit coupling [1].

[1] S. Tölle, C. Gorini, and U. Eckern, arXiv:1409.1809 (2014) (accepted for publication in Phys. Rev. B).

HL 8.3 Mon 10:00 A 053

Phonon Skew Scattering — •Cosimo Gorini[1], Ulrich Eckern[2], and Roberto Raimondi[3] — [1]Institut für Theoretische Physik, Universität Regensburg — [2]Institut für Physik, Universität Augsburg — [3]Dipartimento di Fisica, Università Roma Tre

In spin injection/extraction experiments in metallic systems, the observed temperature behaviour of the (inverse) spin Hall effect is used to determine the dominant spin-orbit mechanism in the sample. This is a fundamental issue of high practical importance.

The current understanding of the high-T behaviour is based on a phenomenological extrapolation from the low-T theory. The latter predicts that (i) a T-independent (inverse) spin hall signal is a signature of dominant side-jump, and (ii) its scaling as the mobility indicates dominant skew scattering.

Our quantum field theoretical (Keldysh) calculation shows, however, that at typical experimental temperatures phonon-induced skew scattering also leads to a T-independent signal – just as side-jump does. Thus, discerning between the two appears a more complicated issue than until now expected.

HL 8.4 Mon 10:15 A 053

Single atom memory described by the quantum master equation: Ho on Pt(111) — •Christian Karlewski[1,2], Michael Marthaler[1], Wulf Wulfhekel[3], and Gerd Schön[1,2] — [1]TFP, Karlsruher Institut für Technologie — [2]INT, Karlsruher Institut für Technologie — [3]PHI, Karlsruher Institut für Technologie

Miniaturizing current memory bits to optimize the storage density is an important task of information technology research. The ultimate goal are single atoms as one bit. Single magnetic holmium atoms on a platinum (111) surface have been investigated in Nature 503, 242 (2013) and have highly stable magnetic moments, in or out of the plane. Stability can be maintained for several minutes, making holmium a great candidate as single atomic storage. The theoretical description of this system is based on the quantum master equation of open quantum systems. We will show that even if the system in total behaves as a classical bit with two states, a full quantum mechanical description is needed to catch the dynamics properly. The dependence of the lifetime of this system on different parameters is investigated and we will show that it might be possible to improve the properties of our system even further by understanding the mechanisms which at present limit the lifetimes.

HL 8.5 Mon 10:30 A 053

Observation of spatial fluctuations of the Rashba parameter by scanning tunneling spectroscopy — •Jan Raphael Bindel[1], Marcus Liebmann[1], Jascha Ulrich[2], Eugene Sherman[3], and Markus Morgenstern[1] — [1]II. Institute of Physics B, RWTH Aachen University, Aachen, Germany — [2]Institute for Quantum Information, RWTH Aachen University, Aachen, Germany — [3]Basque Foundation for Science, Ikerbasque, Bilbao, Spain

We investigate a 2DES induced by Cs surface doping of p-type InSb(110) and evaluate the Rashba parameter on the local scale. The Rashba effect is one of the possibilities to manipulate spins by external gate voltages which led to the proposal of the spin transistor. As a local property, however, the Rashba effect is prone to disorder as ubiquitous in semiconductors, which, in turn, induces spatial fluctuations of the strength of the Rashba effect, and, thus, spin dephasing [1]. Recently, we have shown that the Rashba effect can be probed by STS in magnetic fields as an additional contribution to the spin splitting [2]. Here, we investigate the correlations between the electrostatic potential and the Rashba effect on the local scale. A detailed magnetic field dependence analysis of the spin splitting is required in order to disentangle the Rashba parameter from the Zeeman effect and the spatially fluctuating exchange enhancement. Moreover the nodal structure of the wave functions has to be considered in higher Landau levels, where it leads to multiple peak structures [3].

[1] Glazov et al., Physica E 42, 2157 (2010).
[2] Becker et al., PRB 81, 155308 (2010).
[3] Hernangómez-Pérez et al., PRB 88, 245433 (2013).

15 min. break.

HL 8.6 Mon 11:00 A 053

Magnetoresistance in Weyl semimetals — •Janina Klier[1,2], Igor Gornyi[1,3], and Alexander Mirlin[1,2,4] — [1]Institute for Nanotechnology, Karlsruher Institute for Technology, Karlsruhe, Germany — [2]Institute for Theoretical Condensed Matter physics, Karlsruher

Institute for Technology, Karlsruhe, Geermany — [3]A.F. Ioffe Physico-Technical Institute, St. Petersburg, Russia — [4]Petersburg Nuclear Physics Institute, St. Petersburg, Russia

We theoretically study the magnetoresistvity of a Weyl semimetal within two disorder models: pointlike impurities and charged impurities. Impurity scattering is treated using a self-consistent Born approximation. We find an unusual broadening of Landau levels which leads to a rich structure of various regimes in temperature-magnetic field plane. In particular, the magnetoresitance shows non-monotonous behavior. In the limits of strongest magnetic fields for pointlike impurities, this leads to a vanishing magnetoresistance. For charged impurities, broadening of Landau levels is less important in high magnetic fields. This leads to a positive linear magnetoresistance in strongest magnetic fields.

HL 8.7 Mon 11:15 A 053

Spin-orbit induced longitudinal spin transport in non-magnetic solids — •Sebastian Wimmer, Marten Seemann, Kristina Chadova, Diemo Ködderitzsch, and Hubert Ebert — Ludwig-Maximilians-Universität München, München, Deutschland

A group-theoretical scheme is presented that allows investigating the symmetry properties of response tensors relevant to the field of spintronics. For the spin conductivity tensor it is shown that only the magnetic Laue group has to be considered in this context. In this case non-vanishing transverse elements, found without making reference to the two-current model, give rise to the spin Hall and Edelstein effects in non-magnetic as well as magnetic solids. In the latter case non-vanishing longitudinal elements cause among others the spin-dependent Seebeck effect. For non-magnetic solids having low symmetry non-vanishing longitudinal elements are shown to exist as well. These give rise to spin-orbit induced *longitudinal* spin transport that has not been considered before. Numerical studies confirm these findings and demonstrate that the longitudinal spin conductivity may be in the same order of magnitude as the conventional transverse one.

HL 8.8 Mon 11:30 A 053

Topological transitions in the geometric phase in spin interferometers — •Henri Saarikoski[1], Enrique Vazquez[2], Jose Pablo Baltanás[2], Diego Frustaglia[2], Fumiya Nagasawa[3], and Junsaku Nitta[3] — [1]RIKEN Center for Emergent Matter Science (CEMS), Saitama 351-0198, Japan — [2]Departamento de Física Aplicada II, Universidad de Sevilla, E-41012 Sevilla, Spain — [3]Department of Materials Science, Tohoku University, Sendai 980-8579, Japan

An electronic spin transported around a circuit acquires a phase factor that depends on the geometry of the path in the parameter space. In the adiabatic limit this is the Berry phase and it has been argued that it can undergo an abrupt transition via manipulation of the topology of the path [1]. However, spin transport in mesoscopic structures is usually nonadiabatic, which is associated with the Aharonov-Anandan geometric phase. Here we identify the characteristic signatures of topological transitions in nonadiabatic spin transport by 1D and 2D calculations of mesoscopic loops. We find that the topological transition is characterized by an *effective* Berry phase due to correlations between dynamic and geometric phases close to the region where the transition occurs. This effective Berry phase is related to the topology of the field texture rather than the spin-state structure. The transition manifests as a distinct dislocation of the interference pattern in the quantum conductance. The phenomenon is robust, and can be observed in mesoscopic arrays of loops where phase coherence is significant.

[1] Y. Lyanda-Geller, Phys. Rev. Lett. 71, 657 (1993).

HL 8.9 Mon 11:45 A 053

Use of resonant tunneling in spin transfer torque magnetic tunnel junctions — •Bhaskaran Muralidharan[1], Niladri Chatterji[2], and Ashwin Tulapurkar[1] — [1]Department of Electrical Engineering, IIT Bombay, Powai, Mumbai-400076, India — [2]Department of Physics, IIT Bombay, Powai, Mumbai- 400076, India

We propose a novel device that uses resonant tunneling to enhance the spin-transfer torque switching characteristics of magnetic tunnel junctions. The proposed device structure is a resonant tunneling magnetic tunnel junction based on a MgO-semiconductor heterostructure sandwiched between a fixed magnet and a free magnet [1]. We employ the non-equilibrium Green's function formalism coupled self consistently with the Landau-Lifshitz-Gilbert-Slonczewski equation to demonstrate that the physics of resonant tunneling leads to improved tunnel magneto-resistance characteristics as well as lower switching voltages in comparison with traditional trilayer devices. Using this framework, we also demonstrate a novel spin torque oscillator design at zero applied magnetic field, by simply engineering parallel and perpendicular spin torques.

[1] N. Chatterji, A. A. Tulapurkar and B. Muralidharan, ArXiv: 1411.6454, (2014).

HL 9: Quantum dots: Optical properties

Time: Monday 10:00–13:00 Location: EW 203

HL 9.1 Mon 10:00 EW 203

Advanced in-situ elctron-beam lithography on pre-selected quantum dots by cathodoluminescence spectroscopy — •Arsenty Kaganskiy, Manuel Gschrey, Alexander Schlehahn, Jan-Hindrik Schulze, Ronny Schmidt, Tobias Heindel, Sven Rodt, André Strittmatter, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, D-10623

Future quantum technology will rely crucially on the development of sources for indistinguishable and entangled photon pairs based on self-assembled quantum dots (QDs). To boost their photon extraction efficiency QDs need to be embedded in a precise and controlled way into photonic structures. In order to meet this requirement we developed and further advanced a deterministic technology platform named in-situ cathodoluminescence lithography (CLL) [1]. In the advanced CLL technique we are now able to fully characterize single QDs in a pre-registering process before integrating them with high alignment accuracy, e.g. into microlenses. The pre-characterization comprises measurement of the fine-structure splitting, time resolved luminescence, and second-order photon autocorrelation. Thus, advanced CLL combines the advantage of integrating individual QDs deterministically into nanostructures with a thorough pre- and post-characterization process. Within this scheme it is possible to directly evaluate the change in optical properties, e.g. in terms of the Purcell effect induced by the photonic structures.

[1] M. Gschrey et al., APL 102, 251113 (2013).

HL 9.2 Mon 10:15 EW 203

Processing and optical characterisation of InGaN quantum dots with AlGaN barrier layers — •Elahe Zakizadeh, Carsten Laurus, Stephan Figge, Kathrin Sebald, and Jürgen Gutowski — Institute of Solid State Physics, University of Bremen, Germany

InGaN quantum dots are promising candidates to realize single photon emission at elevated temperatures due to their large bandgap and high exciton binding energies. Single line emission from InGaN quantum dots was already observed up to 150 K.

Here, we report on samples for which an additional AlGaN barrier layer was grown below the InGaN quantum dot layer by metal organic vapor phase epitaxy in order to increase the carrier confinement which might result in single photon emission at elevated temperatures.

For single quantum dot spectroscopy the optically excited quantum dots density must be reduced. One possibility is the creation of shadow masks on the sample. In this contribution different lithographic methods for producing the shadow masks and micro-photoluminescence measurements on the InGaN quantum dots will be presented.

HL 9.3 Mon 10:30 EW 203

Dissipative preparation of the exciton and biexciton in a single self-assembled quantum dot — •Lukas Hanschke[1], Manuel Koller[1], Per-Lennart Ardelt[1], Kevin A. Fischer[2], Kai Müller[2], Alexander Kleinkauf[1], Alexander Bechtold[1], Tobias Simmet[1], Jakob Wierzbowski[1], Gerhard Abstreiter[1], and Jonathan J. Finley[1] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany — [2]E. L. Ginzton Laboratory, Stanford University, Stanford, California 94305, USA

Pulsed resonant fluorescence is used to probe ultrafast phonon-assisted exciton and biexciton preparation in individual self-assembled InGaAs quantum dots. By driving the system using large area ($>10\pi$) near resonant optical pulses, we experimentally demonstrate how phonon mediated dissipation within the manifold of dressed excitonic states can be used to prepare the neutral exciton with a fidelity 70%. By comparing the phonon-assisted preparation with resonant Rabi oscillations we show that the phonon-mediated process provides the higher fidelity preparation for large pulse areas and is less sensitive to pulse area variations. By detuning the laser with respect to the exciton transition we map out the spectral density for exciton coupling to the bulk LA-phonon continuum. Similar phonon mediated processes are shown to facilitate direct biexciton preparation via two photon biexciton absorption, with fidelities $> 80\%$. Our results are found to be in very good quantitative agreement with simulations that model the quantum dot-phonon bath interactions with Bloch-Redfield theory.

HL 9.4 Mon 10:45 EW 203

Neutral and charged biexciton-exciton-cascade of near-telecom wavelength MOVPE-grown InGaAs QDs — •Jan Kettler, Matthias Paul, Fabian Olbrich, Katharina Zeuner, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und funktionelle Grenzflächen (IHFG), Universität Stuttgart, Allmandring 3, 70569 Stuttgart

The implementation of large-scale fiber-based quantum information networks requires sources of single and entangled photons that show little absorption and dispersion in standard glass fibers. InGaAs quantum dots (QDs) have shown to be bright and flexible sources of non-classical light with typical emission wavelengths below 1 μm.

Here we demonstrate InGaAs QDs grown by industrial standard metal-organic vapor phase epitaxy (MOVPE) that are covered with a thin Indium-rich layer, leading to red-shifted emission wavelengths. The QDs can be grown with an ultra-low lateral density ($< 10^7$ cm^{-2}) and show single-photon emission at the telecom O-band (1.3 μm). We further investigate cascaded photon emission from the biexciton-exciton cascade which is a prerequisite to the generation of polarization-entangled photon pairs.

HL 9.5 Mon 11:00 EW 203

Exciton dynamics in a single site-controlled quantum dot — •Ole Hitzemann, Andrei Schliwa, André Strittmatter, Jan-Hindrik Schulze, David Quandt, Waldemar Unrau, Udo W. Pohl, and Axel Hoffmann — Institut für Festkörperphysik, Technische Universität Berlin, Germany

Direct and phonon-mediated channels of optical excitation are studied on a single isolated site-controlled InGaAs/GaAs quantum dot (QD). The nucleation site was precisely defined by a distant buried stressor formed by controlled partial oxidation of a sandwiched AlGaAs layer as part of a mesa structure.

Above a sub-micrometer aperture we observe sharp luminescences lines, originating from a single QD as demonstrated by autocorrelation measurements. Micro photoluminescence excitation spectroscopy shows and coupling with phonon modes as well as distinctively different photoluminescence spectra for different excitation energies. Excitation power dependent measurements reveal the saturation behavior of excitonic and high excitation luminescence lines. The decay dynamics of different exciton related luminescence lines are studied by time-resolved micro photoluminescence spectroscopy.

HL 9.6 Mon 11:15 EW 203

Infrared transmission spectroscopy to measure intersublevel spacings in InAs self-assembled quantum dots — •Shovon Pal[1,2], Sascha R. Valentin[1], Nadezhda Kukharchyk[1], Hanond Nong[2], Alireza B. Parsa[3], Gunther Eggeler[3], Arne Ludwig[1], Nathan Jukam[2], and Andreas D. Wieck[1] — [1]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Germany. — [2]AG Terahertz Spektroskopie und Technologie, Ruhr-Universität Bochum, Germany. — [3]Institut für Werkstoffe, Ruhr-Universität Bochum, Germany.

For over a decade, zero-dimensional semiconductor quantum dots have broadened the horizon of device applications from simple electronic memories to many optoelectronic devices like single photon emitter and photodetectors. The working principle of all these devices relies on the quantization resulting from confinement in such nanostructures. In this study, we employ Fourier transform infrared transmission spectroscopy to investigate the intersublevel spacings in the conduction band of self-assembled InAs quantum dots. Epitaxial, complementary-doped and semi-transparent electrostatic gates are grown on top of the sample within the ultra high vacuum conditions of the molecular beam epitaxy. These gates enable voltage tuning of the device with a better optical transmission [1].

[1] S. Pal et al., Infrared transmission spectroscopy of charge carriers in self-assembled InAs quantum dots under surface electric fields, J. Phys.: Condens. Matter 26 (2014) 505801.

Coffee break

HL 9.7 Mon 11:45 EW 203

Applying pump-probe quantum state tomography to a semiconductor optical amplifier — •Nicolai B. Grosse[1], Nina Owschimikow[1], Roland Aust[2], Benjamin Lingnau[2], Alexej Koltchanov[1], Mirko Kolarczik[1], Kathy Lüdge[2], and Ulrike Woggon[1] — [1]Institut für Optik und Atomare Physik, Technische Universität Berlin, Germany — [2]Institut für Theoretische Physik, Technische Universität Berlin, Germany

We have combined the techniques of pump-probe and quantum state tomography to observe how an In(Ga)As based quantum-dot semiconductor optical amplifier can transform the quantum state of a probe pulse that is tuned to the quantum dots' ground state, while optically pumping the quantum dots' excited state. From the Wigner functions thus obtained, the device gain, the amplified noise, and the excess noise due to amplified spontaneous emission could be measured relative to the quantum noise limit and on an ultrafast time scale. This information was used to infer the degree of population inversion in the gain medium, which revealed a depletion and recovery of the population inversion on the sub-picosecond time scale.

HL 9.8 Mon 12:00 EW 203

Pulsed ODNMR in (In,Ga)As/GaAs-QDs — •Eiko Evers[1], Tomasz Kazimierczuk[1,2], Steffen Varwig[1], Alex Greilich[1], Dmitri Yakovlev[1,3], Dirk Reuter[4,5], Andreas Wieck[5], and Manfred Bayer[1,3] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Institute of Experimental Physics, Faculty of Physics, University of Warsaw, ul. Hoza 69, 00-681 Warszawa, Poland — [3]Ioffe Physical-Technical Institute, Russian Academy of Sciences, 194021 Saint Petersburg, Russia — [4]Department Physik, Universität Paderborn, Warburger Straße 100, 33098 Paderborn, Germany — [5]Angewandte Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany

The spin of electrons in singly charged quantum dots is surrounded by a nuclear spin-bath, which limits the spin-coherence time T_{2,e^-}. The spin dynamics of surrounding isotopes in an ensemble of self-assembled (In,Ga)As/GaAs QDs is investigated using a combination of optically detected e^--spin polarization via Faraday rotation and pulsed, coherent radio frequency NMR control of nuclear-spin orientation. This allows to directly observe the influence of the nuclear-spin bath on the e^--spin polarization in the time domain and to identify the isotopes interacting with the electron spin. We measured a coherence time $T_{2,^{75}\mathrm{As}}$ of up to 6 ms.

HL 9.9 Mon 12:15 EW 203

Random-alloying induced optical fingerprints in colloidal quantum dots — •Daniel Mourad[1], Tangi Aubert[2], Antoine Guille[2], Edouard Brainis[2], Zeger Hens[2], and Gabriel Bester[1] — [1]Institut für Physikalische Chemie, Universität Hamburg — [2]Physics and Chemistry of Nanostructures, Ghent University

Monodisperse, homogeneously alloyed quantum dots (QDs), which can be grown by means of colloidal synthesis, allow for a tayloring of the absorption/emission properties by variation of the composition. However, distinguishing a random alloy from, e.g., a core/shell nanocrystal is difficult and requires advanced characterization tools such as Raman spectroscopy [Aubert *et al.*, Chem. Mater. 25(12), 2388 (2013)]. We show that randomly alloyed Cd(Se,S) QDs exhibit fingerprints of random alloying in their absorption spectrum. Furthermore, we demonstrate that a stochastical empirical tight-binding scheme can reproduce these features without additional free parameters and link them to symmetry breaking intrinsic to random alloying [Mourad *et al.*, Chem. Mater., DOI: 10.1021/cm5035408]. When complemented by many-particle calculations in the configuration interaction framework, excited-state properties like the bowing of the optical gap are also in very good agreement with the experiment. Since symmetry breaking is inherent to random alloys, our method may provide a general framework where theory can be used to predict random alloying fingerprints

in absorption spectra of different nanomaterials. We discuss the effects of size variations, different composition profiles and further material systems.

HL 9.10 Mon 12:30 EW 203

Electron-Phonon coupling in colloidal CdSe/CdS quantum dots — •Steffen Westerkamp, Axel Hoffmann, and Andrei Schliwa — Institut für Festkörperphysik, TU Berlin

The Huang-Rhys-factors of electron-phonon coupling in colloidal CdSe/CdS quantum dots are calculated for various sizes, core-shell ratios, and interface transitions both for the zincblende and the wurtzite phase. Electron and hole wavefunctions are obtained using strain dependent 8-band-kp theory. Phonon eigenmodes and frequencies are calculated using an atomistic model employing pseudopotentials. In particular we discuss the consequences of the lower symmetry of the wurtzite phase compared to zincblende with respect to the electronic spectrum, the phonon frequencies and the coupling strength.

HL 9.11 Mon 12:45 EW 203

Radiation pattern for epitaxial Quantum Dots — Ludwig Albrecht Thorsten Greif, Stefan Jagsch, Axel Hoffmann, and •Andrei Schliwa — TU Berlin, Germany

Effective interaction between an exciton (X_0) localized in a quantum dot (QD) and a cavity mode (CM) requires i) resonance between X_0 and CM, ii) optimal spatial overlap of QD and CM, and iii) a transition dipole moment which is collinear to the electric field of the CM. The latter is closely related to the angular-resolved radiation characteristics of the X_0, which will be discussed here for epitaxial QDs of different chemistry, crystal structure and shape using eight-band kp theory.

HL 10: Photovoltaics: Kesterites and less widely used materials (with DF)

Time: Monday 11:15–13:00 Location: ER 164

HL 10.1 Mon 11:15 ER 164

Optical properties of Cu-chalcogenide photovoltaic absorbers from self-consistent GW and the Bethe-Salpeter equation — •Sabine Körbel[1,2], David Kammerlander[2], Rafael Alejandro Sarmiento Pérez[2,3], Miguel Alexandre Lopes Marques[1], and Silvana Botti[3] — [1]Martin-Luther-Universität Halle-Wittenberg, Germany — [2]Université Claude Bernard Lyon 1, France — [3]Friedrich-Schiller-Universität Jena, Germany

Self-consistent *GW* and the solution of the Bethe-Salpeter equation are currently the best approaches to accurately simulate electronic excitations in a vast class of materials, ranging from molecules to solids. However, numerical instabilities, caused by a vanishing band gap in density-functional theory, make it impossible to use the common implementations of these techniques to calculate optical absorption spectra of the best-known thin-film absorbers for solar cells: $Cu(In,Ga)(S,Se)_2$ chalcopyrites and $Cu_2ZnSn(S,Se)_4$ kesterites/stannites. Here we solve this problem by using a finite-difference method in k-space to evaluate the otherwise diverging dipole matrix elements, obtaining excellent agreement with experiment. Having established the validity of this approach, we use it then to calculate the optical response of the less-studied, but promising, $Cu_2ZnGe(S,Se)_4$ compounds, opening the way to predictive calculations of still unknown materials.

HL 10.2 Mon 11:30 ER 164

Formation of Single-Phase Cu_2ZnSnS_4 Thin Films by Control of Secondary Phases in a Solid State Reaction — •Justus Just[1,2], Jan-Christoph Hebig[1,2], Roland Mainz[1], Dirk Lützenkirchen-Hecht[2], Ronald Frahm[2], and Thomas Unold[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Bergische Universität Wuppertal, Gaußstraße 20, 42109 Wuppertal, Germany

The conversion efficiency of Cu_2ZnSnS_4(CZTS) based solar cells significantly depends on deposition conditions and specifically the composition of the material. Although best material qualities are observed for Cu-poor and Zn-rich conditions, it has been shown that the compositional region of single phase CZTS is rather small, inevitably leading to a segregation of secondary phases, especially ZnS for Zn-rich material. To overcome this, but still maintain Cu-poor and Zn-rich growth we have developed a two stage co-evaporation process including a thermal treatment. In this process CZTS is formed by a cation interdiffusion process during a solid state reaction of ZnS with ternary Cu_2SnS_3. By oversupplying ZnS the chemical potential of Zn is higher than needed for stoichiometric CZTS, while an uncontrolled segregation of ZnS within the CZTS layer is avoided. This method allows the synthesis of single phase CZTS as shown by X-ray absorption spectroscopy. The final absorber layers show a homogenous distribution of atoms indicating that the solid state reaction is fully completed. To investigate the diffusion kinetics as well as the recrystallization mechanism in-situ real-time X-ray diffraction measurements were performed.

HL 10.3 Mon 11:45 ER 164

Reversible band gap changes in $Cu_2ZnSn(S,Se)_4$ solar cells induced by post-annealing — •Christoph Krämmer[1], Christian Huber[1], Christian Zimmermann[1], Mario Lang[1], Thomas Schnabel[2], Tobias Abzieher[1,2], 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, 70565 Stuttgart, Germany

The absence of the environmentally problematic and expensive metals indium and gallium makes the kesterite $Cu_2ZnSn(S,Se)_4$ (CZTSSe) material system a promising alternative to the established $Cu(In,Ga)Se_2$. Recent publications demonstrated that the amount of Cu_{Zn}+Zn_{Cu} antisite defect pairs can be influenced by post-annealing experiments. This has a direct impact on the band gap E_g of the material. We demonstrate that this effect can be used to reversibly tune E_g within a range of over 100 meV – even in finished solar cell devices. These reversible band gap shifts are detected using electroreflectance. We demonstrate that the band gap of the material is directly correlated to the amount of Cu–Zn disorder and follows the stochastic Vineyard model.

HL 10.4 Mon 12:00 ER 164

Effect of post-annealing on $Cu_2ZnSn(S,Se)_4$ solar cells studied by photoluminescence spectroscopy — •Christian Zimmermann[1], Christoph Kraemmer[1], Christian Huber[1], Mario Lang[1], Thomas Schnabel[2], Tobias Abzieher[1,2], 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

In contrast to the established absorbers for thin-film solar cells such as $Cu(In,Ga)Se_2$ and CdTe, thin-film solar cells based on kesterite absorbers like $Cu_2ZnSn(S,Se)_4$ (CZTSSe) require less toxic and scarce constituents. Recently it has been shown by Scragg *et al.*, that a thermal processing can lead to a change in the ordering of the kesterite Cu–Zn planes (Appl. Phys. Lett. **104**, 041911 (2014)), which could lead to a change in the density of the defect pair Cu_{Zn}+Zn_{Cu}. The density and nature of intrinsic defects have a huge influence on the recombination characteristics of kesterites. Hence we use photoluminescence spectroscopy to investigate the influence of post-annealing of solar cells based on solution-processed CZTSSe. Our results lead to the conclusion, that electrostatic potential fluctuations still play a major role in CZTSSe solar cells regardless of the Cu–Zn ordering.

HL 10.5 Mon 12:15 ER 164

Theoretical and experimental approach to optoelectronic study of Nb3O7(OH) — •Wilayat Khan[1], Sophia Betzler[2], Christina Scheu[2], and Jan Minar[1,3] — [1]New Technologies-Research Center, University of West Bohemia, Univerzitní 8, 306 14 Plzeň, Czech Republic — [2]Department of Chemistry, Ludwig-Maximilians-Universität and Center for NanoScience (CeNS), Butenandtstraße 11, 81377 Munich, Germany — [3]Dept. of Chemistry, University of Munich, Germany

Recently, Nb3O7(OH) single crystal has been recommended as a high performing Dye-Sensitized Solar Cell. Theoretical and experimental studies of the Nb3O7(OH) single crystals are performed. The theoretical study were performed by using the full potential linearized

augmented plane wave (FP-LAPW) method to calculate the electronic properties The experimental studies were carried out by characterizing this material by EELS [1]. We also performed theoretical calculations using the multiple-scattering Spin-Polarized Relativistic-KKR (SPR-KKR) code to investigate Ok and NbL2,3 egde, in order to support the EELS spectroscopy. The calculated band using the modified Becke Johnson approximation (mBJ) is 2.32 eV which is in comparison to the experimental band gap. The electronic density of states around the Fermi level is dominated by the H-1s and Nb-4p states (VB) and Nb-5d states (CB), which play an important role in optical transition resulting in maximum peaks in the imaginary part of dielectric function. [1] Sophia B. Betzler et al., J. Mater. Chem. A, 2014,2, 12005-12013.

HL 10.6 Mon 12:30 ER 164

Modelling of octahedral tilts in NBT by first-principles — •Kai-Christian Meyer, Melanie Gröting, and Karsten Albe — TU Darmstadt, Jovanka-Bontschits-Str 2, 64287 Darmstadt

In this work we deal with the structural configuration of Sodium Bismuth Titanate (NBT) on a atomistic level by first-principles studies and we link our results to the experimentally observed dielectric properties. NBT is a lead-free relaxor ferroelectric with interesting physical properties around the temperature range from 100-200 °C, where it shows a broad frequency dependent peak in the dielectric constant. Around 200°C the tetragonal and rhombohedral (and octahedral) phase are simultaneously present. We believe that a connection between polar nanoregions (PNR) and planar octahedral defects in a rhombohedral matrix exist. We show among other things that certain chemical orders enhance the probability for PNRs to occur.

HL 10.7 Mon 12:45 ER 164

Formation of n-type defect levels in 1.0 eV GaInNAs layers and their influence on GaInNAs solar cell performance — •Fabian Langer, Svenja Perl, Sven Höfling, and Martin Kamp — Technische Physik and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, University of Würzburg, Am Hubland, D97074 Würzburg, Germany

The semiconductor material GaInNAs can be grown lattice matched to GaAs/Ge by molecular beam epitaxy (MBE) with a broad degree of freedom in its bandgap. Besides emerging applications like telecommunication light sensing requiring bandgaps below 0.95 eV, GaInNAs material with a 1.0 eV wide bandgap is of increasing interest for the solar cell industry. Up to now the market for space or concentrator photovoltaic (CPV) is dominated by solar cells made of the material combination GaInP/(In)GaAs/Ge. However, this type of solar cell has reached its practical average efficiency limit. But further improvement by the integration of a 1.0 eV GaInN(Sb)As junction could already be shown. In this presentation we report on the investigation of n-type defects formed during the GaInNAs growth and analyze their influence on the performance of 1.0 eV GaInNAs solar cells. Utilizing these defects we achieved very high internal quantum efficiencies above 90 % due to a compensation effect of the background p-doping in the GaInNAs layer. However, this comes along with a strongly increased dark current generated by the defect states within the bandgap and results in reduced open-circuit voltages of about 0.2 V.

HL 11: Transition-metal dichalcogenides and boron nitride (with O)

Time: Monday 11:45–13:00 Location: ER 270

HL 11.1 Mon 11:45 ER 270

$\mathbf{k}\cdot\mathbf{p}$ theory for two-dimensional transition metal dichalcogenide semiconductors — •Andor Kormanyos and Guido Burkard — University of Konstanz

We present $\mathbf{k}\cdot\mathbf{p}$ Hamiltonians (for a review see [1]) parametrised by ab initio density functional theory calculations to describe the dispersion of the valence and conduction bands at their extrema (the K, Q, Γ, and M points of the hexagonal Brillouin zone) in atomic crystals of semiconducting monolayer transition metal dichalcogenides. We review the parametrisation of the essential parts of the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonians for MoS_2, $MoSe_2$, WS_2, and WSe_2, including the spin-splitting and spin-polarisation of the bands We use $\mathbf{k}\cdot\mathbf{p}$ theory to analyse:

i) optical transitions in two-dimensional transition metal dichalcogenides over a broad spectral range;

ii) to discuss magnetotransport properties of the charge carriers in the K and $-K$ valleys.

[1] A. Kormányos, G. Burkard et al, arXiv:1410.6666

HL 11.2 Mon 12:00 ER 270

Coulomb-Induced Valley Coupling in Transition Metal Dichalcogenides — •Gunnar Berghäuser, Andreas Knorr, and Ermin Malic — Institut für Theoretische Physik, Nichtlineare Optic und Quantenelektronik, Technische Universität Berlin, Germany

Within a microscopic model we investigate the impact of Coulomb-induced intervalley coupling on the optical properties of transition metal dichalcogenides (TMDs). Our approach is based on the density matrix formalism and allows an analytical treatment of the excitonic absorption under the influence of intervalley coupling. We find that the strong Coulomb interaction in these atomically thin 2-dimensional materials couples resonant excitonic states in K and K' valleys [1]. This coupling leads to a splitting of excitonic absorption peaks in the range of the trion binding energy. We further investigate the impact of experimentally accessible parameters, such as doping, dielectric environment, and the detuning of resonant states in the K and K' valley, on the intervalley coupling. The gained insights are of crucial importance for the application of TMDs in valleytronics.

[1] Gunnar Berghäuser and Ermin Malic, "Analytical approach to excitonic properties of MoS_2", Phys. Rev. B 89, 125309 (2014)

HL 11.3 Mon 12:15 ER 270

Coupled spin-valley-dynamics in singlelayer transition metal dichalcogenides — •Gerd Plechinger, Nicola Paradiso, Philipp Nagler, Sven Gelfert, Christoph Strunk, Christian Schüller, and Tobias Korn — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany

Single layers of transition metal dichalcogenides (TMDCs) like MoS_2 and WS_2 can be produced by simple mechanical exfoliation. Offering a direct bandgap at the K-points in the Brillouin zone, they represent a promising semiconductor material for flexible and transparent optoelectronic applications. Due to inversion symmetry breaking together with strong spin-orbit-interaction, the valley and spin degrees of freedom are coupled in singlelayer TMDCs. Via circularly polarized optical excitation, an efficient polarization of the K^+ or the K^- valley can be generated. Here, we optically investigate the dynamics of these coupled spin-valley polarizations in singlelayer MoS_2 and singlelayer WS_2 by means of time-resolved Kerr rotation (TRKR) and display the dependence of the spin lifetime on the temperature and the excitation energy. Moreover, we probe the influence of mild annealing on the lifetimes.

HL 11.4 Mon 12:30 ER 270

Low-temperature photoluminescence of 2D Dichalcogenides and indirect excitons in their heterostructures — •Philipp Nagler[1], Gerd Plechinger[1], Philipp Tonndorf[2], Steffen Michaelis de Vasconcellos[2], Rudolf Bratschitsch[2], Christian Schüller[1], and Tobias Korn[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040, Regensburg, Germany — [2]Physikalisches Institut, Westphälische Wilhelms-Universität Münster, 48149, Münster, Germany

Two-dimensional transition-metal dichalcogenides (TMD) have recently emerged as a promising class of direct-gap semiconductors. Here, we present low-temperature photoluminescence (PL) measurements of four different monolayer TMDs, namely MoS_2, $MoSe_2$, WS_2 and WSe_2. The diselenides show a clear splitting of neutral exciton and trion which enables us to deduce the binding energy of the trion. Furthermore, by using a deterministic transfer technique we are able to fabricate van-der-Waals heterostructures consisting of different 2D TMDs. At room temperature, we observe indirect excitons at the interface which probably stem from a spatial separation of electrons and holes. Power-dependent PL measurements on the heterostructures al-

low us to alter the excitonic regime and to probe saturation effects of the system.

HL 11.5 Mon 12:45 ER 270

Synthesis of atomically thin hexagonal boron nitride films on polycrystalline nickel substrates using MBE — •Siamak Nakhaie, Joseph M. Wofford, Timo Schumann, Uwe Jahn, João Marcelo Lopes, and Henning Riechert — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

Hexagonal boron nitride (h-BN) has recently been the subject of an intense research effort. This has in large part been driven by the suitability of h-BN for integration into heterostructures with other 2-dimensional materials, such as graphene [1]. We report the synthesis of h-BN on polycrystalline Ni foils by molecular beam epitaxy (MBE) from elemental B and N. The presence of a well-ordered, crystalline h-BN film on the Ni foil substrate was confirmed using Raman spectroscopy, which revealed a sharp peak at 1365 cm^{-1}. The ubiquity of wrinkle structures in numerous atomic force microscopy scans, together with the uninterrupted observation of the h-BN Raman signal, offer strong evidence of a continuous h-BN film. Using shorter duration depositions we were able to gain insight into the nucleation and growth behavior of h-BN before forming a closed film. According to scanning electron microscopy (SEM) images, we observed the morphology of sub-monolayer h-BN islands to evolve from star-shaped to much larger compact triangles with increasing growth temperature. SEM micrographs also clearly showed points of increased contrast at the approximate geometric centers of the islands, suggesting that the h-BN nucleated heterogeneously. [1] C.R. Dean et al., Nat. Nanotechnol. 5 (2010) 722

HL 12: Graphene: mostly Theory (with O/TT)

Time: Monday 15:00–17:15 Location: ER 164

HL 12.1 Mon 15:00 ER 164

The decoupling of epitaxial graphene on SiC by hydrogen intercalation: an *ab initio* study — •Lydia Nemec[1], Patrick Rinke[1,2], Volker Blum[3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Aalto University, Helsinki, Fi — [3]Duke University, Durham, NC, USA

Large-scale ordered epitaxial graphene can be grown on various substrates, out of which silicon carbide (SiC) is one of the most promising. The exact material properties of graphene depend on the growth conditions and its interaction with the substrate. By hydrogen intercalation of epitaxial graphene on the Si-face of SiC the graphene layer decouples from the substrate forming quasi-free-standing monolayer graphene (QFMLG) [1].

We performed an density functional theory study of QFMLG on the polar 6H-SiC(0001) surface based on a van der Waals corrected semi-local exchange-correlation functional using the all-electron numeric atom-centered basis function code FHI-aims. We find an adsorption height in excellent agreement with X-ray standing wave experiments, a very low buckling of the graphene layer, and a very homogeneous electron density at the interface. All these features improve the electronic properties of QFMLG compared to epitaxial graphene.

Using the insight gleaned on the Si-face, we present the structure of a hypothetical QFMLG phase on the C-face of SiC. We find that hydrogen intercalation is a promising option to control the SiC-graphene interface.

[1] C. Riedl, *et. al*, PRL 103, 246804 (2009).

HL 12.2 Mon 15:15 ER 164

Two-dimensional analysis of the double-resonant 2D Raman mode in bilayer graphene — •Felix Herziger[1], Matteo Calandra[2], Paola Gava[2], Patrick May[1], Michele Lazzeri[2], Francesco Mauri[2], and Janina Maultzsch[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany — [2]IMPMC, Université Pierre et Marie Curie, CNRS, 75252 Paris, France

The double-resonant 2D-mode Raman process in bilayer graphene has been discussed controversially in recent years. In this context, different models were proposed to explain the complex lineshape observed in experiments.

Using a two-dimensional first-principles calculation, we investigate the dominant contributions to the double-resonant Raman scattering cross-section of the 2D mode in bilayer graphene [1]. In contrast to previous works, we demonstrate that so-called 'inner' processes are, by far, the most dominant processes, as in single-layer graphene. Moreover, we show that the splitting between the two TO-derived phonon branches in bilayer graphene cannot be neglected for a consistent understanding of the 2D-mode lineshape. Additionally, we investigate the contributions from both TO branches to the symmetric and antisymmetric scattering processes. Our results answer the long-standing question regarding the different contributions to the 2D-mode lineshape in bilayer graphene.

[1] F. Herziger, M. Calandra, P. Gava, P. May, M. Lazzeri, F. Mauri, and J. Maultzsch, Phys. Rev. Lett. 113, 187401 (2014)

HL 12.3 Mon 15:30 ER 164

Edge effects in the Raman spectra of atomically precise graphene nanoribbons: an ab-initio study — Marzio De Corato[1,2], •Deborah Prezzi[2], Alice Ruini[1,2], and Elisa Molinari[1,2] — [1]Department of Physics, Mathematics, and Informatics, University of Modena and Reggio Emilia, 41125 Modena, Italy — [2]CNR-Nanoscience Institute, S3 Center, 41125 Modena, Italy

Bottom-up techniques have proven successful to achieve ultra-narrow and structurally well-defined graphene nanoribbons (GNRs) [1-2], where different edge shapes and terminations can be obtained by varying the molecular precursors. In this work we perform density-functional perturbation theory calculations to investigate the vibrational properties of GNRs with cove-type edge structure and variable width, similar to those produced in Ref. 2. By comparison with other prototype systems, we show that the phonon modes and the Raman spectra of these systems strongly depend on the specific edge morphology. This is particularly evident in the acoustic region, where the Radial-Like Breathing Mode (RLBM) shows sensible changes when the edge termination is modified. This makes the Raman spectrum of these GNRs very different from the case of both carbon nanotubes and ribbons with ideal armchair or zigzag edges, where the breathing mode depends on the lateral size only. Our results are in very good agreement with recent experimental data [2].

[1] J. Cai et al., Nature (London) 466, 470 (2010). [2] A. Narita et al., Nature Chem. 6, 126 (2014).

HL 12.4 Mon 15:45 ER 164

Controlling the localization of electrons in bilayer graphene — •Maximilian Fleischmann, Sam Shallcross, and Oleg Pankratov — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

Two mutually rotated layers of graphene exhibit an electronic structure that depends profoundly on the rotation angle. The small angle regime in particular is associated with significant changes of the electronic properties of the bilayer: one finds localization on the moiré lattice and a significant reduction in the Fermi velocity near the Dirac point [1]. We investigate how the electronic properties in the small angle limit may be controlled by an external electric field directed perpendicular to the bilayer. We consider a uniform field as well as modulated fields with a period chosen to "connect" the Dirac cones of the two layers in momentum space. The latter electrostatic potentials may be realized by a proper choice of substrate. We find that electric fields can be used to control the degree of localization of the quasiparticles in the bilayer. A uniform field tends to delocalize the electron states; this effect is generally less pronounced for energies close to the Dirac point. In contrast, a modulated field favours electron localization throughout the low-energy spectrum.
[1] S. Shallcross et al., Phys. Rev. B 87, 245403, 2013.

HL 12.5 Mon 16:00 ER 164

Magnetic interactions in bilayer graphene — •Nicolas Klier, Sam Shallcross, and Oleg Pankratov — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

The indirect exchange interaction between magnetic impurities, known

as the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction, is governed by the static spin susceptibility of the host system and therefore depends sensitively on the host electronic structure. For this reason, this interaction is particularly interesting for materials in which the underlying electronic spectrum is novel, such as single layer and bilayer graphene. We investigate the RKKY interaction for bilayer graphene at zero and at finite temperature, as well as for the case in which the bilayer is biased by a perpendicular electric field. At the edge of the energy gap between the two conduction (or valence) bands at the Dirac point we find a remarkable transition in the form of the RKKY interaction. For Fermi energies on either side of the gap the interaction takes asymptotically two different forms: the oscillatory or the antiferromagnetic. We show that at the Dirac point the sign of the RKKY interaction (ferromagnetic vs anti-ferromagnetic) can be controlled by an external electric field.

HL 12.6 Mon 16:15 ER 164

Is deformed graphene described by the Dirac-Weyl equation on a curved space-time? — •Fabian Rost, Sam Shallcross, and Oleg Pankratov — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

It is well known that, at low energies, the quasiparticles of graphene are described by the wave equation of massless neutrinos: the Dirac-Weyl equation. Less well understood is whether the elastically deformed graphene can be described as the DW equation on a curved space-time as suggested in [1]. To answer this question we consider both a space-time description, and a low energy treatment derived from the tight-binding model, and compare them term by term in an expansion in the deformation tensor. We find that the low energy theory contains an infinite class of deformation-dependent terms that are absent in the space-time approach. Yet all terms present in the curved-space approach can be found in the low energy theory which follows from the tight-binding model.

[1] F. de Juan, A. Cortijo, and M.A.H. Vozmediano, *P*hys. Rev. B **76**, 165409, 2007.

HL 12.7 Mon 16:30 ER 164

Phase diagram of honeycomb lattice in Iionic-Hubbard model — •Sahar Nabavi and Morad Ebrahimkhas — Department of Science, Mahabad Branch, Islamic Azad University, Mahabad 59135, Iran

Tight binding electrons on a honeycomb lattice are described by an effective Dirac theory at low energies. An alternate ionic potential (Δ) generates a single-particle gap in the spectrum. We employ the dynamical mean field theory- iterative perturbation theory (DMFT-IPT) technique, to study the effect of on-site electron correlation (U) on energy gap of a honeycomb system. For a fixed ionic potential Δ, we find that beyond a critical value $U_{c1}(\Delta)$ massive Dirac fermions become massed and we have gapped energy bands. Further increasing U beyond $U_{c2}(\Delta)$, there will be another phase transition to the Mott insulating state. Therefore the competition between the single-particle gap parameter, Δ, and the Hubbard U between $U_{c1}(\Delta) < U < U_{c2}(\Delta)$ restores the semi-metallic nature. The width of the intermediate semi-metallic regime shrinks by increasing the ionic potential. However, at small values of Δ, there is a wide interval of U values for which the system remains semi-metal. The phase diagram and energy gap of the system are identified

HL 12.8 Mon 16:45 ER 164

Antiferromagnetic coupling of vacancies in graphene on SiO_2 — •Stephan Zimmermann[1], Sven Just[2], Marco Pratzer[2], Markus Morgenstern[2], Vladislav Kataev[1], and Bernd Büchner[1] — [1]IFW Dresden, Institute of Solid State and Materials Research, 01069 Dresden, Germany — [2]II. Institute of Physics B and JARA-FIT, RWTH Aachen, 52074 Aachen, Germany

Monolayer graphene grown by chemical vapor deposition and transferred to SiO_2 is used to introduce vacancies by Ar^+ ion bombardment at a kinetic energy of 50 eV. The density of defects visible in scanning tunneling microscopy is considerably lower than the ion fluence, implying that most of the defects are single vacancies as expected from the low ion energy. The vacancies are characterized by scanning tunneling spectroscopy on graphene and highly oriented pyrolytic graphite (HOPG). A peak close to the Dirac point is found within the local density of states of the vacancies similar to the peak found previously for vacancies on HOPG. The peak persists after air exposure up to 180 min, such that electron spin resonance (ESR) at 9.6 GHz can probe the vacancies exhibiting such a peak. After an ion flux of 10/nm^2, we find an ESR signal corresponding to a g factor of 2.001-2.003 and a spin density of 1-2 spins/nm^2. The peak width is as small as 0.17 mT indicating exchange narrowing. Consistently, the temperature-dependent measurements reveal antiferromagnetic correlations with a Curie-Weiss temperature of -10 K. Thus, the vacancies preferentially couple antiferromagnetically, ruling out a ferromagnetic graphene monolayer at ion induced spin densities of 1-2 nm^2.

HL 12.9 Mon 17:00 ER 164

Behaviour of the edge states of the $\nu = 0$ lowest Landau level in graphene beyond SU(4)-symmetry — •Angelika Knothe[1,2] and Thierry Jolicoeur[2] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg — [2]Université Paris Sud, CNRS, LPTMS, UMR 8626, Orsay 91405 France

The $\nu = 0$ quantum Hall state of an infinite sheet of graphene is known to exhibit various different phases when the SU(4)-symmetry of spin and valley/sublattice isospin is broken by interactions and the Zeeman-effect [1]. The situation becomes even richer when considering the edge states close to the sharp boundaries of a finite piece of graphene: Recent theoretical [2] and experimental [3] works suggest that in finite samples the properties of the spin and isospin-texture and its excitations depend on the position within the lattice with respect to its edge. With the help of numerical Hartree-Fock calculations we theoretically investigate the behaviour of the edge modes of a $\nu = 0$ quantum Hall state of graphene. In our model-Hamiltonian we account for both, the influence of SU(4)-symmetric terms and such that break the symmetry, as well as for the presence of the boundary of the lattice. In doing so, we are able to understand the behaviour of different spin and isospin configurations as compared to the phases in the bulk or the predictions of a non-interacting single-electron theory [4].

[1] M. Kharitonov, Phys. Rev. B **85**, 155439 (2012) [2] G. Murthy *et al.*, Phys. Rev. B **90**, 241410(R) (2014) [3] G. Li *et al.*, Nature Commun. **4**, 1744 (2013) [4] D. A. Abanin *et al.*, Phys. Rev. Lett. **96**, 176803 (2006)

HL 13: Focus Session (with TT): Functional semiconductor nanowires II

This is the continuation of the morning session "Functional semiconductor nanowires I".

Organization: Carsten Ronning (FSU Jena), Martin Eickhoff (JLU Giessen), Tobias Voss (TU Braunschweig)

Time: Monday 15:00–18:45 Location: EW 201

Invited Talk HL 13.1 Mon 15:00 EW 201

Light-matter interaction in wire cavities - from Purcell effect to Bose-Einstein condensates — •Rüdiger Schmidt-Grund — Universität Leipzig, Inst. für Exp. Physik II, Leipzig, Germany

I will discuss effects emerging in different regimes of light-matter interaction in, basically, ZnO-based nano- and micro-wire cavities of various type. The superior crystal quality along with very smooth surfaces of that self-organized structures allows for the observation of bosonic quantum effects like parametric mixing and multi-mode bosonic final state stimulation respective Bose-Einstein condensation (BEC), which in particular benefit from the rich mode structure of such cavities.

Depending on the photonic confinement strength lasing arises gained by electron-hole plasmas [1], from coherent photonic states fed by stimulated exciton-phonon scattering [2], and from BECs of exciton-polaritons [3]. Further, lateral conformal coating with concentric distributed Bragg reflector (DBR) shells prevents lateral losses and causes Purcell enhancement of the states lifetime in typical micropillar cavities

[4]. The involved photonic modes are of one-dimensional Fabry-Perot and Whispering-Gallery type. In bare wires, usually modes of only one of these types can be observed. In DBR coated nano-wire cavities, both can coexist being at the same time in the strong and weak coupling regime with the electronic system.
[1] C. Czekalla *et al*, phys. stat. sol. b **247**, 1282 (2010). [2] T. Michalsky *et al*, Appl. Phys. Lett. **105**, 211106 (2014). [3] C.P. Dietrich *et al*, Phys. Rev. B: Rapid Comm. (2015). [4] T. Jakubczy *et al*, ACS Nano **8**, 9970 (2014).

HL 13.2 Mon 15:30 EW 201

GaAs/AlGaAs core shell nanowire lasers and their integration on Si — •Sabrina Sterzl[1], Benedikt Mayer[1], Lisa Janker[1], Bernhard Loitsch[1], Gerhard Abstreiter[1,2], Christopher Gies[3], Gregor Koblmüller[1], and Jonathan Finley[1] — [1]Walter Schottky Institut and Physik Department, TU München, Garching, Germany — [2]Institute of Advanced Studies, TU München, Garching, Germany — [3]Institute for Theoretical Physics, University of Bremen, Bremen, Germany

We present lasing from individual GaAs/AlGaAs core shell nanowires (NWs) under pulsed and continuous wave (CW) optical excitation. The tailored composition profile of the NW lasers studied by photolumines- cence measurements reveals highly efficient fundamental mode lasing with emission coupling efficiencies (β) up to 0.1, ultrafast pulse emission down to 5ps as well as CW operation. Monolithic integration of the NW lasers is achieved by a universally applicable porous dielectric SiO2 reflection layer on top of the Silicon growth substrate. The SiO2 layer maintains direct contact of the NW core to the substrate and provides sufficient reflectivities for lasing operation directly on Si. The fast pulse emission found in our experiments are in good agreement with theoretical calculations predicting possible repetition rates up to 33GHz. The findings demonstrate the versatility and high functionality of the coherent on-chip NW light sources.

HL 13.3 Mon 15:45 EW 201

Time-resolved optical spectroscopy of InGaN/GaN 3D-LEDs — •Linus Krieg[1], Johannes Dühn[1], Kathrin Sebald[1], Jürgen Gutowski[1], Christian Tessarek[2], Martin Heilmann[2], Silke Christiansen[2], and Tobias Voss[3] — [1]Institute of Solid State Physics, University of Bremen — [2]Max-Planck-Institute for the Science of Light, Erlangen — [3]Institute of Semiconductor Technology, TU Braunschweig

GaN is an efficient and widely established material for optoelectronic devices, especially light-emitting diodes (LEDs). Core-shell InGaN/GaN nano- and microrod structures are supposed to further improve the efficiency and spectral range of conventional GaN-based structures leading to LEDs in the green-to-ultraviolet spectral region. Using optical spectroscopy, we perform a characterisation of self-assembled GaN micro- and nanorods with an embedded threefold InGaN quantum well (QW). The GaN rod structures were grown in a vapour-liquid-solid (VLS) growth mode. Afterwards, InGaN QWs were deposited around the rods. After using time-integrated photoluminescence measurements to analyse the concentration and homogeneity of the indium, we focus on time-resolved optical spectroscopy and determine the temperature dependent decay times. The tip of the micro- and nanorods is partly covered with a GaN pyramid. By using micro-PL measurements, we can determine the InGaN distribution on the tip as well as the impact of the GaN pyramid. Our results show a clear decrease of decay time with rising temperature and a spectral shift of the luminescence originating from the tip.

HL 13.4 Mon 16:00 EW 201

Surface functionalization and its influence on excitonic emission of ZnO nanowires — •Lisa Schade[1], Sebastian Resch[2], Sascha Creutzburg[1], Robert Röder[1], Davide Cammi[1], Siegfried R. Waldvogel[2], and Carsten Ronning[1] — [1]Institut für Festkörperphysik, FSU Jena, Max-Wien-Platz 1, 07743 Jena — [2]Institut für Organische Chemie, JGU Mainz, Duesbergweg 10-14, 55128 Mainz

Semiconductor nanowires (NW) are expected to serve as a basis for next-generation high performance devices as they serve as functional and the electrical or optical connection unit for new devices with enhanced properties. This implementation has already succeeded for NW field effect transistors as well as photonic devices like LEDs, waveguides and lasers. The combination of inorganic semiconductors and organic molecules promises hybrid systems with superior functionality. Electrical and optical properties of semiconductor NWs are very sensitive to the treatment of the surface due to the high surface-to-volume ratio, thus especially the surface bound exciton becomes a dominant feature in low temperature photoluminescence spectra, indicating information about the surface properties. For that reason ZnO NWs were coated with organic molecules and photoluminescence measurements were taken before and after the functionalization. There are some anchor-groups, which are suited for functionalization: e.g. -COO-Bu_4N^+ and -Si$(C_2H_5O)_3$ allowing the link of different chains like e.g. C_6F_{12}-C_2H_4- and C_8- . Further functionality increase will be achieved by linking organic dyes for photonic devices.

HL 13.5 Mon 16:15 EW 201

Carrier dynamics in GaN-nanowire based AlN/GaN heterostructures doped with Germanium — •Nils Rosemann[1], Pascal Hille[2], Jan Müssener[2], Pascal Becker[2], María de la Mata[3], César Magén[4], Jordi Arbiol[3,5], Jörg Teubert[2], Jörg Schörmann[2], Martin Eickhoff[2], and Sangam Chatterjee[1] — [1]Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, D-35392 Gießen, Germany — [3]Institut de Ciencia de Materials de Barcelona, ICMAB-CSIC, Campus de la UAB, ES-08193 Bellaterra, CAT, Spain — [4]Laboratorio de Microscopas Avanzadas, Instituto de Nanociencia de Aragon-RAID, Universidad de Zaragoza, ES-50018 Zaragoza Spain — [5]Institucio Catalana de Recerca I Estudis Avantas (ICREA), ES-08010 Barcelona, CAT, Spain

Wide gap materials based on AlN/GaN are promising candidates for opto electronic devices in the UV-range. Here, nanowires (NWs) are of particular interest as they exhibit a significantly reduced potential for structural defects compared to bulk due to efficient strain-relaxation during the self-assembled growth. We investigate the influence of Ge doping which has a much larger covalent radius than Si or Mg on a series of AlN/GaN structures based on GaN NWs using a streak-camera setup with high spatial resolution.

HL 13.6 Mon 16:30 EW 201

Luminescence dynamics of hybrid ZnO nanowire/CdSe quantum dot structures — •Stephanie Bley[1], Friederike Albrecht[1], Michael Diez[1], Alejandra Castro-Carranza[1], Jürgen Gutowski[1], and Tobias Voss[2] — [1]Institute of Solid State Physics, Semiconductor Optics, University of Bremen, 28359 Bremen, Germany — [2]Institute of Semiconductor Technology , Braunschweig University of Technology, 38106 Braunschweig, Germany

The development of cheap and efficient hybrid solar cells, which show high absorption, and a fast and efficient conversion of the incident photon energy into electrical energy is of paramount interest for regenerative energy applications. To achieve that, colloidal CdSe quantum dots with different organic linker molecules were attached to ZnO nanowires to study the luminescence dynamics and the electron transfer inside these hybrid nanostructures via time-resolved photoluminescence and photoconductivity experiments. Photo-induced electron tunneling from an excited state of the QD into the nanowire becomes visible by a particular decrease of the QD decay time. This will be discussed by introducing an appropriate rate equation model. The electron tunneling is further clearly verified by a strong enhancement of the photocurrent which can be controlled by different linker molecule lengths. Further, the influence of surface oxidation on the luminescence dynamics and electron transfer will be discussed by studying polymethylmethacrylate- and polystyrene-passivated hybrid structures.

Coffee break

Invited Talk HL 13.7 Mon 17:00 EW 201

Quantum Transport in Core/Shell Semiconductor Nanowires — •Thomas Schäpers, Fabian Haas, Patrick Zellekens, Torsten Rieger, Tobias Wenz, Yusuf Günel, Önder Gül, Natalia Demarina, Mihail Lepsa, Hans Lüth, and Detlev Grützmacher — Peter Grünberg Institute (PGI- 9) and JARA-Fundamentals of Future Information Technology, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

The transport properties of GaAs/InAs core/shell nanowires is investigated, where the highly conductive InAs shell is wrapped around an insulating GaAs core nanowire. At low temperatures pronounced flux periodic (h/e) magnetoconductance oscillations are observed, when the magnetic field is oriented along the nanowire axis. These very regu-

lar oscillations are explained by the formation of closed-loop quantum states in the tube-like InAs shell comprising a flux periodic energy spectrum. The magnetoconductance oscillations are even observed at temperatures as high as 50K. When the GaAs/InAs core/shell nanowire is contacted by two superconducting Nb electrodes the carrier transport is governed by phase-coherent Andreev reflection processes. Here, the observed oscillation period in the magneto-transport corresponds to half a flux quantum (h/2e).

HL 13.8 Mon 17:30 EW 201

Influence of growth parameters on electrical transport characteristics in InAs Nanowires — •Jonathan Becker[1], Stefanie Morkötter[1], Phillip Geselbracht[1], Julian Treu[1], Simon Hertenberger[1], Max Bichler[1], Gerhard Abstreiter[1,2], Jonathan J. Finley[1], and Gregor Koblmüller[1] — [1]Walter Schottky Institut und Physik Department, TU München, Garching, Germany — [2]Walter Schottky Institut and Physik Department, TU München, Garching, Germany

In this work we present recent results on the electrical transport of nominally undoped MBE grown InAs nanowires (NWs). In particular we explore the influence of growth parameters, microstructure, aspect ratio and contact metal on the electrical properties of the NWs. Four-terminal measurements on planar, back-gated NW field effect transistor (NWFET) devices revealed room-temperature mobilities ranging from 500 to 2000 cm^2/Vs and on-off ratios of $>10^3$ at 4.2K. The obtained electron densities are in the order of $10^{17}cm^{-3}$. A strong effect of the diameter and the microstructure, altered by growth parameters, on the mobility was observed. The latter was investigated by HRTEM, simulations and temperature-dependent measurements in high detail. Here, the impact of band discontinuieties induced by stacking faults and WZ/ZB crystal phase boundaries on electron scattering is evaluated.

HL 13.9 Mon 17:45 EW 201

Giant Magnetoconductance Oscillations in Hybrid Superconductor - Semiconductor Core/Shell Nanowire Devices — •Fabian Haas[1,2], Önder Gül[1,2], Haci Yusuf Günel[1,2], Hans Lüth[1,2], Torsten Rieger[1,2], Tobias Wenz[1,2], Patrick Zellekens[1,2], Mihail Lepsa[1,2], Gregory Panaitov[1,2], Detlev Grützmacher[1,2], and Thomas Schäpers[1,2] — [1]Peter Grünberg Institute (PGI-9 and PGI-8), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]JARA - Fundamentals of Future Information Technology

In GaAs/InAs core/shell nanowires the electrons are confined in the cylindrical conductive InAs shell. In recent publications we have shown that this InAs nanotube allows the observation of h/e flux periodic oscillations in the nanowires magnetoconductance, when a magnetic field is aligned in parallel with the nanowire axis.

In this contribution, we present novel magnetotransport measurements of GaAs/InAs core/shell nanowires, this time contacted with two superconducting Nb electrodes. We observe regular $h/2e$ half-flux periodic oscillations with amplitudes in the order of e^2/h, which is larger by two orders of magnitude than observed for the h/e oscillations in a reference sample contacted with Ti/Au leads.

Phase-coherent resonant Andreev reflections at the Nb-nanowire interface, where interfering electron-hole trajectories enclose the penetrating magnetic flux, can explain these strongly enhanced oscillations as well as the $h/2e$ flux periodicity.

HL 13.10 Mon 18:00 EW 201

Heterogenous Assembly of Silicon Nanowires for Battery Applications — •Andreas Krause[1,2], Matthias Grube[1], Jan Brückner[3], Susanne Dörfler[3], Ulrike Langklotz[4], Tony Jaumann[5], Florian M. Wisser[6], Thomas Mikolajick[1,2,7], and Walter M. Weber[1,2] — [1]Namlab gGmbh, 01187 Dresden — [2]Center for Advancing Electronics Dresden (CfAED), TU Dresden — [3]Fraunhofer Institute for Material and Beam Technology (IWS), 01277 Dresden — [4]Fraunhofer Institute for Ceramic Technologies and Systems (IKTS), 01277 Dresden — [5]Chemistry of Functional Materials (IKM), Leibniz Institute for Solid State and Materials Research (IFW), Dresden — [6]Department for Inorganic Chemistry I, Dresden University of Technology, Germany — [7]Chair of Nanoelectronic Materials, Institute of Semiconductor and Microsystems Technology, TU Dresden

Silicon is a promising anode material for Lithium storage due to its high theoretical specific capacity surpassing 4200 Ah/kg, but with a large volume expansion of 400 per cent. We show innovative anode assemblies composed of a forest of free standing Si nanowires conformally integrated on a carbon fiber network. The morphology of Si nanowires allows a volume expansion and compression lowering strain incorporation. TEM micrographs of samples before and after cycling in a battery stack show the morphology change of the incorporated nanowires. A detailed electrochemical analysis is done on various samples and shows an increased stability of Si with a remaining effective capacitance above 2000 Ah/kg(Si) after 225 full charge/discharge cycles.

HL 13.11 Mon 18:15 EW 201

Monitoring cation exchange from CdSe to Ag_2Se in individual nanowires. — •Cornelius Fendler[1], August Dorn[1], Hauke Heller[2], Andreas Kornowski[2], Robert Schön[2], and Robert Blick[1] — [1]Center for Hybrid Nanostructures, Institutes of Nanostructure and Solid State Physics, University of Hamburg, Jungiusstrasse 11c, 20355 Hamburg, Germany — [2]2Institut for physical chemistry, Grindelallee 117, 20146 Hamburg

Cation exchange is a relatively simple tool to broaden the range of material compositions available in nanostructures.[1] With sufficient monitoring tools, partial cation exchange can be used to tune the material properties to desired values.[2]

In this study we investigated the correlation between the electrical conductivity and the degree of the exchange from CdSe to Ag_2Se on individuelal nanowires. We used the solution-liquid-solid (SLS) process to directly grow CdSe nanowires off bismuth thin films on Si/SiO_2-substrates. Single CdSe wires with diameters of 30 nm to 100 nm and lengths exceeding 10 μm were contacted with titanium electrodes by confocal laser lithography. The conductivity of the individual nanowires was monitored in situ during the cation exchange reaction from CdSe to Ag_2Se. At different stages of the cation exchange reaction the samples were removed from solution, the voltage-current-characteristics were measured and the material composition was determined by wavelength-dispersive X-ray spectroscopy (WDS).

[1] J.B. Rivest et al., Chem. Soc. Rev.,2013, 42, 89.
[2] A. Dorn et al., Nano Lett. 2010, 10, 3948-3951.

HL 13.12 Mon 18:30 EW 201

Charge transport along GaAs nanowires: Surface conductivity and band bending — •Stefan Korte[1], Matthias Steidl[2], Weihong Zhao[2], Werner Prost[3], Felix Lüpke[1], Vasily Cherepanov[1], Bert Voigtländer[1], Peter Kleinschmidt[2], and Thomas Hannappel[2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and JARA-Fundamentals of Future Information Technology — [2]Photovoltaics Group, Institute for Physics, Technische Universität Ilmenau, 98684 Ilmenau, Germany — [3]CeNIDE and Center for Semiconductor Technology and Optoelectronics, University of Duisburg-Essen, 47057 Duisburg, Germany

Using a multi-tip STM as nanoprober to explore the electrical transport properties of freestanding p-doped GaAs nanowires, we revealed a highly increased resistivity in the nanowire base, which caused bad contact to the substrate. This high resistance can be explained by a charge carrier depletion through the whole nanowire cross section due to Fermi level pinning at surface states. To explore this, Zn-doped GaAs nanowires were grown by Au-assisted metal-organic vapor-phase epitaxy (MOVPE) in the vapor-liquid-solid growth mode with different growth procedures. We measured and analyzed I/V characteristics and resistance profiles to understand the conduction mechanisms and band bending along these nanowires.

HL 14: Organic photovoltaics and electronics - mostly cell design (with DS)

Time: Monday 15:00–16:45 Location: EW 202

HL 14.1 Mon 15:00 EW 202

Polymer/cathode interface barrier limiting the open circuit voltage in polymer:fullerene organic bulk heterojunction solar cells — •Jairo Cesar Nolasco — Energy and Semiconductor Research Laboratory, Department of Physics, Carl von Ossietzky University of Oldenburg, D-26111, Germany

Factors which limit the open circuit voltage Voc in polymer bulk heterojunction solar cells is still a topic of controversy. Fundamentally, the Voc is determined by the balance of photogeneration and recombination, with recombination occurring either at the internal donor/aceptor interface or at the contacts. In case of ohmic contacts the losses have been mainly attributed to the donor/acceptor interface, whereas for the case of non-ohmic contacts, the dominant losses have been discussed in terms of minority carrier surface recombination occurring at the acceptor/cathode interface. In this contribution it is demonstrated the existence of a majoritary free carrier recombination occurring at the polymer/cathode barrier interface [1].

[1] J. C. Nolasco, G. Ramos-Ortiz, J.L. Maldonado, O. Barbosa-Garcia, B. Ecker, E. Von Hauff, Appl. Phys. Lett., 104, 043308 (2014).

HL 14.2 Mon 15:15 EW 202

Accurate Characterization of Serial Tandem Organic Solar Cells — •Toni Meyer, Ronny Timmreck, Christian Körner, Koen Vandewal, and Karl Leo — Institut für Angewandte Photophysik, TU Dresden, Germany

A well known concept for further improvement of the efficiency of solar cells are tandem solar cells. The most common representative of this concept are the serial tandem solar cells (sTSC) where the subcells are connected electrically in series. Due to Kirchhoff's law this leads to a current limitation of the whole device by the subcell generating less current under a specific spectrum. For scientific comparison and practical application it is inevitable to determine the exact performance of such a device under different illumination conditions. However, the current limitation of a sTSC represents a major challenge for their characterization.

The spectrometric characterization, developed by Meusel et. al, represents a precise method of determining the performance of sTSC for any given illumination spectrum by using a multi-source sun simulator. We apply this method to a state of the art vacuum deposited sTSC with complementary absorbers and compare it to the minimal requirements of the standard ASTM E2236-05 for characterizing multijunction photovoltaic devices. We show that in case of differing fill factors of the subcells of the sTSC it is not sufficient to use only a single source sun simulator, which does usually not yield correct results for the solar cell efficiency in accordance with the standard reporting conditions.

HL 14.3 Mon 15:30 EW 202

Investigation of semiconducting polymers with thermally cleavable side chains for application in multilayer devices II: Spectroscopy — •Sabina Hillebrandt[1,5], Janusz Schinke[2,5], Torben Adermann[3], Eric Mankel[4,5], Robert Lovrincic[2,5], Manuel Hamburger[3,5], Tobias Glaser[1,5], Wolfram Jaegermann[4], Wolfgang Kowalsky[2,5], and Annemarie Pucci[1,5] — [1]Kirchhoff-Institut für Physik, Universität heidelberg — [2]Institut für Hochfrequenztechnik, Technische Universität Braunschweig — [3]Organisch-Chemisches Institut, Universität Heidelberg — [4]Institut für Materialwissenschaften, Technische Universität Darmstadt — [5]Innovationlab GmbH, Heidelberg

Conjugated polymers are a promising material class for solution processed organic electronic devices. A major challenge in solution processing of multi-layer devices is the limited number of options regarding orthogonal solvents. Therefore solubility alteration of the functional layers is crucial for facilitating device fabrication. In this talk the removal of side-chains of novel naphthalene tetracarboxydiimide based semiconducting polymers by thermal treatment is analyzed by infrared transmission spectroscopy, photoelectron spectroscopy and charge transport characteristics in organic field effect transistors. Side chain residuals in the films are correlated to temperature and duration of the thermal treatment. Solvent stability is tested by washing the films after thermal treatment. Our findings show that although side chains can be removed completely after washing the thermally treated films, the charge transport strongly depends on the parameters used for this treatment.

HL 14.4 Mon 15:45 EW 202

Understanding thickness dependent onset voltage shifts in OLED IV-characteristics I: Internal electric field distributions — •Maybritt Kühn[1,2], Eric Mankel[1,2], Christof Pflumm[3], Thomas Mayer[1,2], and Wolfram Jaegermann[1,2] — [1]Technische Universität Darmstadt, Institute of Materials Science — [2]InnovationLab GmbH, Heidelberg — [3]Merck KGaA, Darmstadt

Steady-state IV measurements are used as important characterization method for organic light-emitting diodes (OLEDs). Surprisingly, in some OLED devices the current onset voltage increases significantly depending on the emission layer (EML) thickness by approximately 2.7 V/100nm. For experimental investigations of this phenomenon we focus on a three layer device architecture, using two different isomers synthesized by Merck as transport material in the EML - one showing changes in onset voltage (EML-A) the other (EML-B) not. To investigate the onset voltage shift the mean electric fields in the respective layers are determined in dependence of the current density. Therefore, systematic layer thickness variations of the injection layers and both EML materials were performed and the respective IV characteristics were evaluated. In contrast to EML-B a large field enhancement in EML-A can be identified induced by discontinuities of the electric field at the EML-A contacts. Using a simple drift model both EML field distributions and the discontinuities can be described quantitatively. Furthermore they can be allocated to a lack of bulk charge carriers, probably induced by an energetic interface barrier or trapped interface charges. A further consideration of the topic will be done in part 2.

HL 14.5 Mon 16:00 EW 202

Understanding thickness dependant onset voltage shifts in OLED IV-characteristics II: Equilibrium band alignments and their impact on the steady-state situation — •Eric Mankel[1,2], Maybritt Kühn[1,2], Christof Pflumm[3], Thomas Mayer[1,2], and Wolfram Jaegermann[1,2] — [1]TU Darmstadt, Darmstadt — [2]InnovationLab GmbH, Heidelberg — [3]Merck KGaA, Darmstadt

Steady-state IV measurements are used as important characterization method for organic light-emitting diodes (OLEDs). Surprisingly, in some OLED devices the current onset voltage increases significantly depending on the emission layer (EML) thickness by approximately 2,7 V/100 nm. In part 1 we used two isomers - one showing changes in onset voltage (EML-A) the other (EML-B) not - and concluded that enhanced internal electric fields explain this unexpected behavior. Here in part 2 we present how interface band offsets (a), interface dipoles (b) and space charge regions (c) influence the field distribution under steady-state conditions. First we show the impact of a, b and c on the electric and the electrochemical potential distribution as well as the IV-characteristic of a two layer model device. Then we allocate these results to the measured interface discontinuities of the electric field shown in part 1. Finally we present the interface band diagrams of the EML layers and the respective contact layers measured by XPS layer-by-layer experiments. The values for a, b and c were used to model the IV-characteristics of both, EML-A and EML-B containing devices. The described onset voltage shift can successfully be reproduced.

HL 14.6 Mon 16:15 EW 202

SWNT:Fullerene solar cells — •Alexey Gavrik[1], Stefan Väth[1], Andreas Sperlich[1], Imge Namal[2], Florian Späth[2], Tobias Hertel[2], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Physical and Theoretical Chemistry II, Julius Maximilian University of Würzburg, 97074 Würzburg — [3]ZAE Bayern, 97074 Würzburg

Single-wall carbon nanotubes (SWNTs) are a promising material for application in organic solar cells due to their attractive properties: solution processability, broadband absorption, high charge carrier mobility. Moreover, by selecting SWNTs of one chirality, it is possible to choose the energy gap, which determines the light absorbtion spectrum and therefore, solar cell performance.

In this study, solar cells were prepared using blends of (6,5)-SWNTs

and the soluble fullerene $PC_{60}BM$. External quantum efficiency (EQE) spectra show spikes at ca. 570, 870 and 1000 nm, which correlates with absorbtion bands of SWNTs. This proves that charge carriers in SWNTs contribute to the photocurrent. Moreover, SWNTs are showing high performance of converting light into electricity: even at low SWNTs:fullerene ratios (1:100) the current from SWNTs in the EQE spectrum is comparable to the fullerenes' contribution.

This study shows the potential for the application of (6,5)-SWNTs as an active material in organic solar cells. While the device performance is still limited by film thickness and overall device characteristics, we were able to fabricate solar cells with reasonable efficiency.

HL 14.7 Mon 16:30 EW 202

Effective injection barriers of organic Schottky diodes — •Thorsten Arnold and Frank Ortmann — Institute for Materials Science and Dresden Center for Computational Material Science, TU Dresden, Germany

We describe electron transport through organic semiconductors connected to two metallic electrodes. The microscopic approach is based on a dynamic master-equation and Poisson equation describing the space charge potential. Disorder is modeled by a Gaussian site energy distribution. The current-voltage characteristic depends on the effective height of the injection barrier at the metal-semiconductor interface, which can be influenced by several effects, and the bulk properties.

The model is applied to a Schottky diode with different work functions of the electrodes. The influence of bulk and surface disorder on the rectification of the diode are analyzed for various temperatures. Furthermore, the influence of the space charge on the effective injection barrier height is investigated.

HL 15: Invited Talk Fritz Henneberger

Time: Monday 15:00–15:30 Location: EW 203

Invited Talk HL 15.1 Mon 15:00 EW 203

Semiconductor-based plasmonics — •Fritz Henneberger, Sascha Kalusniak, and Sergey Sadofev — Humboldt Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin

When targeting the infrared spectral range in plasmonics, traditional metals like gold and silver suffer from strong losses and weak localization. We show that heavily doped n-type ZnO (and other oxide semiconductors) are excellent alternatives including even telecommunication wavelengths. Using MBE, free carrier concentrations of almost 10^{21} cm^{-3} can be generated by Ga-doping of ZnO without significant deterioration of the crystalline structure. In this way, a metallic permittivity emerges with losses at least one order of magnitude lower than for traditional metals and a negative real part tuneable from mid infrared wavelengths to 1.2 μm. Epitaxial multi-layer structures with different doping level enable the demonstration of novel surface plasmon polaritons (SPPs) with dispersions that can be engineered in a unique way. In particular, SPPs at metal/metal-type interfaces exhibit finite frequencies in the long-wavelength limit, in marked contrast to metal/dielectric SPPs. Further, we resonantly and coherently couple these SPP states to molecular vibrations and observe profound changes of the molecular line shape when adjusting the resonance detuning. Negative refraction at 1.55 μm is achieved by strong SPP-photon coupling in a microcavity setting formed by multi-layer film structures, as commonly used in waveguide optics. Increasing the layer number towards the effective-medium regime, a compact hyperbolic metamaterial is built-up exhibiting, e.g., extraordinary transmission.

HL 16: Transport: Quantum coherence and quantum information systems - Experiments (TT with HL)

Time: Monday 15:00–17:15 Location: H 0110

HL 16.1 Mon 15:00 H 0110

Coplanar microwave resonators for superconductor/cold atom hybrid devices — •Daniel Bothner, Dominik Wiedmaier, Benedikt Ferdinand, Martin Knufinke, Helge Hattermann, Patrizia Weiss, József Fortágh, Dieter Koelle, and Reinhold Kleiner — Physikalisches Institut and Center for Collective Quantum Phenomena in LISA$^+$, University of Tübingen, Germany

Recently, it has been demonstrated that ultracold atomic clouds can show very long coherence times on the order of 10 sec in close proximity to a superconducting chip surface [1]. Due to these extraordinarily long coherence times, atomic clouds are promising candidates as long-lived quantum memory in a future hybrid quantum processor. The realization of such a fully functioning hybrid system, however, poses severe challenges regarding the design and optimization of the superconducting chip. We will briefly discuss the relevant experimental boundary conditions and present strategies to comply with them on the way towards coherent coupling between ultracold atomic ensembles and on-chip microwave resonators. We in particular focus on how mixing normal conducting and superconducting components can outperform purely superconducting chips with respect to the requirements of the aspired hybrid system.

[1] S. Bernon *et al.*, Nature Commun. **4**, 2380 (2013)

HL 16.2 Mon 15:15 H 0110

Circuit QED with a gradiometric tunable-gap flux qubit — •Frank Deppe[1,2,3], Manuel J. Schwarz[1,2,3], Max Haeberlein[1,2,3], Jan Goetz[1,2,3], Alexander Baust[1,2,3], Peter Eder[1,2,3], Friedrich Wulschner[1,2,3], Edwar Xie[1,2,3], Ling Zhong[1,2,3], Kirill Fedorov[1,2,3], Edwin P. Menzel[1,2,3], Achim Marx[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

In circuit quantum electrodynamics or quantum simulation experiments, superconducting quantum bits must combine good coherence with high in situ tunability. Often, a large anharmonicity is also desirable. Other than the popular transmon, the gradiometric tunable-gap flux qubit meets all three of these requirements. Here, we fabricate and characterize such a qubit and demonstrate its first implementation into a transmission line resonator. We show spectroscopy and first time domain results.

This work is supported by the DFG via SFB 631 and the EU projects CCQED and PROMISCE.

HL 16.3 Mon 15:30 H 0110

Flux qubit to a transmission line — •Max Haeberlein[1,2,3], Gustav Anderson[1,2], Lujun Wang[1,2], Alexander Baust[1,2,3], Peter Eder[1,2], Michael Fischer[1,2], Jan Goetz[1,2], Edwar Xie[1,2], Manuel Schwarz[1,2], Karl Friedrich Wulschner[1,2], Ling Zhong[1,2,3], Frank Deppe[1,2], Kirill Fedorov[1,2], Hans Hübl[1,2], Achim Marx[1], Edwin Menzel[1,2], and Rudolf Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), Schellingstraße 4, 80799 München, Germany

Within the last decade, superconducting qubits coupled to microwave resonators have been extensively studied within the framework of quantum electrodynamics. Ultimately, quantum computing seems within reach in such architectures. However, error correction schemes are necessary to achieve the required fidelity in multi-qubit operations, drastically increasing the number of qubits involved.

In this work, we couple a flux qubit to a transmission line where it interacts with itinerant microwave photons granting access to all-optical quantum computing. In this approach, travelling photons generate entanglement between two waveguides, containing the qubit information.

In this presentation, we show experimental data on flux qubits cou-

pled to transmission lines. Furhtermore, we will discuss entanglement generation between two separate paths.

This work is supported by the DFG via SFB 631 and EU projects CCQED and PROMISCE.

HL 16.4 Mon 15:45 H 0110

Ultrastrong coupling of a flux qubit — •A. Baust[1,2,3], E. Hoffmann[1,2,3], M. Haeberlein[1,2,3], M. J. Schwarz[1,2,3], P. Eder[1,2,3], J. Goetz[1,2,3], F. Wulschner[1,2,3], E. Xie[1,2,3], L. Zhong[1,2,3], K. G. Fedorov[1,2,3], E. P. Menzel[1,2,3], F. Deppe[1,2,3], A. Marx[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

Circuit quantum electrodynamics has not only become a versatile toolbox for quantum information processing, but is also a powerful platform for the investigation of light-matter interaction. The coupling strength between microwave resonators and qubits acting as artificial atoms can be tuned over several orders of magnitude and can even reach the regime of ultrastrong coupling. We present spectroscopic data of a flux qubit coupled galvanically to the signal lines of two coplanar stripline resonators. We discuss the complex mode spectrum and show that the coupling strength between the qubit and one resonant mode reaches 17% of the respective mode frequency. Noticably, the high coupling strength is reached solely by the geometric layout of the qubit without utilizing additional coupling elements such as Josephson junctions. Our data exhibit a pronounced Bloch-Siegert shift and therefore represent an experimental evidence for the breakdown of the Jaynes-Cummings model.

This work is supported by the DFG via SFB 631 and EU projects CCQED and PROMISCE.

HL 16.5 Mon 16:00 H 0110

Characterization of superconducting transmission line resonators — •Jan Goetz[1,2], Philipp Summer[1,2], Sebastian Meier[1,2], Marta Krawczyk[1], Max Häberlein[1,2], Alexander Baust[1,2,3], Karl Friedrich Wulschner[1,2], Edwar Xie[1,2,3], Peter Eder[1,2], Michael Fischer[1,2], Manuel Schwarz[1,2], Ling Zhong[1,2,3], Frank Deppe[1,2], Kirill Fedorov[1,2], Hans Hübl[1,2], Achim Marx[1], Edwin Menzel[1,2], 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

Superconducting transmission line resonators are widely used in circuit quantum electrodynamics experiments as quantum bus or storage devices. For these applications, long coherence times, which can be linked to the internal quality factor of the resonators, are crucial. Here, we show a systematic study of the internal quality factor of niobium thin film resonators. We analyze different cleaning methods and substrate parameters for coplanar waveguide as well as microstrip geometries. In addition, we investigate the impact of a niobium-aluminum interface which is necessary for galvanically coupled flux qubits made from aluminum. This interface can be avoided by fabricating the complete resonator-qubit structure using $Al/AlO_x/Al$ technology during fabrication.

This work is supported by the DFG via SFB 631 and EU projects CCQED and PROMISCE.

HL 16.6 Mon 16:15 H 0110

Superconducting on-chip microwave interferometers — •Edwin P. Menzel[1,2,3], Michael Fischer[1,2,3], Christian Schneider[1,2,3], Alexander Baust[1,2,3], Peter Eder[1,2,3], Jan Goetz[1,2,3], Max Haeberlein[1,2,3], Manuel Schwarz[1,2,3], Karl Friedrich Wulschner[1,2,3], Edwar Xie[1,2,3], Ling Zhong[1,2,3], Frank Deppe[1,2,3], Kirill Fedorov[1,2,3], Hans Huebl[1,2,3], Achim Marx[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

In the realm of all-microwave quantum computation, information is encoded in itinerant microwave photons propagating along transmission lines. In such a system unitary operations are implemented by linear elements such as beam splitters or interferometers. However, for two-qubit operations non-linear gates, e.g., c-phase gates are required. In this work, we investigate superconducting interferometers as a building block of a c-phase gate. We experimentally characterize their scattering properties and compare them to simulation results. Finally, we discuss our progress towards the realization of a c-phase gate.

This work is supported by the DFG via SFB 631 and the EU projects CCQED and PROMISCE.

HL 16.7 Mon 16:30 H 0110

Towards chains of tunable and nonlinear superconducting microwave resonators — •Michael Fischer[1,2], Friedrich Wulschner[1,2], Udo Schaumburger[1,2], Max Haeberlein[1,2], Manuel Schwarz[1,2,3], Peter Eder[1,2,3], Edwin Menzel[1,2,3], Kirill Fedorov[1,2], Jan Goetz[1,2], Edwar Xie[1,2], Ling Zhong[1,2,3], Frank Deppe[1,2,3], Achim Marx[1], and Rudolf Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), 80799 München, Germany

We present an experimental feasibility study of chains of tunable and nonlinear superconducting microwave resonators within the realm of circuit QED. We describe the fabrication and experimental characterization of the components required to realize nonlinear resonators with tunable anharmonicity, capacitively coupled resonator chains and on-chip parallel plate capacitors. We discuss possible error sources in the fabrication and characterization processes. Furthermore, simulations based on existing theories are performed to identify accessible parameter ranges.

This work is supported by the DFG via SFB 631 and the EU projects CCQED and PROMISCE.

HL 16.8 Mon 16:45 H 0110

Probing the Interaction of Microscopic Material Defects with Quasiparticles using a Superconducting Qubit — •Alexander Bilmes[1], Jürgen Lisenfeld[1], Andreas Heimes[2], Sebastian Zanker[2], Gerd Schön[2], Georg Weiss[1], and Alexey V. Ustinov[1] — [1]PI, Fakultät für Physik, KIT, Wolfgang-Gaede-Straße 1, 76131 Karlsruhe, Germany — [2]TFP, Fakultät für Physik, KIT, Wolfgang-Gaede-Straße 1, 76131 Karlsruhe, Germany

Two-Level-Systems (TLS) are one of the main sources of decoherence in superconducting nano-scale devices such as SQUIDs, photon detectors, resonators and quantum bits (qubits), although the TLS' microscopic nature remains unclear. We use a superconducting phase qubit to detect TLS contained within the tunnel barrier of the qubit's Josephson junction. We coherently operate *individual* TLS by resonant microwave pulses and access their quantum state by utilizing their strong coupling to the qubit. Our previous measurements of TLS coherence in dependence of the temperature indicate that quasiparticles may give rise to TLS energy loss and dephasing. Here, we probe the TLS-quasiparticle interaction using a reliable method of *in-situ* quasiparticle injection via an on-chip dc-SQUID that is pulse-biased beyond its critical current. The quasiparticle density is calibrated by measuring associated characteristic changes to the qubit's resonance frequency and energy relaxation rate [1]. We will present experimental data that clearly show the influence of quasiparticles on TLS coherence.

[1] M. Lenander et al., Phys.Rev. B 84, 024501 (2011).

HL 16.9 Mon 17:00 H 0110

Incoherent Two-Level Fluctuators inside the Josephson junction of a Superconducting Qubit — •Saskia Meissner, Jürgen Lisenfeld, Alexey V. Ustinov, and Georg Weiss — Physikalisches Institut, KIT Karlsruhe

Spectroscopy on qubits based on Josephson junctions reveals the precence of defects like quantum coherent tunneling systems (TS) as well as two-level fluctuators (TLF). TLF are incoherent tunneling particles which are described by dissipative quantum tunneling theory. Due to the coherent interaction of qubit and the TS, it is possible to probe individual TLF that themselves are coupled to a tunneling system.

Here we perform high resolution defect spectroscopy by tuning the TS and TLF asymmetry energies with external strain applied to the qubit chip. Slow fluctuators induce telegraph noise in the resonance frequency of TS. Fast fluctuators create double resonances of TS in the manner of two frequency branches. Apparently, the two-level fluctuator causes a rapid modulation of the asymmetry energy of the tunneling system on top of the static strain tuning. We perform time domain analyses of TS resonance frequencies with the goal of reconstructing the TLF deformation potential and the TLF-TS interaction potentials.

HL 17: Transport: Topological insulators 1 (TT with DS/HL)

Time: Monday 15:00–17:45 Location: A 053

Invited Talk HL 17.1 Mon 15:00 A 053

The Wires' Approach to Topological Insulators — •Yuval Oreg — Weizmann Institute of Science, Rehovot, Israel

We suggest a construction of a large class of topological states using an array of quantum wires. We will show how to construct a Chern insulator using an array of alternating wires that contain electrons and holes, correlated with an alternating magnetic field. A generalization to wires, with alternating spin-orbit couplings which give rise to integer and fractional (Abelian and non-Abelian) topological insulators, is then straightforward.

Following this construction we will discuss suggestions for two possible experiments which give rise to a fractional Josephson-effect and in addition a novel spin-resolved current correlation effect.

HL 17.2 Mon 15:30 A 053

Helical Majorana surface states of strongly disordered topological superconductors with time-reversal symmetry — •Raquel Queiroz and Andreas Schnyder — Max Planck Instutute for Solid State Research, Stuttgart, Germany

Noncentrosymmetric superconductors with strong spin-orbit coupling and the B phase of ^{3}He are possible realizations of topological superconductors with time-reversal symmetry. The nontrivial topology manifests itself at the material's surface in terms of linearly dispersive helical Majorana modes protected by symmetry from disorder weaker than the superconducting gap. Using extensive numerical simulations, we investigate the stability and properties of these Majorana states under strong surface disorder, which influences both bulk and surface states. A critical crossover from weak to strong disorder is observed in both two and three dimensions, through which an extended state exactly at zero energy always persists. The localization properties of the ingap states are studied through the distribution of the local density of states and level repulsion statistics.

HL 17.3 Mon 15:45 A 053

Intrinsic conduction through topological surface states of insulating Bi_2Te_3 epitaxial thin films — •Katharina Hoefer[1], Christoph Becker[1], Diana Rata[1], Jesse Swanson[1,2], Peter Thalmeier[1], and Liu Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden — [2]University of British Columbia, Vancouver

Topological insulators represent a new state of matter that open up new opportunities to create unique quantum particles. Many exciting experiments have been proposed by theory, yet, the main obstacle for their execution is material quality and cleanliness of the experimental conditions. The presence of tiny amounts of defects in the bulk or contaminants at the surface already mask these phenomena.

We present the preparation, structural and spectroscopic characterisation of MBE-grown Bi_2Te_3 thin films that are insulating in the bulk. Moreover, temperature dependent four-point-probe resistivity measurements of the Dirac states on surfaces that are intrinsically clean were conducted. The total amount of surface charge carries is in the order of $10^{12}\,\mathrm{cm}^{-2}$ and mobilities up to $4600\,\mathrm{cm}^2/\mathrm{Vs}$ are observed.

Importantly, these results are achieved by carrying out the preparation and characterisation all in-situ under ultra-high-vacuum conditions [1].

[1] K. Hoefer et al. PNAS, 2014, 111(42), 14979-14984.

HL 17.4 Mon 16:00 A 053

Quantum interference of edge supercurrents in a two-dimensional topological insulator — •Grigory Tkachov, Pablo Burset, Björn Trauzettel, and Ewelina Hankiewicz — Würzburg University

Josephson weak links made of two-dimensional topological insulators (TIs) exhibit magnetic oscillations of the supercurrent that are reminiscent of those in superconducting quantum interference devices (SQUIDs). We propose a microscopic theory of such a TI SQUID effect [1]. The key ingredient of our model is the exact treatment of the influence of an external magnetic field on the edge supercurrents. We show that this influence has the form of a 1D Doppler effect that describes the flux-controlled interference of the edge currents with superimposed suppression of Andreev reflection. Both long and short junctions are discussed. In particular, for long junctions the theory shows a temperature-driven crossover from the normal Φ_0-periodic SQUID pattern to a $2\Phi_0$-quasiperiodic pattern consisting of a series of alternating even and odd peaks (where $\Phi_0 = ch/2e$ is the magnetic flux quantum). The predicted even-odd effect is the signature of gapless (protected) Andreev bound states with a sawtooth dependence on the magnetic flux. Our findings may shed some light on the recently observed even-odd interference pattern in InAs/GaSb-based TI Josephson junctions, suggesting new operation regimes for nano-SQUIDs.

[1] G. Tkachov, P. Burset, B. Trauzettel, and E. M. Hankiewicz, arXiv:1409.7301.

HL 17.5 Mon 16:15 A 053

Rashba spin-orbit coupling at the quantum spin Hall edge — •Florian Geissler, Francois Crepin, and Björn Trauzettel — Universität Würzburg, Institut für Theoretische Physik und Astrophysik, Germany

Not only since the discovery of the quantum spin Hall effect, and up to most recent questions in the context of topological insulating materials, transport through one-dimensional systems is a problem of great importance and interest. In a quantum spin Hall system, electron transport occurs in conducting edge channels, that are spin-filtered with respect to their direction of motion, and was shown to be topologically protected by time-reversal symmetry. We use the helical Luttinger liquid model to study transport in such systems, when the perfect conductance is perturbed. Particularly, we show that a potential source of backscattering is provided by the combination of a Rashba spin-orbit coupling (SOC) impurity and electron-electron interactions, even though time-reversal symmetry remains preserved. Based on both renormalization group and Keldysh calculations, the scaling of the conductance with the external bias is derived at zero temperature. Moreover, we illustrate, that such SOC-impurities may give rise to interesting effects when being present in an interface of a Luttinger liquid connected to a superconductor.

15 min. break.

HL 17.6 Mon 16:45 A 053

Coexisting edge states and gapless bulk in topological states of matter — Yuval Baum[1], •Thore Posske[2], Ion Cosma Fulga[1], Björn Trauzettel[2], and Ady Stern[1] — [1]Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 76100, Israel — [2]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany

We consider two dimensional systems in which edge states coexist with a gapless bulk. Such systems may be constructed, for example, by coupling a gapped two dimensional state of matter that carries edge states to a gapless two dimensional system in which the spectrum is composed of a number of Dirac cones. We find that in the absence of disorder the edge states could be protected even when the two systems are coupled, due to momentum and energy conservation. We distinguish between weak and strong edge states by the level of their mixing with the bulk. In the presence of disorder, the edge states may be stabilized when the bulk is localized or destabilized when the bulk is metallic. We analyze the conditions under which these two cases occur. Finally, we propose a concrete physical realization for one of our models on the basis of bilayer Hg(Cd)Te quantum wells.

HL 17.7 Mon 17:00 A 053

Spin texture of generic helical edge states — •Alexia Rod[1], Thomas L. Schmidt[2], and Stephan Rachel[1] — [1]Institut für Theoretische Physik, TU Dresden, Germany — [2]Department of Physics, University of Basel, Switzerland

Edge states of time-reversal topological insulators can be described as helical Luttinger liquids. The generic helical liquid is the most general model of a time-reversal invariant helical liquid without axial spin symmetry. This symmetry is usually broken in experimental realizations, and it has been shown that its absence changes the transport properties significantly [1]. For a translation invariant system, the breaking of axial spin symmetry manifests itself in a momentum-dependent rotation of the spin quantization axis. Its manifestation in real space has remained, however, elusive so far.

Here we show that one can extract the rotation of spin quantization axis also in real space, e.g. for topological insulator disks with broken spin symmetry but also other geometries which are not rotationally invariant [2]. This suggests that the concept of a generic helical liquid is independent of the microscopic model and the considered geometry.

[1] T.L. Schmidt, S. Rachel, F. von Oppen, L. Glazman, Phys. Rev. Lett. 108, (2012).
[2] A. Rod, T.L. Schmidt, S. Rachel, manuscript in preparation.

HL 17.8 Mon 17:15 A 053

Manipulation of helical edge state transport by a quantum magnet — •Peter Silvestrov[1], Patrik Recher[1], and Piet Brouwer[2] — [1]Institute for Mathematical Physics, TU Braunschweig — [2]Dahlem Center for Complex Quantum Systems, FU Berlin

Application of a magnetic field is usually considered as a way to open the gap in the spectrum of helical edge states, leading to a blocking of the edge current. Nevertheless, it was shown recently that the current is fully transmitted through the gapped region in case of interaction with a quantum magnet[1]. Here we consider other interesting features of the helical edge state current interacting with the magnet. First, we notice that although the current is transmitted, all electrons with energies close to the Fermi energy are fully reflected. The actual current is carried by the electrons with energies below the gap and well below the Fermi energy. This suggests that the magnet while allowing passing the current, fully blocks the thermal transport thereby acting as a cooler for the injected electron beam. Our second setup consists of two helical edges covered by the same magnet. The current injected into one edge creates a non-equilibrium magnetization driving a current in the second edge. The current in the first edge is now half-reflected and half-transmitted by the magnet. However, the partial reflection of the current does not cause any shot noise.

[1] Q.Meng, S.Vishveshwara, T.L.Hughes, arXiv:1312.7303.

HL 17.9 Mon 17:30 A 053

Probing spin-polarized edge state superconductivity by Andreev reflection in in-plane magnetic fields — •Rolf W. Reinthaler, Grigory Tkachov, and Ewelina M. Hankiewicz — Faculty of Physics and Astrophysics, University of Würzburg, Würzburg, Germany

Finding signatures of unconventional superconductivity in Quantum Spin Hall systems is one of the challenges of solid state physics. Here we induce superconductivity in a 3D topological insulator thin film to cause the formation of helical edge states, which are protected against backscattering even in finite magnetic fields. Above a critical in-plane magnetic field, which is much smaller than the critical field of typical superconductors, the quasi-particle gap closes, giving rise to energy-dependent spin polarization. In this regime the spin-polarized edge state superconductivity can be detected by Andreev reflection. We propose measurement setups to experimentally observe the spin-dependent excess current and dI/dV characteristics.

HL 18: Plasmons, plasmonic laser, and spaser

Time: Monday 15:45–17:15 Location: EW 203

HL 18.1 Mon 15:45 EW 203

Metal-Organic Microcavities: Utilizing Tamm-Plasmon-Polaritons for Observing Photonic Bloch States — •Andreas Mischok[1], Robert Brückner[1], Alexander A. Zakhidov[1,2], Vadim G. Lyssenko[1], Hartmut Fröb[1], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr Str. 1, 01069 Dresden — [2]Texas State University, 601 University Drive, San Marcos, Texas, United States

Organic small molecule semiconductors provide large oscillator strengths, high quantum efficiencies and broad tunable emission spectra, ideal for an application in low-threshold microcavity lasers. We fabricate such cavities and add a photolithographically patterned silver layer next to the organic emitter system. Embedding metallic layers into such a microcavity leads to the interaction of the optical cavity-state in the organic layer and the neighbouring metal which red-shifts the cavity resonance, creating a Tamm-Plasmon-Polariton state. A patterning of the metal can in turn be exploited to fabricate deep photonic wells of micron-size, that efficiently confine light in the lateral direction [1]. In periodic arrays of silver wires we can create a Kronig-Penney-like optical potential in the cavity and in turn observe optical Bloch states spanning over several of these photonic wires [2]. We modify the Kronig-Penney theory to analytically describe the full far-field emission dispersion of our cavities and show the emergence of either zero- , π-, or 2π- phase-locking in the system [3].
[1] APL **105**, 051108; [2] Advanced Optical Materials **2**(8), 746;
[3] Nature Photonics **6**, 322.

HL 18.2 Mon 16:00 EW 203

Influence of Tamm plasmons on the light-matter interaction in ZnSe-based microcavities — •SK. Shaid-Ur Rahman[1], Merle Cornelius[1], Thorsten Klein[2], Carsten Kruse[2], Detlef Hommel[2], Jürgen Gutowski[1], and Kathrin Sebald[1] — [1]Semiconductor Optics — [2]Semiconductor Epitaxy, Institute of Solid State Physics, University of Bremen, P.O. Box 330440, 28334 Bremen, Germany

Strong light-matter interactions in semiconductor microcavities (MCs) introduce cavity polaritons. ZnSe-based MCs are very promising to realize polariton devices at elevated temperatures due to high oscillator strengths and large excitonic binding energies. By depositing a metallic layer on the DBR, electromagnetic modes called Tamm plasmons can be formed at the semiconductor-metal interface. We will discuss the influence of Tamm plasmons on the optical properties of ZnSe-based MCs. The cold MC consists of a 12-fold bottom DBR, a $\lambda/2$ cavity and a 1.5-fold top DBR. The hot unfolded MC is built of an 18-fold bottom DBR and a λ cavity including 3 ZnSe QWs. Ag layers with thicknesses between 30 and 50 nm are deposited on the MC samples. Micro-reflectivity measurements on the cold MC covered by a 30 nm Ag layer show a shift of the cavity resonance of about 26 meV compared to the metal-free areas, due to the influence of Tamm plasmons. For the hot MC, besides the shift an anticrossing between the generated cavity resonance and QW excitons is observed in temperature dependent measurements. The observed energy shift and the anticrossing are in agreement with simulations based on the transfer-matrix method.

HL 18.3 Mon 16:15 EW 203

Photonic and plasmonic coupled CdS nanowire lasing — •Lukas Trefflich[1], Robert Röder[1], Themistoklis Sidiropoulos[2], Rupert F. Oulton[2], and Carsten Ronning[1] — [1]Institut für Festkörperphysik, Friedrich- Schiller- Universität Jena, Max- Wien- Platz 1, 07743 Jena — [2]Imperial College London, Prince Consort Road, UK-SW7 2BZ London, UK

Conventional electronic circuitry has driven the technological progress for decades by progressive miniaturization of the structure. However, facing its limits concerning the minimal size of the structures an alternative approach might be provided utilizing nanophotonic elements. The building of such devices for optical data processing urgently requires nanoscale light sources like nanolasers. Compound semiconductor nanowires made of zinc oxide (ZnO) or cadmium sulfide (CdS) are well known as coherent nano-lightsources. Especially, CdS nanowires emitting in the green spectral range show room temperature lasing as well as cw operation [Geburt et al, Nanotechnology 23, 365204 (2012), Röder et al, Nano Letters 13, 3602 (2013)]. However, these nanowire lasers are limited in size and maximal switching speed due to the diffraction limit and the relatively slow light-matter interactions. Confining the guided electric field by coupling it to surface plasmons accelerates the spontaneous and stimulated emission through the Purcell- effect, making ultrafast, sub- wavelength nanolasers possible. Therefore, the polarization properties as well as the temporal dynamics of cadmium sulfide nanowires on photonic and plasmonic surfaces are investigated.

HL 18.4 Mon 16:30 EW 203

Theoretical studies on a plasmonic nano-laser: plasmon excitation and emission line narrowing due to the presenec of many molecules — •Yuan Zhang and Volkhard May — Institut für Physik, Humboldt Universität zu Berlin, Netonstraße 15, D-12489 Berlin, Germany

Strong plasmon excitation and photon emission is demonstrated for a plasmonic nano-laser (SPASER) consisting of a gold nano-sphere coated by many dye molecules. An exact description of this system in the framework of density matrix theory becomes possible if all molecules are treated as identical units. Due to their external and simultaneous excitation the molecules overcome the huge plasmon damping. By increasing the number of molecules, the photon emission intensity increases and the emission line-shape becomes narrowed. Thus, such results can be related to plasmonic lasing. Beside optical pumping of the molecules also a mechanism of electrical pumping is considered. It is realized via electron transfer between the molecules and two leads forming a molecular junction. The exact quantum-dynamics simulations are extended up to 20 molecules covering the nano-sphere.

HL 18.5 Mon 16:45 EW 203

Atomistic Modeling of Excitation Energy Transfer in a Metal Semiconductor Core Shell Nanostructure — •Dirk Ziemann and Volkhard May — Institut für Physik, Newtonstr. 15, Humboldt Universität zu Berlin, D-12489 Berlin, Germany

The interaction of metal nanoparticle plasmons with semiconductor excitons is well studied in literature. As a consequence of this coupling the properties of semiconductor excitons are strongly modified. In this talk special attention is paid to the combination of both systems in close proximity, particularly a core shell system with a metal core and a semiconductor shell. The influence of the metal on the electronic structure of the semiconductor nanostructure is modeled on an atomistic level and the interaction of semiconductor excitons and metal plasmons is discussed. It is shown that exciton quenching due to excitation energy transfer from the semiconductor shell to the metal core is in line with recent experiments (ACS Nano 8(2014),352-361).

HL 18.6 Mon 17:00 EW 203

Numerically exact solution of the many emitter – cavity laser problem: application to the fully quantized spaser emission — •Michael Gegg, T. Sverre Theuerholz, Andreas Knorr, and Marten Richter — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Open many body quantum systems consisting of N quantum emitters (QEs), e.g. dye molecules or quantum dots, coupled to a lossy cavity/optical mode have been subject to extensive research for decades. These systems are described by a Tavis-Cummings/Dicke model in the Lindblad formalism for open quantum systems. This provides access to a manifold of interesting applications, such as lasers, parametric amplifiers, atomic coherent states etc.

For instance, in the field of quantum plasmonics, the model system was utilized to address the feasibility of spasing – i.e. surface plasmon amplification by stimulated emission of radiation. In this context, we develop an exact and numerically scalable solution to the Tavis-Cummings/Dicke Lindblad equation.

HL 19: Organic photovoltaics and electronics - mostly properties of the absorber (with DS)

Time: Monday 17:00–19:00 Location: EW 202

HL 19.1 Mon 17:00 EW 202

Structural and electronic properties of planar organic heterojunction interfaces and their impact on diode characteristics — •A. Opitz[1], A. Wilke[1], N. Koch[1,2], U. Hörmann[3], W. Brütting[3], R. Hansson[4], and E. Moons[4] — [1]Humboldt-Universität zu Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany — [3]University of Augsburg, Germany — [4]Karlstad University, Sweden

The structural and electronic properties of organic heterojunction interfaces are of paramount importance. Here two prototypical interfaces are discussed: diindenoperylene (DIP) combined with fullerene (C60) and copper-phthalocyanine combined with its perfluorinated analog. Angle dependent near edge X-ray absorption fine structure measurements were performed to determine the molecular orientation and compared to measurements of the frontier level alignment by ultraviolet photoelectron spectroscopy.

The orientation of the rod-like DIP molecules is unaffected upon deposition of spherical C60 molecules on top and vacuum level alignment appears. In contrast, cofacial lying interface layers with π-orbital stacking of the two phthalocyanines is observed together with energy level bending. These results will be related to the solar cell performance [1,2]. The combined experimental approach results in a comprehensive model of the investigated interface. The presence of a π-orbital stacking is also of interest for ground-state charge transfer.

[1] J. Wagner et al., Adv. Funct. Mater. 20 (2010) 4295.
[2] A. Opitz et al., Org. Electron. 10 (2009) 1259.

HL 19.2 Mon 17:15 EW 202

Unified model approach for hybrid charge transfer states in organic-organic heterostructures — Tino Meisel, •Paul Beyer, Georg Heimel, Norbert Koch, and Andreas Opitz — Humboldt-Universität zu Berlin, Germany

There are different electronic coupling mechanisms for organic-organic heterostructures, which ultimately determine the charge separation in solar cells or the doping efficiency in blended systems. Here, these charge transfer mechanisms are investigated in blends of diindenoperylene (DIP) with different acceptor materials, namely core functionalized perylene alkyldiimide with cyano groups (PDIR-CN_2) and perfluoronaphthalene-diylidene dimalononitrile (F6TCNNQ), which show compatible optical gaps. To scrutinize the interplay between these molecules a combination of atomic force microscopy (AFM), UV/Vis/NIR absorption spectroscopy and electrical conductivity measurements is used.

From absorption spectroscopy the formation of new absorption features is clearly seen in blends with both acceptors. An increase in electrical conductivity is observed for DIP:F6TCNNQ blends, which is absent in the DIP:PDIR-CN_2 case. The formation of distinct islands in AFM shows a difference in morphology between pristine and blended films. From these investigations we conclude the appearance of new charge transfer states and a unified hybridization model is applied to explain the different regimes of charge transfer behavior.

HL 19.3 Mon 17:30 EW 202

New Insights on traps states in organic semiconductor devices using transient current measurements on metal-insulator-semiconductor capacitors — Hippolyte Hirwa and •Veit Wagner — Jacobs University, Bremen, Germany

A Transient current measurement technique utilizing metal-insulator-semiconductor (MIS) capacitors is developed, which does not need a light stimulus. The technique offers insights on carrier trapping states such as capture time of trapping states and the attempt-to-escape frequency of trapped carriers. For the analysis of the measurements Fourier transformation of imepdance-based circuit models to the time domain as well as direct numerical simulation of transient current of MIS capacitors were used. Numerical simulations allow to go beyond the usual assumptions of negligable extraction time for de-trapped carriers. It is shown, that re-trapping events are relevant in order to extract the proper band tail density of states and the corresponding characteristic parameters. For e.g. P3HT an exponential density of states with a total density of $4 \cdot 10^{17}$ cm^3 and a width of 50 meV was found to be representative for the band tail. Analyzing the multiple trap and release behavior in the numerical simulation, the average capture time and the attempt-to-escape frequency of band tail states were found to be 10^{-10} s and 10^8 s^{-1}, respectively.

HL 19.4 Mon 17:45 EW 202

Influence of trap distribution on the electrical characteristics of organic solar cells — •Alexander Wagenpfahl, Robert Hanfland, and Carsten Deibel — Chemnitz University of Technology, Institute of Physics, 09126 Chemnitz, Germany

Charge carrier traps have a strong impact on the performance of organic solar cell devices. It remains unclear, however, if either a Gaussion or an exponential distribution of the density of states (DOS) describes most organic photovoltaic devices better. In our work, we apply a macroscopic drift–diffusion simulation in combination with the multiple-trapping and release model to examine how the DOS distribution influences the current-voltage characteristics, diode ideality factor

and effective charge carrier mobility of organic solar cells. We compare our findings to corresponding experimental data from different types of organic solar cells to determine the likely DOS shape. Its impact on the experimental device characteristics will be discussed.

HL 19.5 Mon 18:00 EW 202

Investigation of DCV5T-Me Solar Cells on Presence of Traps — •Natalia Sergeeva[1], Janine Fischer[1], Paul Pahner[1], Lorenzo Burtone[1,2], Christian Körner[1], Koen Vandewal[1], and Karl Leo[1] — [1]Institut für Angewandte Photophysik Technische Universität Dresden, Germany — [2]Globalfoundries, Dresden, Germany

Traps play an important role in the performance of organic solar cells (OSC). They influence the mobility, the amount of extracted charge carriers at the electrodes and lead to trap assisted recombination. Better understanding of traps is necessary to further improve the efficiency of OSC. We investigate bulk heterojunction OSC based on the donor material DCV5T-Me with regards to the presence of traps by performing Impedance spectroscopy (IS) and temperature stimulated currents (TSC) measurements. We discuss the observed impedance and TSC spectra, evaluate the density and distribution of trap states and the attempt to escape frequency.

HL 19.6 Mon 18:15 EW 202

Charge transport: Mobility in organic donor-acceptor blends for photovoltaics — •Johannes Widmer, Julia Oelker, Janine Fischer, Christian Koerner, and Karl Leo — IAPP (Institut für Angewandte Photophysik), TU Dresden, Germany

The charge carrier mobility μ is the key parameter describing charge transport in semiconductors. In amorphous material with predominating hopping transport, the effective mobility is affected by disorder. The resulting μ varies with electric field strength F and charge carrier density n, and is influenced by the layer morphology.

In this contribution, we analyze the mobility of various small molecule organic semiconductors in neat as well as blend layers. The mobility is measured by means of electric potential mapping (POEM), varying the thickness of single carrier devices and evaluating them at constant current density.[1] This measurement technique allows for resolving the field dependence and the density dependence of $\mu(F, n)$ independently of each other, separately for electrons and holes.

Substrate heating during the deposition of donor-acceptor blend layers is known to substantially improve the device performance of solar cells, and we show which role the charge carrier mobility plays in this context. Furthermore, the influence of the blend ratio on μ is investigated, which allows for a refined interpretation of the role of the acceptor phase in hole transport. These findings improve the understanding of charge transport in organic solar cells and inspire paths for efficient further improvement of device performance.

[1] Widmer et al., OrgEl 14, p. 3460 (2013)

HL 19.7 Mon 18:30 EW 202

Mobility Relaxation in PTB7:PC_{70}BM on nanosecond timescale — •Andreas Fritze[1], Andreas Sperlich[1], Carsten Deibel[2], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz — [3]ZAE Bayern, 97074 Würzburg

For photovoltaics, charge carrier lifetime is an essential parameter due to its influence on short circuit current, and thus on power conversion efficiency. In organic photovoltaics, for several material systems, charge carrier lifetime exceeds predictions from recombination models by orders of magnitude. In literature, this phenomenon is discussed in the context of reduced langevin recombination, for instance the high-efficiency bulk heterojunction polymer fullerene solar cell PTB7:PC_{70}BM, it is shown that recombination is also reduced. However, the physical processes responsible for these low recombination rates, such as mobility relaxation, energetic traps, and morphological traps, are hard to observe separately. Here, we present simultaneous transient absorption (TA) and transient microwave conductivity (TRMC) measurements on PTB7:PC_{70}BM films. From the experimental data we calculate time dependent mobility, since TA is sensitive to charge carrier density and TRMC is sensitive to conductivity. A relaxation of mobility on these time scales is measured the first time separately. Thus, we can distinguish mobility relaxation from other recombination influencing processes in PTB7:PC_{70}BM.

HL 19.8 Mon 18:45 EW 202

OTRACE: The technique to study charge carrier mobility and lifetime in organic thin film solar cells under real operating conditions — •Andreas Baumann[1], Andreas Zusan[2], and Vladimir Dyakonov[1,2] — [1]Bayerisches Zentrum für Angewandte Energieforschung, Am Galgenberg 87, D-97074 Würzburg — [2]Experimentelle Physik 6, Julius-Maximilians-Universität Würzburg, Am Hubland, D-97074 Würzburg

For the development and design of new promising semiconducting materials for organic electronics material parameters like the mobility and the lifetime of photogenerated charge carriers need to be investigated and optimized. Usually, techniques such as TOF, SCLC, or photo-CELIV are used to study the charge carrier transport. Especially, the latter technique principally enables one to study both charge carrier mobility and lifetime. However, all of these techniques are not really suited to study real solar cell devices under ambient conditions. With our newly developed experimental method of open circuit corrected transient charge extraction (OTRACE)[1] it is feasible to easily determine the charge carrier mobility and lifetime under operating conditions of the solar cell device. In addition, the mobility determined by OTRACE is the most relevant one for organic solar cells at open circuit conditions without suffering from injected charge carriers, which would result in major RC limitations. In combination with IV measurement this technique can be easily used for material screening producing fast output of relevant solar cell parameters. [1] Baumann et. al., AM, 2012. 24(32): p. 4381-4386.

HL 20: Poster IA (Ultrafast phenomena; Optical properties; Transport; Theory)

Presenters are kindly requested to be near their poster for at least one hour in the time between 17:00-19:00 or to leave a note about their availability for discussions.

Time: Monday 15:00–20:00 Location: Poster B

HL 20.1 Mon 15:00 Poster B

Laser induced Tellurium formation detected by THz oscillations in plasmonic crystals — •Jonas Vondran[1], Lars E. Kreilkamp[1], Martin Pohl[1], Maciej Wiater[2], Tomasz Wojtowicz[2], Grzegorz Karczewski[2], Boris. A Glavin[3], Leonid Litvin[4], Axel Rudzinski[4], Michael Kahl[4], Ilya A. Akimov[1,5], Dmitri R. Yakovlev[1,5], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, D-44221 Dortmund, Germany — [2]Institute of Physics, Polish Academy of Sciences, PL-02668 Warsaw, Poland — [3]Lashkaryov Institute of Semiconductor Physics, 03028 Kyiv, Ukraine — [4]Raith GmbH, Konrad-Adenauer-Allee 8, 44263 Dortmund, Germany — [5]A. F. Ioffe Physical-Technical Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia

We study the differential reflectivity of a CdMgTe structure in pump-probe experiments on a femtosecond timescale under below bandgap excitation. In the transient data oscillations with frequencies in the 3.6 - 3.8 THz range are observed. We attribute this to coherent oscillation of optical phonons in a thin Tellurium layer on the sample surface which is formed on the II-VI semiconductor due to a surface reconstruction induced by the pump beam. Changes in frequency and amplitude with increasing exposure time allow to monitor the build-up process of the Tellurium layer.

We show that the oscillatory signal is enhanced by one order of magnitude via patterning of a plasmonic grating with a period of several hundreds of nanometers.

HL 20.2 Mon 15:00 Poster B

Electron dynamics driven by light carrying orbital angular momentum — •Jonas Wätzel and Jamal Berakdar — Institut für Physik, Martin-Luther Universität Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3, 06120 Halle

The feasibility of light carrying orbital angular momentum (OAM) opened new opportunities in photonics [1] but also in optoelectronics. When interacting with matter, OAM beams may transfer a torque to the carrier with an amount governed by the topological charge l. This allows to steer the orbital [2] as well as the spin dynamics [3]. Indeed, an OAM beam irradiating an injected electronic wave packet in a 2D semiconductor stripe results in an edge charge-density accumulation that can be steered by the OAM beam [2].

Here, we present results for an isolated mesoscopic 2D ring driven by OAM laser. The calculations reveal that due to the transferred torque a directed current can be generated and controlled by the sign and the strength of the topological charge l. We also discuss technological applications of these phenomena.

[1] L. Allen, S. M. Barnett, and M. Padgett, Optical Angular Momentum (Institute of Physics Publishing, Bristol, 2003).

[2] J. Wätzel, A. S. Moskalenko and J. Berakdar, Opt. Express 20, 27992 (2012)

[3] G. F. Quinteiro and J. Berakdar, Opt. Express 17, 20465 (2009)

HL 20.3 Mon 15:00 Poster B

Ab-initio MD-simulations of the response of titanium dioxde after fs-laser exciation — •Sergej Krylow[1], Fairoja Cheenicode Kabeer[1,2], Eeuwe S. Zijlstra[1], and Martin E. Garcia[1] — [1]Theoretical Physics II, University of Kassel — [2]Theory Department, Fritz Haber Institute Berlin

The response of titanium dioxide was determined by using our in-house Code for Highly-excIted Valence Electron Systems(CHIVES), which is based on electronic temperature dependent density functional theory using pseudopotentials and localized atom-centered basis functions. We are especially interested in the decay of the A1g phonon mode as well as the phonon-phonon interaction causing this decay. We show that the dynamics of the decay is dependent on the applied fs-laser fluence and we comapre the result with recent experiments [1]

[1] E. M. Bothschafter , A. Paarmann , E. S. Zijlstra, N. Karpowicz, M. E. Garcia, and R. Ernstdorfer: Ultrafast evolution of the excited-state potential energy surface of TiO_2 single crystals induced by carrier cooling

HL 20.4 Mon 15:00 Poster B

Ultrafast carrier dynamics and coherent oscillations in PbTe — •Prashant Padmanabhan[1], Kestutis Budzinauskas[1], Kiran H. Prabhakara[1], Benoît Fauqué[2], Kamran Behnia[2], and Paul H. M. van Loosdrecht[1] — [1]Physics Institute 2, University of Cologne, 50937 Cologne, Germany — [2]LPEM (UPMC-CNRS), Ecole Supérieure de Physique et de Chimie Industrielles, 75005 Paris, France

PbTe is a leading thermoelectric material that, in addition to its low thermal conductivity, shows unusually large carrier mobilities at very low doping levels. Here, we report on ultrafast pump-probe experiments on PbTe that shed light on these, as of yet, ill-understood properties. By employing time-resolved differential reflectivity measurements, the dynamics of electron-electron and electron-phonon interactions on the femtosecond time-scale are studied. The influences of sample temperature and pump fluence on the time constants of the various scattering pathways are also investigated. In addition, our experiments have revealed the presence of coherent oscillations in the differential reflectivity with a frequency close to those associated with LA+TO excitations; these may provide a means to further study the giant anharmonic coupling that is central to the low thermal conductivity of PbTe.

HL 20.5 Mon 15:00 Poster B

Plasmon-Exciton coupling in stacked 2D Perovskite Semiconductors — •David Leipold[1], Wendy Niu[2], Lindsey Ibbotson[2], G. Vijaya Prakash[3], Jeremy J. Baumberg[2], and Erich Runge[1] — [1]Technische Universität Ilmenau, Germany — [2]University of Cambridge, UK — [3]Indian Institute of Technology Delhi, India

The coupling of plasmons and non-linear materials is a vital part in the developement of future plasmonic devices. Strong coupling and the formation of new plasmon-exiton quasiparticles called Excimons was previously observed in metal-semiconductor hybrid systems and organic dye coated metal-gratings. Here, we discuss $(C_6H_9C_2H_4NH_3)_2PbI_4$ (CHPI) as a candidate material for active plasmonic devices. In contrast to other materials, CHPI shows strong excitonic response and high stability even at room temperature. It can viably be processed from solution and forms regular stacks of semiconducting sheets. We present experiments and calculations for the optical properties of CHPI on nanostructured metal-gratings. We observe the formation of collective grating-exciton modes that are coupled with a Rabi splitting of 125-150meV. The role of the interaction of the CHPI exciton with its image-exciton in the metal is discussed as an additional interesting effect.

HL 20.6 Mon 15:00 Poster B

Surface plasmons at semiconductor/dielectric interfaces — •Dalibor Blažek[1,2], Michael Čada[2,1], and Jaromír Pištora[1] — [1]Nanotechnology Centre, VŠB - Technical University of Ostrava, 17. listopadu 15, Ostrava - Poruba, Czech republic — [2]Department of Electrical and Computer Engineering, Dalhousie University, Halifax, NS B3H 4R2, Canada

Plasmonic structures are a promising solution for developing novel integrated optics devices. While metals have shown to support plasmon oscillations at optical frequencies, heavily doped semiconductors may support surface plasmons (SP) at infrared frequencies. In order to fully understand the resulting SP characteristics, one needs to investigate properties of the lattice permittivity, the plasma frequency, and the damping.While these material properties may be regarded as the material constants, the relevant SP properties are dispersive. Focusing on the SP of a chosen wavelength, its characteristics may be tuned by a semiconductors doping level. While a minimum dopant concentration is required to support a chosen SP, as the doping concentrations increase, the secondary effects, such as decreasing electron mobility and increasing effective mass, will significantly affect plasmon damping.

This contribution presents the influence of doping levels on the SP properties. The calculations are based on the Drude model using the real semiconductor properties. It is shown that the propagation length of the SP increases monotonically with increasing doping levels despite the extremely large damping.

HL 20.7 Mon 15:00 Poster B

Control of Lasing from Bloch-States in Microcavity Photonic Wires via Selective Excitation and Gain — •Andreas Mischok[1], Robert Brückner[1], Alexander A. Zakhidov[1,2], Hartmut Fröb[1], Vadim G. Lyssenko[1], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr Str. 1, 01069 Dresden — [2]Texas State University, 601 University Drive, San Marcos, Texas, United States

Organic microcavities comprising the host:guest emitter system Alq_3:DCM offer an interesting playground to experimentally study the full dispersion characteristics of laterally patterned surface emitting lasers due to the broad emission spectrum and high quantum efficiency of the organic dye. By structuring directly on top of the bottom distributed Bragg reflector, we are able to precisely manipulate the mode structure and influence the coherent emission properties of the device. Adding SiO_2 photonic wire structures into an organic microcavity, we create an additional lateral confinement and a Bloch-like band-structure in the dispersion of periodically patterned cavities. We experimentally observe spontaneous and stimulated emission from the ground and different excited discrete states at room temperature. By changing the spatial gain distribution via a two beam interference, we are able to directly control the laser emission from both extended and confined modes of such organic photonic wires. Both spatial distribution and dispersion exhibit coherent emission from tunable modes, which we describe with an analytical model and numerical simulations, in perfect agreement with our measurements.

HL 20.8 Mon 15:00 Poster B

Towards coupling of photonic crystal cavities and waveguides as an integrated deterministic single-photon source in quantum photonic networks — •Stefan Hepp, Ulrich Rengstl, Matthias Paul, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen and Center for Integrated Quantum Science and Technology IQ^{ST}, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

The generation and control of deterministic single photons is crucial for quantum photonic technologies like quantum teleportation, quantum computation and quantum cryptography. The requirements for such an on-demand single-photon source are a near unity photon-extraction and excitation efficiency coupled with a high degree of indistinguishability and an easy implementation in quantum photonic networks. Semiconductor quantum dots (QDs) have been proven as excellent candidates due to their outstanding optical properties and their easy integration in semiconductor nanophotonic devices. One main approach for an on-demand single-photon source is the positioning of QDs in photonic crystal cavities and waveguides for the coupling

of the QD emission into guided modes, which is required for on-chip integration. An additional benefit of this approach is the exploitation of cavity quantum electrodynamic effects (cQED) to improve and manipulate the optical properties of the quantum dot emission. Here we present a way to an integrated on-demand single-photon source based on InAs/GaAs QDs positioned in a L3 photonic crystal cavity coupled to a waveguide for in-plane single-photon emission at 910nm.

HL 20.9 Mon 15:00 Poster B

Lasing Dynamics in ZnO & CdS Nanowires — •Marcel Wille[1], Tom Michalsky[1], Robert Röder[2], Carsten Ronning[2], Rüdiger Schmidt-Grund[1], and Marius Grundmann[1] — [1]Institut für Experimentelle Physik II, Universität Leipzig, Linnéstraße 5, 04103 Leipzig — [2]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena

The knowledge of the turning-on characteristic as well as of the laser dynamics itself is of great importance for the application of semiconductor nanowires (NWs) as on-chip integrated nanolaser. In this work we investigated the laser dynamics of high quality, CVD grown ZnO and CdS NWs using time-resolved micro photoluminescence technique. Experiments at room temperature clearly demonstrate the formation of an electron-hole plasma in both semiconductor materials accompanied by a spectral red shift of the PL emission as well as the drop of the decay constant above laser threshold. After the high exciting laser pulse the propagating NW laser modes exhibit a red shift in time, what can be explained with the increase of the refractive index with decreasing carrier density. Remarkably, modes closer to the excitonic energy exhibit a stronger red shift than lower energetic modes. In fact the modal shift depending on the initial mode energy is significantly higher in ZnO compared to CdS NWs.

HL 20.10 Mon 15:00 Poster B

Exciton polariton modes of a planar resonator in magnetic fields — •Steffen Richter, Chris Sturm, Helena Franke, Rüdiger Schmidt-Grund, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig, Germany

Exciton-polaritons have gained large interest during the last years especially due to their ability to undergo Bose-Einstein-like condensation. Magnetic fields are important as they can be be used to control the polariton and resonator properties, e.g. in order to decrease condensation thresholds. Here, we show a theoretical study of the evolution of the polariton eigenmodes and their polarization properties (pseudo spin) in a planar resonator in the presence of a magnetic field. Thereby no restrictions of the direction of the magnetic field with respect to the polariton wave vectors are assumed. A 4×4 transfer matrix approach enables numerical application of the respective mode conditions with full polarization treatment at arbitrary in-plane wavevectors.

HL 20.11 Mon 15:00 Poster B

Temperature dependent dielectric function of hexagonal $YMnO_3$ — •Steffen Richter[1], Rüdiger Schmidt-Grund[1], Carsten Bundesmann[2], Stefan Ebbinghaus[3], and Marius Grundmann[1] — [1]Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig, Germany — [2]Leibniz-Institut für Oberflächenmodifizierung e.V., Permoserstr. 15, 04318 Leipzig, Germany — [3]Martin-Luther-Universität Halle-Wittenberg, Institut für Chemie, Kurt-Mothes-Str. 2, 06120 Halle, Germany

Rare earth manganites are promising due to the occurrence of multiferroic properties. Hexagonal $YMnO_3$ is ferrolectric up to high temperatures. Furthermore, it is antiferromagnetic below a Néel temperature of around 90K. Both features are coupled by the configuration of the manganese ions. In order to study a possible coupling to its optical properties we examine the uniaxial dielectric function of h-$YMnO_3$ in the NIR-VUV spectral range for temperatures from 10 to 300K. The measurements are performed at an *a*-plane oriented single crystal sample, grown by the optical floating zone technique. The temperature dependence of some Mn-related transitions gives hint to the occurence of a soft mode related to the antiferromagnetic phase transition.

HL 20.12 Mon 15:00 Poster B

Interference measurements on exciton-polariton Bose-Einstein Condensates — •Alexander Holm, Martin Thunert, Helena Franke, Chris Sturm, Tom Michalsky, Marius Grundmann, and Rüdiger Schmidt-Grund — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig, Germany

We report on interference measurements to investigate the coherence properties of exciton-polariton Bose-Einstein condensates (BECs) in a ZnO-based planar microcavity at T = 10 K. The photoluminescence signal of the Fourier plane was sent to a Michelson interferometer in mirror-retroreflector (RR) configuration. The RR image is a centrosymmetric counterpart of the mirror arm image. In the resulting interferogram we superimpose the emission with opposite wavevectors.

By means of analyzing the fringe visibility of the interferogram as a function of the path length difference of both interferometer arms, a BEC coherence time at least (500 ± 200) fs could be deduced. This is about four times larger than the BEC lifetime demonstrating the coherence conservation during the multiple reabsorption and reemission process of this quantum system.

HL 20.13 Mon 15:00 Poster B

Impact of disorder on the coherence of a polariton condensate in dependence on the temperature — Martin Thunert[1], •Stefan Lange[1], Helena Franke[1], Chris Sturm[1], Alexander Janot[2], Bernd Rosenow[2], M. Dolores Martín[3], Luis Viña[3], Marius Grundmann[1], and Rüdiger Schmidt-Grund[1] — [1]Uni Leipzig, Inst. für Exp. Physik II, Linnéstr. 5, 04103 Leipzig — [2]Uni Leipzig, Inst. für Theor. Physik, Brüderstr. 16, 04103 Leipzig — [3]Universidad Autónoma de Madrid, Departamento de Física de Materiales, C/ Francisco Tomás y Valiente, n* 7, 28049 Madrid, Spain

We report on the impact of disorder on the coherence proterties of an exciton-polariton Bose-Einstein condensate (BEC) in a ZnO-based bulk planar microcavity (MC). In general, disorder leads to reduced long-range correlations of the BEC, which may eventually result in frequency desynchronization or even in spatially separated condensate fragments. In our MC, the momentum space intensity distribution of the BEC emission is strongly affected by disorder even at high excitation powers and for a wide range of temperatures and detunings. We found theoretically that this lack of BEC stabilization relies on the driven dissipative nature of the condensate, leading to disorder-induced density-independent phase fluctuations. We analyzed the interference pattern of the condensate emission pattern in momentum space for excitation powers slightly above the condensation threshold and a large range of temperatures up to 160 K. These measurements show that the emission from a certain energy state arises from a temporally coherent condensate rather than of uncorrelated BEC fragments.

HL 20.14 Mon 15:00 Poster B

Optical Properties of a Palladium-Tin Clusters as a Model System for Interfaces on a Molecular Scale — •Andre Rinn, Niklas Rinn, Stefanie Dehnen, and Sangam Chatterjee — Philipps-Universität Marburg, Germany

Palladium-containing compound-materials are of great interest for their catalytic properties. We have successfully grown a new Pd-Sn cluster with an organic shell which is a promising candidate for a next-generation heterogenic catalyst. From a more fundamental point of view, the interaction of the Pd and Sn core with the outer organic shell makes this cluster an interesting model system for internal interfaces on a molecular scale.

The compound crystalizes into micrometer-sized, well-ordered single-crystalline needles which are relatively ambient-insensitive. To characterize their optical response we perform linear absorption and steady-state PL under vacuum conditions in a microscopy setup containing all-reflective optics. Next, we study the transfer between the Pd-containing core and the outer shell for various excitation energies and fluencies to identify the charge-transfer mechanisms. Furthermore, the influence of different ambient conditions is investigated to explore surface adhesion effects on the optical response.

Financial support by the German Research foundation in the Framework of SFB 1083 is gratefully acknowledged.

HL 20.15 Mon 15:00 Poster B

Optical properties of organotin sulfide clusters — •Nils Rosemann[1], Jens Eussner[2], Stefanie Dehnen[2], and Sangam Chatterjee[1] — [1]Faculty of Physics and Material Science Center, Philipps-Universität Marburg, Renthof 5,D-35032 Marburg, Germany — [2]Faculty of Chemistry and Material Science Center, Philipps-Universität Marburg, Hans-Meerweinstraße,D-35043 Marburg, Germany

Chalcogenide-based clusters offer a large variety of structural and physical properties which can be further functionalized by adding various different ligands. By changing the combination of cluster and ligand, their properties can be tuned to fit the desired purpose, e.g., opti-

mized light harvesting in organic solar cells or enhancing the efficiency of electrolysis of water for hydrogen production. To identify the impact of different ligands, we study a series of three different organotinsulfide clusters, based on the same core but with different functional groups. Only by changing the ligand, the optical properties change drastically, e.g., disabling optical activity or changing from optical activity to dichroism.

HL 20.16 Mon 15:00 Poster B

Time-resolved photoluminescence spectroscopy on silicon doped AlN, iron doped GaN and nominally undoped ZnO using correlational analysis — •Matthias Lamprecht[1], Benjamin Neuschl[1], Sebastian Bauer[1], Ramón Collazo[2], Martin Klein[3], Ferdinand Scholz[3], Zlatko Sitar[2], and Klaus Thonke[1] — [1]Institute of Quantum Matter / Semiconductor Physics Group, Ulm University, 89081 Ulm, Germany — [2]Department of Materials Science and Engineering, North Carolina State University, Raleigh, North Carolina 27606, USA — [3]Optoelectronics Department, University of Ulm, 89069 Ulm, Germany

We present results of time-resolved photoluminescence investigations using correlational analysis on a time scale of microseconds and milliseconds. Modulation of the pumping HeCd laser with a pseudorandom binary sequence yields correlational properties similar to white noise. Via cross correlation of the detected signal and the pseudorandom binary sequence the photoluminescence decay is computed. We applied this method to several defect-related photoluminescence bands in silicon doped AlN, iron doped GaN and nominally undoped ZnO and discuss the characteristics, and temperature dependencies.

HL 20.17 Mon 15:00 Poster B

Activated transport in nanoporous titanium dioxide under hydrogen exposure — •Sonja Allani[1], Thomas Heinzel[1], Mihai Cerchez[1], and Klaus Schierbaum[2] — [1]Solid State Physics Laboratory (IPkM), Heinrich-Heine-Universität Düsseldorf, 40204 Düsseldorf, Germany — [2]Materials Science Laboratory (IPkM), Heinrich-Heine-Universität Düsseldorf, 40204 Düsseldorf, Germany

Nanoporous titanium dioxide is reduced to $TiO_{2-\delta}$ by thermal annealing. The oxygen vacancies act as donors and increase the conductivity. This material has been used for hydrogen sensing in the ppm range, [1] but the hydrogen-induced transport mechanism is not fully understood. Here, we present temperature dependent transport experiments of this material in the presence of atomic hydrogen. We observe a strongly decreasing conductivity as the temperature is decreased from 300 K to 40 K. The temperature dependence is consistent with both activated transport and variable range hopping within experimental uncertainties. Moreover, the current-voltage characteristics are nonlinear, incidating that reduced titanium dioxide does not become metallic under hydrogen exposure that is typical for sensing applications.

[1] M. Cerchez, H. Langer, M. El Achhab, T. Heinzel, D. Ostermann, H. Lüder, and J. Degenhardt, Appl. Phys. Lett. 103, 033522 (2013).

HL 20.18 Mon 15:00 Poster B

Asymmetric Hall cross junction — •Michael Szelong[1], Arne Ludwig[2], Andreas D. Wieck[2], and Ulrich Kunze[1] — [1]Werkstoffe und Nanoelektronik, Ruhr-Universität Bochum — [2]Angewandte Festkörperphysik, Ruhr-Universtät Bochum

We are analysing the influence of a geometrical asymmetry in a cross junction on Hall voltage in ballistic linear and nonlinear transport regime in a perpendicular magnetic field of up to 15 T. The cross junction consists of a straight current channel while two voltage probes merge into the middle of the current channel at an angle of 45°. All four emerging branches have the same length of 900 nm and the same width of 330 nm. A top-gate has not been processed to prevent threshold voltage shifts during measurements. The device has been processed on a high-mobility GaAs/AlGaAs heterostructure with a two-dimensional electron density of $n = 4.1 \cdot 10^{11}\mathrm{cm}^{-2}$ and a mobility of $\mu_n = 5.5 \cdot 10^5\mathrm{cm}^2/\mathrm{Vs}$, both at 4.2 K, resulting in an elastic mean free path of 5.8 μm.

A current through the current channel induces, with application of a perpendicular magnetic field, a Hall voltage in the 45-degree branches which is expected to be current polarity dependent, larger where electrons can easier enter the tilted branches, smaller in the opposite case. It is found that in non-linear regime this expectation is met whereas in weak non-linear regime it is sometimes turned upside down.

HL 20.19 Mon 15:00 Poster B

Hall effect in an asymmetric ballistic cross junction — •Joeren von Pock[1], Ulrich Wieser[1], Thomas Hackbarth[2], and Ulrich Kunze[1] — [1]Lehrstuhl für Werkstoffe und Nanoelektronik, Ruhr-Universität Bochum, D-44780 Bochum — [2]DaimlerChrysler Forschungszentrum Ulm, D-89081 Ulm

Low-temperature ($T = 4.2$ K) Hall measurements up to $B = 15$ T are performed on a ballistic cross junction consisting of 220 nm wide channels on a high mobility Si/SiGe heterostructure ($\mu_{2D} = 18.3\ \mathrm{m}^2\mathrm{V}^{-1}\mathrm{s}^{-1}$, $n_{2D} = 6.3 \cdot 10^{15}\ \mathrm{m}^{-2}$ at 1.4 K). A non-centrosymmetric Hall geometry is formed by a straight current channel and oblique voltage probes attached to the channel under 45° in the same direction. A Pd gate electrode covers the whole structure. In the nonlinear transport regime (current $I \approx 1$ μA) at low magnetic fields ($B \leq 1$ T) the absolute value of the Hall voltage depends on the current direction [1]. This is explained in terms of ballistic cyclotron orbits propagating into the oblique probe channels. Surprisingly, the polarity dependence persists up to magnetic fields up to $B = 15$ T, where the cyclotron diameter shrinks to 13 nm, which is less than the effective channel width.

[1] U. Wieser *et al.*, Physica E **40**, 2179 (2008).

HL 20.20 Mon 15:00 Poster B

Hartree-Fock Ground State Phase Diagram of the Two-Dimensional Electron Gas with Spin-Orbit Interaction — •Akash Chakraborty, Paul Wenk, and John Schliemann — Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

The two-dimensional electron gas (2DEG) has served as a prototype for the understanding of electrons in solid state and condensed matter physics, such as in the quasi two-dimensional semiconductor heterostructures. However, the quantum mechanical many-body nature of these systems increases the complexities and the Hartree-Fock (HF) approximation plays a fundamental role in tackling this problem. Starting from the early works of Overhauser[1], the HF ground state of the 2DEG has been studied over the years but the effects of spin-orbit interaction have not been studied extensively. We calculate the ground state of the 2DEG within the HF approximation in the presence of Rashba and Dresselhaus spin-orbit coupling. Based on an earlier work[2], which included only the Rashba term, we try to identify two competing phases, a ferromagnetic one with partial out-of-plane polarization and a paramagnetic one with in-plane spin. A phase diagram in terms of the electron density and the relative intensities of the spin-orbit couplings with respect to the Coulomb interaction is also presented.

[1] A. W. Overhauser, Phys. Rev. Lett. 4, 462 (1960); Phys. Rev. 128, 1437 (1962).

[2] L. O. Juri and P. I. Tamborenea, Phys. Rev. B 77, 233310 (2008).

HL 20.21 Mon 15:00 Poster B

Effect of B/N co-doping on optical properties of Graphene — •Pooja Goyal — Dep. of Physics, Panjab University, Chandigarh — DAV College Chandigarh

Ab-initio calculations based on density functional theory (DFT) have been performed to study the optical properties of pure graphene as compared BN co-doped graphene sheet. The effect of doping has been investigated by varying the concentrations of dopants from 6.25 % (one atom of the dopant in 32 host atoms) to 75 % for BN co-doping also varying the doping sites. The dielectric function has been calculated within the random phase approximation (RPA) using VASP (Vienna ab-initio Simulation Package) code. The dielectric function, absorption spectrum and energy loss-function of single layer graphene sheet have been calculated for light polarization parallel and perpendicular to the plane of graphene sheet and compared with doping graphene. The calculated dielectric functions and energy-loss spectra are in reasonable agreement with the available theoretical and experimental results. It has been found that there is significant red shift in absorption towards visible range of the radiation at high doping concentration. The results suggest further investigations in this direction for application of graphene in photonics in visible region of light.

HL 20.22 Mon 15:00 Poster B

***Ab-Initio* Studies of X-Ray Absorption in Kesterites** — •Archana Manoharan, Lorenzo Pardini, Karsten Hannewald, and Claudia Draxl — Humboldt-Universität zu Berlin, Institut für Physik und IRIS Adlershof, Zum Großen Windkanal 6, 12489 Berlin, Germany

The kesterite Cu_2ZnSnS_4 (CZTS) is considered as good absorber material for solar-cell applications because it contains only non-toxic and inexpensive metals. In the present work, we study the structural and electronic properties of CZTS using density-functional theory within the generalized gradient approximation (GGA-PBEsol). X-ray absorption spectra are obtained by solving the Bethe-Salpeter equation of many-body perturbation theory. We explore the sulfur K and $L_{2,3}$ edges in CZTS as well as in binary phases like ZnS etc. The *ab-initio* calculations are carried out by the all-electron full-potential code *exciting*. A detailed analysis of the observed spectral signatures is performed by comparison with available experimental data.

HL 21: Poster IB (Oxide semiconductors; II-VI and group IV semiconductors; Nanotubes and Buckyballs)

Presenters are kindly requested to be near their poster for at least one hour in the time between 17:00-19:00 or to leave a note about their availability for discussions.

Time: Monday 15:00–20:00 Location: Poster B

HL 21.1 Mon 15:00 Poster B

Multi-beam sputtering approach for creation of material libraries — •Martin Becker, Angelika Polity, and Bruno K. Meyer — 1st Physics Institute, Justus-Liebig-University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

Ion beam sputter deposition (IBSD) has been under focus of research for a number of years due to the flexibility it provides in the deposition of novel thin film materials. One of the characteristics, making IBSD unique, is the ability to deposit multi-component or multi-layered materials using a multi-target single ion gun scheme. This is accomplished by sequentially positioning selected targets in front of the ion source. Furthermore the demand of new combinatorial capabilities for both the synthesis of new solid state opto-electronics and optimization of existing materials has driven the interest in multi-beam arrangements. Important materials for applications include semiconductors, transparent conductors, energy storage materials and more.

We report on the application of single beam and combinatorial approach to the specific material type of transparent conducting oxides (TCOs). In this case, libraries are generated by ion beam sputtering. The application of a combinatorial approach to this materials area can greatly accelerate the rate of discovery and optimization of new materials and the optimization of devices. Initial collection of characterization tools for investigation of optical and structural properties includes UV/VIS/NIR transmission/reflection, Raman scattering and X-ray diffraction.

HL 21.2 Mon 15:00 Poster B

An X-ray photoelectron spectroscopy (XPS) study on intrinsic and nitrogen doped tin oxides — •Fabian Michel, Benedikt Kramm, Martin Becker, Jie Jang, Angelika Polity, and Bruno K. Meyer — 1. Physikalisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, 35392 Gießen

This work is an XPS study on intrinsic and nitrogen doped tin oxide. We fabricated SnO_x thin films by ion beam sputtering and epitaxial growth. By sputtering we produced a series with varying stoichiometrie by changing the oxygen flow and/or the substrate temperature. Using the second method we made a series of SnO_2 with different nitrogen concentrations. By X-ray photoelectron spectroscopy (XPS) we identified the phases in the SnO_x thin films. Therefore, we took a look at the relative atomic concentration of tin and oxygen in the stoichiometrie series and especially at the relative atomic concentration of nitrogen in the samples produced by epitaxial growth. We also investigated the variation of the valence band position in relation to the treatments mentioned above. Thus we analyzed the chemical shifts of the photoelectron and the Auger electron lines. Furthermore the effects of the nitrogen doping on the valence band maximum and on the work function were investigated using ultraviolet photoelectron spectroscopy (UPS).

HL 21.3 Mon 15:00 Poster B

Ohmic contacts to In2O3 single crystals — •Maryam Nazarzadehmoafi[1], Mattia Mulazzi[1], Christoph Janowitz[1], Stephan Machulik[1], Zbigniew Galazka[2], and Recardo Manzke[1] — [1]Institut für Physik, Humboldt Universität zu Berlin, Newtonstraße 15, 12489 Berlin, Germany — [2]Leibniz Institut für Kristallzüchtung, Max Born Str. 2, 12489 Berlin, Germany

It is known that the barrier formation at the interface between metals and ionic semiconductors usually follows the Schottky-Mott rule. In contrast, this model fails for the several metal-In2O3 interfaces, and this is commonly attributed to an electron accumulation layer at the surface of In2O3, believed to prevent the Schottky contact formation. In order to have a deeper insight into the metal-In2O3 contacts, the barrier heights of In and Cu on the melt-grown In2O3(111) single crystals were studied by means of ARPES at room temperature (RT) and low temperature (LT). The growth of Copper on In2O3 (111) is ordered and homogenous at RT, as suggested by the presence of a distinct surface state for thick Cu films. In the case of Indium, we observed an electronic state near the Fermi level at small coverages, blurring out for increasing the metal thicknesses, what is a signature of an interface state. The ohmic behavior of both interfaces is evident at RT and LT for both metals, contrary to the prediction of the Schottky-Mott rule, with a stronger discrepancy for Cu/In2O3. We interpret the results in terms of surface electron and hole-doping of the semiconductor and with the presence of a significant density of electronic states within the band gap that is responsible for the reduction of the barrier height.

HL 21.4 Mon 15:00 Poster B

Investigations on simple copper vacancies and split vacancies in Cu_2O based on density functional theory — •Raphael Knecht and Christian Heiliger — 1. I. Physikalisches Institut, Justus Liebig University Giessen, Germany

We present investigations on simple copper vacancies V_{Cu} and split vacancies V_{Cu}^{split} in Cu_2O based on density functional theory. Both defects are simulated in a 2x2x2 supercell of Cu_2O. We determine the influence of these defects on structural and electronic properties using the LDA+U functional and compare them with properties of defect free Cu_2O. Since both vacancies come along with an electron hole state, we further investigate the localization of this defect state. In order to do so we calculate Born effective charges, magnetic moments and density-differences for both defect structures.

HL 21.5 Mon 15:00 Poster B

Ab initio Raman Spectra of $Zr_{1-x}Ce_xO_2$ and of Ceria with oxygen vacancies — •Michael Bachmann and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

Although the phase diagram of $Zr_{1-x}Ce_xO_2$ has been investigated a while ago with Raman spectroscopy [1] it is still not fully understood. We perform DFT supercell calculations of $Zr_{1-x}Ce_xO_2$ for different phases. For each concentration we average over a number of supercells with different configurations. We present the concentration dependence of the lattice constants, the band gaps, and the Raman spectra. All quantities are obtained by thermodynamic and statistic weighting. Furthermore, we use a supercell approach to calculate the Raman spectra of ceria with oxygen vacancies as a function of the oxygen vacancy concentration.

[1] Yashima et al. J.Am. Ceram. Soc. 77 1067 (1994)

HL 21.6 Mon 15:00 Poster B

Ab-initio Electronic Structure of Different Tin Oxides — •Bianca Eifert and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

Tin forms two stable oxides, a monoxide and a dioxide, which are already used in application fields ranging from electrochemistry to optoelectronics. Tin dioxide (SnO_2) is a wide-bandgap n-type semiconductor, while tin monoxide (SnO) is usually regarded as a semimetal or a small-bandgap p-type semiconductor. At higher temperatures, SnO disproportionates into Sn and SnO_2, and oxides of other stoichiome-

tries are sometimes observed in experiments during this reaction. This variety of oxide phases with very different electronic properties makes the tin/oxygen system an interesting candidate for electronic components such as p/n junctions, which could be constructed from just two types of atoms. The present work contributes to the theoretical understanding of different tin oxides phases, their stability, and their electronic and optical properties by performing DFT calculations of the structural properties, bandstructures, and Raman spectra of these phases.

HL 21.7 Mon 15:00 Poster B

Ab initio study on structural and optical properties of copper oxide compounds — •Markus Heinemann, Marcel Giar, Bianca Eifert, and Christian Heiliger — I. Physikalisches Institut, Justus-Liebig-Universität, Gießen, Germany

Due to its promising electronic properties, nontoxicity, and vast abundance the p-type semiconductor copper oxide and its related compounds are of broad research interest for various applications ranging from optoelectronics to solar cell design [1]. In this work we use density functional theory (DFT) calculations to investigate structural, electronic, and optical properties of the copper oxide compounds Cu2O, CuO, and Cu4O3. We show that numerical methods beyond the local density approximation are necessary to correctly describe the electronic structure of these compounds and compare different approaches to the exchange- correlation functional. For Cu2O a hybrid functional approach yields best results while for CuO and Cu4O3 the LDA+U method succeeds [2]. We further discuss the performance of self-consistent quasiparticle calculations within the framework of the GW approximation for all three compounds. Optical properties are evaluated by assessing the dielectric function from which optical absorption spectra are derived. We compare these quantities to recent experimental data [1]. As the conduction mechanism for CuO is still under discussion we investigate the influence of the formation of various point defects in this material using a supercell approach.

[1] Meyer et al., pss(b) 249, 1487 (2012)
[2] Heinemann et al., Phys. Rev. B 87, 115111 (2013)

HL 21.8 Mon 15:00 Poster B

NIR-VUV dielectric function of $(Al,In,Ga)_2O_3$ thin films — •Rüdiger Schmidt-Grund, Chris Sturm, Christian Kranert, Hannes Krauss, Holger von Wenckstern, Michael Bonholzer, Jörg Lenzner, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Leipzig, Germany

We present the dielectric function spectra of $(Al,In,Ga)_2O_3$ thin films in a wide composition range obtained by means of spectroscopic ellipsometry in the spectral range from near NIR to vacuum UV and temperatures between 10K and room temperature [1]. By model analysis of the experimental data using a parametric model dielectric function approach we derive the refractive index dispersion in the visible spectral range and the energies of electronic transitions as a function of the composition and temperature. For In incorporation in β-Ga_2O_3 we found that the electronic structure for x<0.3 is dominantly that of monoclinic β-Ga_2O_3 and for x>0.7 that of the cubic bcc-In_2O_3 [2]. In the intermediate composition range, the DF reveals strong signatures of rh-In_2O_3 or rh-In_2O_3II. For increasing In and Al concentration we found a redshift respective a strong blueshift of the transition energies. The thin films with compositional spread were deposited on 2" a-plane sapphire and MgO substrates by means of pulsed laser deposition using segmented targets (consisting of half-segments of binary aluminum oxide respective indium oxide and binary gallium oxide) [3].

[1] R. Schmidt-Grund et al., APL **105**, 111906 (2014); JAP **116**, 053510 (2014). [2] C. Kranert et al., JAP **116**, 013505 (2014). [3] H. von Wenckstern et al., Cryst. Eng. Comm. **15**, 10020 (2013).

HL 21.9 Mon 15:00 Poster B

Bipolar Oxide heterodiodes comprising In_2O_3 thin films — •Steffen Lanzinger, Daniel Splith, Peter Schlupp, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Leipzig, Germany

Recently, the interest on In_2O_3 extends beyond application as transparent electrode and properties of semiconducting In_2O_3 thin films were reported. Different measurements revealed that In_2O_3 tends to form a surface electron accumulation layer, which makes the formation of rectifying contacts non-trivial. Recently, by using reactively sputtered Schottky contacts, highest rectification of about 3 orders of magnitude at room temperature was achieved, which is not sufficient for most applications (e.g. field-effect transistors). Therefore, the exploitation of pn-heterodiodes presents an additional, interesting approach towards higher rectification.

We investigated nominally undoped In_2O_3 thin films with a compensated In_2O_3:Mg surface layer with different thickness (0 nm, about 10 nm and about 100 nm). The thin films were deposited by pulsed-laser deposition at 600°C and 0.016 mbar. On top, NiO and $ZnCo_2O_4$ were deposited at room temperature, forming pn-heterojunction diodes with the In_2O_3. Those diodes were investigated by current-voltage measurements (IV) at room temperature. Best rectifications of p-NiO/n-In_2O_3 and p-$ZnCo_2O_4$/n-In_2O_3 are with 4 orders of magnitude better than that of best Schottky barrier diodes on In_2O_3 thin films grown by molecular beam epitaxy. Further, temperature-dependent IV and the breakdown behavior of the diodes will be discussed.

HL 21.10 Mon 15:00 Poster B

Lattice dynamics of β-Ga_2O_3 mono-crystals — •Marcel Weinhold, Thomas Sander, and Peter Jens Klar — Justus-Liebig-University Giessen, Institute of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Giessen

Ga_2O_3 has attracted great interest, due to its potential use in UV transparent electrodes, photodetectors, and field-effect transistors (FETs). On top of that, Ga_2O_3 offers the opportunity to grow single crystalline substrates. In spite of that, the knowledge about its lattice vibration modes is still limited. We performed Raman studies of monoclinic Ga_2O_3 single crystals and performed a corresponding group theoretical analysis of the Raman activity of the vibrational modes. These results are compared with the Raman spectra obtained at room temperature of $(\bar{2}01)$ and (010) oriented β-Ga_2O_3 grown by the edge-defined film-fed growth method (EFG). To identify the symmetry characteristics of the phonons, the samples were rotated about the axis defined by the excitation laser light coming in at normal incidence. Furthermore, the dependence of the Raman spectra on excitation wavelength in the UV to IR range will be presented.

HL 21.11 Mon 15:00 Poster B

Stark-Effect Measurements on Giant Rydberg Excitons in Cuprous Oxide — •Johannes Thewes[1], Julian Heckötter[1], Marc Assmann[1], Tomasz Kazimierczuk[2], Dietmar Fröhlich[1], and Manfred Bayer[1] — [1]Institut für Physik, Technische Universität Dortmund, D-44221 Dortmund, Germany — [2]Faculty of Physics, University of Warsaw, Poland

We report on Stark-effect measurements of Giant Rydberg excitons[3] in Cu_2O with quantum numbers up to $n = 25$. These excitons have extensions up to 2 μm. As known from hydrogen, the dipole matrix elements for $\Delta n = 0$ and $\Delta l = \pm 1$ grow quadratically with n. In Cu_2O, P-excitons are dipole-allowed. Due to the electric field-induced coupling of P-excitons to S- and D-excitons we observe P/S and P/D resonances in fields as low as $10\,V cm^{-1}$. Measurements are done on a 30 μm sample with a single frequency dye laser ($\Delta E = 1$ neV) at temperatures down to 1.2 K. Contrary to hydrogen, the Stark-effect measurements can be done in a longitudinal configuration ($\mathbf{K}_{\mathrm{laser}} || \mathbf{E}$).

— [3] T. Kazimierczuk et al. Nature 514, 343 (2014)

HL 21.12 Mon 15:00 Poster B

Electrical conductivity and photoconductivity of single-crystalline In_2O_3 thin films — •Julius Rombach and Oliver Bierwagen — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany

Although the gas sensing effect of conductometric metal oxide gas sensors is known to be surface-related, contributions from the bulk and the substrate interface are unclear. Due to the presence of a surface electron accumulation layer (SEAL), electrical conductivity of In_2O_3 thin films usually consists of contributions from the bulk material, the SEAL and the substrate interface. This study aims to disentangle these sources of conductivity using MBE grown single-crystalline In_2O_3 films. By thickness variation and Mg-doping with a subsequent annealing step in Oxygen, the bulk and interface contribution to the overall conductivity was altered. The SEAL contribution was influenced by oxygen plasma treatment of the surface, which removes the SEAL, and by UV illumination during conductivity measurements. In_2O_3 shows photoconductivity in the UV range with photon energies below the fundamental absorption edge, which is believed to be a photoreduction of oxygen adatoms on the In_2O_3 surface. Hence the contribution of the SEAL to overall conductivity can be increased by UV illumination. This can help to get a better understanding of the sensing mechanism of In_2O_3-based gas sensors and to achieve higher sensitivities by specifically influencing the particular contributions to

electrical conductivity.

HL 21.13 Mon 15:00 Poster B

Influence of the preparation of thin indium oxide films on the electronic surface properties — •Theresa Berthold[1], Jochen Räthel[1], Stefan Krischok[1], Marcel Himmerlich[1], Chunyu Wang[2], Volker Cimalla[2], Julius Rombach[3], Marko Perestjuk[3], and Oliver Bierwagen[3] — [1]Institut für Physik and Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, Germany — [2]Fraunhofer-Institut für Angewandte Festkörperphysik, Freiburg, Germany — [3]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

The electronic structure of In_2O_3 can be modified by an oxygen plasma surface treatment, to establish a surface depletion layer [1]. We analyze the influence of different preparation methods, like annealing in vacuum and oxygen environment, oxygen plasma modification as well as indium-flash-off, on In_2O_3 surface composition and electronic properties, such as band bending, electron accumulation and work function. Thin indium oxide films grown by MBE or MOCVD are characterized using PES and the morphology is analyzed by AFM. In the initial state, an electron accumulation layer as well as hydrocarbon and hydroxide adsorbates are observed at the surface. Thermal treatments result in adsorbate removal, while the formation of surface defects can be prevented by annealing in oxygen environment. Oxygen plasma processes as well as other oxidative surface treatments induce a change in the surface composition. In all cases, the electronic surface properties are influenced and changes in band bending and work function are observed. [1] O. Bierwagen et al., Appl. Phys. Lett. 98, 172101 (2011)

HL 21.14 Mon 15:00 Poster B

Conducting mechanism in epitaxial p-type Transparent Conducting Oxide Cr_2O_3:Mg — •Leo Farrell, Karsten Fleischer, David Caffrey, Darragh Mullarkey, Emma Norton, Elisabetta Arca, and Igor Shvets — CRANN, School of Physics, Trinity College Dublin, College Green, Dublin 2, Ireland

p-type transparent conducting oxides (TCOs) are an important material class for many optoelectronic devices. However, p-type TCOs have always exhibited poorer performances than their n-type counterparts. As a result, new p-type materials remain an important area of research. Cr_2O_3 doped with Mg is a candidate p-type TCO material. In this study we improved on the electrical and optical properties of Cr_2O_3:Mg. The samples were epitaxially grown by MBE where the stoichiometry was finely tuned in order to investigate the effect on the structural, electrical and optical properties. The influence of the Mg dopants and the oxygen partial pressure were also investigated by Seebeck and resistivity measurements. Carrier transport properties are examined. The role of polaronic reduction in hole mobility for this material is also discussed. Investigating the fundamental properties in epitaxial material will allow us to add to our understanding of the role of defects in p-type TCOs, helping to improve material grown by other more industrial relevant methods.

HL 21.15 Mon 15:00 Poster B

LEEM and XPEEM studies of MgO films on Ag(100) — •Sabrina Pechmann[1], Gina Peschel[2], Hagen W Klemm[2], Thomas Schmidt[2], and Rainer H Fink[1] — [1]Physical Chemistry, Friedrich-Alexander-University Erlangen-Nuremberg, Germany — [2]Chemical Physics, Fritz Haber Institute of the Max Planck Society Berlin, Germany

Metal oxide thin films on metal supports are important for various technological applications like catalysis or the fabrication of electronic devices. Therefore, it is necessary to understand the electronic properties of the interfaces, as well as microscopic structure and morphology of the films. Especially MgO on Ag(100) serves as an attractive model system as the lattice mismatch between both bulk structures is only 3.1%, allowing epitaxial growth with just a small number of grain boundaries. Nevertheless, defects like non-stoichiometries, or vacancies influence the surface properties of the oxide layer to a large extend. Exposure to X-rays and even low-energy electrons (up to 200 eV), already leads to the formation of so-called color centers. We investigated the growth and structural properties of epitaxial MgO thin films on Ag(100) by LEEM and XPEEM as both techniques provide insight into structural and chemical sensitivity and directly visualize the influence of surface defects, e.g., step bunches. We could observe a strong influence of low-energy electrons and X-rays on the metal oxide layer, like the reversible formation of long-range ordered oxygen vacancies and even quadrangular structures. First results concerning those effects will be presented.

HL 21.16 Mon 15:00 Poster B

Impact of soft x-rays on the field effect in $SrTiO_3/LaAlO_3$ heterostructures — •Martin Zwiebler[1], Enrico Schierle[2], Emiliano Di Gennaro[3], Fabio Miletto Granozio[3], and Jochen Geck[1,4] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Germany — [3]CNR-SPIN and Dipartimento di Fisica Università "Federico II" di Napoli, Italy — [4]Dresden University of Technology, Germany

The two-dimensional electron gas (2DEG), which can be realized at the $SrTiO_3/LaAlO_3$ interface, currently receives a lot of attention. Although both constituent materials are bulk insulators, the 2DEG at the interface exhibits a high carrier mobility and can even become superconducting. Numerous spectroscopic studies aimed at clarifying the electronic properties of the $SrTiO_3/LaAlO_3$ interface. However, the connection of those results to macroscopic quantities often remained controversial. In order to directly relate spectroscopic measurements to transport properties, we combined both techniques into a single experiment. More specifically, we measured the electrical resistivity as well as Ti $L_{2,3}$ x-ray absorption and resonant x-ray reflectivity of $SrTiO_3/LaAlO_3$ field effect devices, while monitoring the electrical resistivity. In this contribution we present first results of these efforts that reveal a strong impact of the soft x-ray radiation on the 2DEG. The implications for previously published studies are also discussed.

HL 21.17 Mon 15:00 Poster B

The Electronic Structure of amorphuos SnOx thin films and SnO2 single crystals — •J. Haeberle[1], D. Gaspar[2], P. Barquinha[2], L. Pereira[2], R. Martins[2], E. Fortunato[2], S. Machulik[3], C. Janowitz[3], R. Manzke[3], and D. Schmeisser[1] — [1]Angewandte Physik/Sensorik, Brandenburgische TU Cottbus,K.-Wachsmann-Allee 17, 03046 Cottbus, Germany — [2]Department of Materials Science Faculty of Sciences and Technology,New University of Lisbon and CEMOP-UNINOVA, Campus de Caparica,2829-516 Caparica, Portugal — [3]AG Elektronische Eigenschaften und Supraleitung, Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

We compare the electronic properties of amorphous p-type SnOx thin film grown by rf magnetron sputtering with those of n-type SnO2 single crystals grown by cvt. We use resPES to study the electronic band structure. We measure the core levels, the VB PES data, partial Integrated Yield (pIY) and the XAS absorption data. From the resPES data recorded at the O1s and the Sn3d edges we derive the VB pDOS and the CB pDOS . The differences are most pronounced in the position of the VBM as for the a-SnOx films there appears a band closer to the Fermi energy. In addition for the SnOx we find in the XAS and pIY data a significant peak that appears right at the Fermi energy. This peak is absent in the single crystalline data. We attribute this to a change in the configuration of the Sn4d states to form a 4d8 configuration instead of 4d9 and 4d10 configurations which are identified in the single crystalline data.

HL 21.18 Mon 15:00 Poster B

Preparation and Characterization of Nitrogen Doped ZnMgO:Al-Thin Films — •Hannes Giese, Philipp Schurig, Limei Chen, Thomas Sander, Angelika Polity, Detlev M. Hofmann, and Bruno K. Meyer — I. Physikalisches Institut, Justus-Liebig-Universität, Giessen, Deutschland

ZnO has a tunable band gap with good abilities for ultraviolet optoelectronic devices. The electrical properties, especially the band gap, of ZnO can be increased by adding MgO and doping with aluminum, for example. In order to yield homojunctions of ZnO, it is necessary to produce a stable and effective p-type doping of this system. A promising way to obtain this is to dope with nitrogen because of its atomic radius and its electrical properties being comparable with oxygen. In this work, thin films were produced by RF-sputter deposition with a ceramic target of Zn(0,72)Mg(0,25)O:Al(0,03). Nitrogen was used with argon as the sputtering gas at different growth temperatures (from room temperature to 700°C) and at constant temperatures with a different nitrogen flows (from 0,02-0,2 sccm). The films were characterized by UV/Vis spectroscopy, XRD and Hall-effect measurements. The results showed a dependence of the optical, structural and electrical properties on the varied parameters. This is accompanied with different colors of the thin films and different crystal structures. Zinc nitride formation was studied as a function of nitrogen partial

pressure and growth temperature. It is assumed that only at very low nitrogen flows (0,02 sccm) the doping was successful, but the results indicate that p-type doping was not achieved.

HL 21.19 Mon 15:00 Poster B

The role of oxygen ambient in the Persistent Photoconductivity of ZnO nanowires — •Florian Huber, Manfred Madel, Martin Dickel, Bruno Amann, and Klaus Thonke — Institute of Quantum Matter / Semiconductor Physics Group, Ulm University

The origin of the Persistent Photoconductivity (PPC) in zinc oxide is a widely discussed topic. The reason for the PPC is frequently attributed to intrinsic defects, especially to oxygen vacancies which are reported to act as deep traps [1]. Besides these defects, the adsorption and desorption of oxygen on the surface of the material influences the PPC strongly.

We investigated in detail especially the kinetics of the slow photo-induced conductivity processes with respect to their photon energy, temperature, oxygen ambient and illumination time dependence. Energy barriers for the decay process after illumination are determined, and the experimental results are discussed in the frame of possible models.

[1] A. Janotti and C.G. Van de Walle, Applied Physics Letters **12**, 122102 (2005)

HL 21.20 Mon 15:00 Poster B

Impact of strain on electronic defects in (Mg,Zn)O thin films — •Florian Schmidt, Laurenz Thyen, Stefan Müller, Holger von Wenckstern, Gabriele Benndorf, Rainer Pickenhain, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Abteilung Halbleiterphysik, Linnéstraße 5, 04103 Leipzig

Ternary MgZnO is an excellent material system for the fabrication of quantum well heterostructures and thus for potential application in exciton-related photonic devices.

We have investigated the impact of strain on the incorporation and the properties of extended and point defects in (Mg,Zn)O thin films by means of photoluminescence, X-ray diffraction, deep-level transient spectroscopy (DLTS) and deep-level optical spectroscopy. The recombination line Y2, previously detected in ZnO thin films grown on an Al-doped ZnO buffer layer and attributed to tensile strain [1], was exclusively found in (Mg,Zn)O samples being under tensile strain and is absent in relaxed or compressively strained thin films. Furthermore a structural defect E3' can be detected via DLTS measurements and is only incorporated in tensile strained samples. Finally it is shown that the omnipresent deep-level E3 in ZnO can only be optically recharged in relaxed ZnO samples [2].

[1] M. Brandt *et al.*, Phys. Rev. B **81**, 073306 (2010).
[2] F. Schmidt *et al.*, J. Appl. Phys. **116**, 103703 (2014).

HL 21.21 Mon 15:00 Poster B

Non-linear deformation potential in highly strained ZnO microwires — •Sherzod Khujanov, Chris Sturm, Marcel Wille, Michael Lorenz und Marius Grundmann — Institut für Experimentelle Physik II, Universität Leipzig, Linnéstr. 5, 04103 Leipzig, Germany

Zinc oxid nano- and microwires are promising building blocks for sensor and generator applications [1]. In this work we present the investigation of the deformation potential of ZnO microwires and the ability of engineering the band gap energy via mechanical stress. The microwires (MW) were prepared by carbothermal evaporation, bent and fixed on Si substrates. Thereby we induced a uniaxial strain up to ±3.5%. The emission properties near the band edge were investigated by using cathodoluminescence. In the unstrained case the MW exhibit a sharp emission from donor bound excitons whereas in the case of an applied strain we observed a broadening and a red (blue) shift of the near band emission for tensile (compressive) strain. For strain values up to ±1.5% we observe a linear dependence between strain and observed energy shift as already reported in the literature [2]. However, for larger strain we observe that this linear relation does not hold anymore and non-linear effects have to be considered. This is supported by the fact that the magnitude of the energy shift is significantly larger for compressive strain compared to the tensile strain.

[1] Z.L. Wang MRS BULLETIN 37, 814 (2012).
[2] C.P. Dietrich et al. Appl. Phys. Lett. 98, 031105 (2011).

HL 21.22 Mon 15:00 Poster B

Effects of functionalization of ZnO nanowire Schottky diodes on their current-voltage characteristics — •Emily T. Tansey[1], Alejandra Castro-Carranza[1], Stephanie Bley[1], Olesea Volciuc[1], Tobias Voss[2], and Jürgen Gutowski[1] — [1]Institute of Solid State Physics, Universität Bremen, Bremen, Germany — [2]Institute of Semiconductor Technology, TU Braunschweig University of Technology, Braunschweig, Germany

Zinc oxide nanowires (ZnO NWs) have shown to be promising as nanoscale building blocks for optoelectronic applications due to their unique semiconductor, optical, piezoelectric, and chemical characteristics. An interesting approach to tailor the optoelectronic properties of ZnO NWs is to form hybrid junctions with other materials, e.g. polymers. It has been proposed that surface defects play a role in the tailor of the ZnO NWs properties. To gain further insight into this physical phenomenon, we explore the current-voltage characteristics of Schottky diodes formed by wet chemical-growth ZnO NW arrays and the p-type polymer Poly(3-hexylthiophene-2,5-diyl). Our results show that the thickness of the P3HT impacts the current transport mechanisms occurring at the junction.

HL 21.23 Mon 15:00 Poster B

ZnO nanowire Schottky diodes on ITO and FTO substrates: study of the junction by electrical characterization — Alejandra Castro-Carranza[1], •Jairo Cesar Nolasco[2], Emily T. Tansey[1], Stephanie Bley[1], Olesea Volciuc[1], Tobias Voss[3], and Jürgen Gutowski[1] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]Energy and Semiconductor Research Laboratory, Carl von Ossietzky University Oldenburg, Germany — [3]Institute of Semiconductor Technology, TU Braunschweig University of Technology, Germany

Zinc oxide nanowires (ZnO NW) have been used in flexible LEDs and solar cells. As important topic for these applications is the study of the junction formed between ZnO NWs and transparent conductive oxides, e.g. fluorine doped tin oxide (FTO) and indium tin oxide (ITO), which are commonly used as front contacts. Their work functions define the nature of the junction with ZnO NWs, i.e. ohmic contacts or Schottky diodes. However, surface defect states on the ZnO NWs can influence such a junction. In the present work we explore the electrical characteristics of junctions based on wet-chemically grown vertical ZnO NW arrays on FTO and ITO by means of their current-voltage characteristics and impedance spectroscopy. We observed that a significant barrier height is formed at the junctions, corresponding to a Schottky diode, and the obtained ideality factors describe that the conduction mechanism occurring at the junctions is affected by tunneling through traps.

HL 21.24 Mon 15:00 Poster B

Simultaneous adsorption of water and molecular oxygen on non-polar ZnO($10\bar{1}0$) surface: a microscopic understanding — Delsuz Hassani, Saied Masoumi, •Ebrahim Nadimi, and Faramarz Hossein-Babaei — Faculty of Electrical Engineering, K N Toosi University of Technology, Tehran, Iran

The surface of different metallic oxides such as ZnO, SnO_2 and TiO_2 are widely used in gas sensing applications. Atomic level modeling are widely employed to explain the sensing mechanism at a microscopic level. The present work is an attempt to apply density functional theory to investigate the adsorption of water and oxygen molecules on non-polar ZnO($10\bar{1}0$) surface. The focus is on the simultaneous adsorption of two molecules which could shed more light on the oxygen sensing at different humidity levels.

HL 21.25 Mon 15:00 Poster B

Field-effect transistors based on printed amorphous zinc-tin-oxide — •Benedikt Sykora and Heinz von Seggern — Technische Universität Darmstadt Fachbereich Materialwissenschaften Fachgebiet Elektronische Materialeigenschaften Alarich-Weiss-Straße 2 64287 Darmstadt Germany Building L2|01 - Room 156 Tel.: +49 (0) 6151 16-6331 Fax: +49 (0) 6151 16-6305

Since the last two decades metal-oxides like ZnO are widely studied as semiconductors for transistor applications. The benefits of these materials are, that they can be processed out of solution, they are transparent and cost efficient. This contribution presents field-effect transistors based on a printed amorphous zinc-tin-oxide (ZTO) semiconductor. Thin films are analysed by XRD, TEM, SEM and absorption measurements. The used ethanol based precursor solution is cheap and easy to process, non-toxic and long term stable. The saturation mobility increases from 0.05 cm^2/Vs, if a single semiconducting layer

is applied, to a value of 7.7 cm^2/Vs for a transistor composed of 8 layers. To the best of our knowledge this is the highest reported value for a printed ZTO transistor. The reason for this huge increase in electron mobility is presumable d an improved film coverage and increased density which could be confirmed by AFM and that is known from other oxide semiconductors (1). The devices also show large output currents, high on/off ratios and low subthreshold voltages.

(1) Walker et al. ACS Appl. Mater. Interfaces 4, 6835-6841 (2012)

HL 21.26 Mon 15:00 Poster B

Determination of the Mn-spin temperature of photo-excited n-doped $Zn_{1-x}Mn_xSe$ by magneto-luminescence and spin-flip Raman spectroscopy — •Alexander Gerhard Knapp[1], Michael Hetterich[2], and Jean Geurts[1] — [1]Universität Würzburg, Experimentelle Physik 3, Würzburg, Germany — [2]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

The wide-gap semiconductor $Zn_{1-x}Mn_xSe$, as a II-VI-based diluted magnetic semiconductor, offers the opportunity for an independent tuning of the magnetic and the electronic properties by variation of either the Mn content or the dopant concentration. The strong s,p-d exchange coupling gives rise to a giant Zeeman splitting in magneto-photoluminescence (PL). Furthermore, magneto-Raman spectroscopy (RS) shows local spin flip excitations on Mn atoms, as well as electronic spin flip excitations of donator atoms in n-type material. The spectral position of the latter reflects the spin-selective energy splitting of the conduction band due to the s-d exchange interaction. We performed polarization-selective magneto-PL and and magneto-RS on $Zn_{1-x}Mn_xSe$ (x = .05 to .06) with various n-doping levels up to 10^{18} cm^{-3}, i.e. up to the range of the Mott density, at T = 1.6 K in Voigt configuration in B-fields up to 7 T. For near-resonant optical excitation in the range of the fundamental energy gap E_0, we investigated the influence of the variation of excitation power on the Mn-spin temperature. For this purpose, the Brillouin-function fit parameters of the PL- and RS-peak positions as well as the Stokes-to-Anti-Stokes intensity ratio of the local Mn spin flip were evaluated.

HL 21.27 Mon 15:00 Poster B

Photon-assisted field emission from a Si tip with applied AC field (10 Hz-10 MHz) — Anna Zaporozhchenko[1], Sergey Chernov[2], Larisa Odnodvorets[1], Boris Stetsenko[3], •Sergej Nepijko[2], Hans-Joachim Elmers[2], and Gerd Schönhense[2] — [1]Sumy State University, Rimsky-Korsakov Str. 2, 40007 Sumy, Ukraine — [2]Institute of Physics, University Mainz, Staudingerweg 7, 55128 Mainz, Germany — [3]Institute of Physics, National Academy of Sciences of Ukraine, pr. Nauki 46, 03028 Kiev, Ukraine

We investigated the field emission current from a p-type silicon tip with large resistivity of 4×10^3 Ω·cm for illumination with a photon energy of 1.3 eV (close to the optical gap) and tip-anode voltages of $(0.7\div5)\times10^3$ V. Variations of the emission current due to an additional AC component of 30-60 V with varying frequency in the range of 10 to 10^7 Hz were observed. We investigated the dependence of this phenomenon on the AC frequency, light intensity and temperature. The resonant-like frequency dependence of the emission current is attributed to a dielectric resonance in the semiconducting tip material. The tip behaves like a driven plasmonic resonator. The results represent an important step forward for the development of high frequency display systems based on electron field emission.

HL 21.28 Mon 15:00 Poster B

Lattice dynamics of defect systems: The test case of Si — •Marcel Giar, Andreas Rühl, and Christian Heiliger — I. Physikalisches Institut, Justus-Liebig-University, D-35392 Giessen, Germany

Our research aims at calculating the vibrational properties, in particular Raman spectra, of defect systems. In order to realize sufficiently small defect concentrations very large supercells have to be considered. As a direct first principles approach is computationally too expensive for very large systems (>1000 atoms) we resort to Molecular Dynamics (MD) simulations for calculating lattice dynamical properties of the defect systems. The required effective potentials for carrying out the MD simulations are still based on *ab initio* data, created in the scope of Force Matching. We test our approach by constructing the respective potential for Si to reproduce phonon spectra obtained from *ab initio* calculations. The dynamical matrix is obtained within the so called small displacement method, which relies on displacing single atoms and calculating the resulting forces.

HL 21.29 Mon 15:00 Poster B

Transport properties of individual photoluminescent silicon quantum dot studied by scanning tunneling microscopy — •Tuhin Shuvra Basu, Simon Diesch, and Elke Scheer — Fachbereich Physik, Universität Konstanz, Universitätsstraße 10, 78457 Konstanz, Germany.

Silicon quantum dot (Si QD) exhibit room temperature photoluminescence (PL) property due to size induced quantum confinement effects in an ensemble measurement. The ensemble measurement of the PL provides average estimation of their excitonic bandgap and is dependent on size and surface protection [1]. Thus it is important to study the band-structure and exciton dynamics of Si QD on a single particle level. It is expected that the charging energy of Si QD will be appreciably high and will exhibit pronounced single-electron tunneling (SET) effects [2]. By studying tunneling spectroscopy, the conduction and valence band states and their degeneracy can be separately probed. In this work, the electronic transport and bandgap modification of Si QD on a single particle level has been studied by scanning tunneling spectroscopy (STS). The dI/dV curves exhibit features corresponding to the excitonic bandgap. Further the STS study of the individual Si QD by changing the size and the temperature (from 300 mK to 30 K) reveals bandgap fluctuations. We discuss our results in terms of correlations between the exciton dynamics, size, and temperature.

References:
[1]X. Cheng et al., Chem. Soc. Rev. 43, 2680 (2014).
[2]B. Weber et al., Nat. Nanotech. 9, 430 (2014).

HL 21.30 Mon 15:00 Poster B

Herstellung und Untersuchung von Bor-dotierten polykristallinen CVD-Diamantschichten — •Regina Berendakova, Nicolas Wöhrl und Volker Buck — Universität Duisburg-Essen und CENIDE, Forsthausweg 2, 47057 Duisburg

Bor-dotierte polykristalline Diamantschichten wurden mittels Mikrowellen-Plasma CVD aus einem Ar-CH_4-H_2 Plasma hergestellt. Die Dotierung der Schichten erfolgte durch Zugabe eines neuartigen flüssigen Bor-Precursors Tripropylboran $B(C_3H_7)_3$. Dieser Precursor wurde zuvor noch nicht für die Dotierung von Diamantschichten verwendet. Es konnte gezeigt werden, dass eine höhere Bor-Konzentration im Plasma auch zu einer höheren Dotierung der resultierenden Diamantschichten führt. Der spezifische elektrische Widerstand der Proben wurde mittels Vier-Punkt-Messung charakterisiert und liegt im Bereich von 10^{-4}-10^{-5} Ωm bei Raumtemperatur. Es wurde ein fast exponentieller Abfall des spezifischen Widerstandes der Proben mit steigendem Bor-Signal in den OES-Spektren des Plasmas festgestellt. Des Weiteren wurde der Einfluss des Bor-Precursors auf die Schichtmorphologie untersucht. In vorangegangenen Arbeiten ohne Bor-Dotierung wurden bei ähnlichen Prozessparametern ultra-nanokristalline Diamantschichten (UNCD) hergestellt. REM-Untersuchungen ergaben, dass alle dotierten Schichten eine deutlich erkennbare kolumnare Struktur aufweisen, was die Proben als mikrokristallinen Diamant (MCD) klassifizieren lässt. Es wurde also ein Übergang vom UNCD zum MCD Wachstum durch die Zugabe des Bor-Precursors ins Plasma beobachtet und charakterisiert.

HL 21.31 Mon 15:00 Poster B

Towards stabilization of the negatively charged nitrogen-vacancy center in diamond — •Samuel Müller[1], Jochen Scheuer[1], Boris Naydenov[1], Junichi Isoya[2], and Fedor Jelezko[1] — [1]Institut für Quantenoptik, Universität Ulm, Ulm, Germany — [2]Research Center for Knowledge Communities, University of Tsukuba, Tsukuba, Japan

The nitrogen-vacancy centers in diamond (NV) are very promising solid state single quantum systems with a wide application as qubits and ultra sensitive nano-scale field sensors. The NV is constantly changing its charged state from NV0 to NV-, whereas the latter is relevant for the applications. We propose a new method of stabilizing the NV- state via doping the diamond with an electron donor (phosphorus) and continuous irradiation with infrared light. We show that the NV- spin state can be measure using an orange laser light, which usually leads to photo-ionization in standard diamond crystals. We performed single shot nuclear magnetic resonance measurements in order to determine the degree of stability in the NV- state [1,2].

[1] Neumann, Philipp, et al. "Single-shot readout of a single nuclear spin." Science 329.5991 (2010): 542-544.

[2] Waldherr, G., et al. "Dark states of single nitrogen-vacancy centers in diamond unraveled by single shot NMR." Physical review letters

106.15 (2011): 157601.

HL 21.32 Mon 15:00 Poster B

Close to surface UHV-preparation of NV centers in diamond — •Stefan Borgsdorf[1], Lina Elber[1], Andreas Kaivers[1], Aniela Scheffzyk[1], Frederico Brandao[2], Dieter Suter[2], and Ulrich Köhler[1] — [1]Experimentalphysik IV, AG Oberflächen, Ruhr-Universität Bochum, Germany — [2]Experimentelle Physik IIIA, Technische Universität Dortmund, Germany

Color centers in diamond, especially NV-centers, are practical single photon emitters due to RT operation and are candidates for applications in quantum computing. NV-centers close to the surface allow electrical addressing and can be used for magnetic sensors. Here we present a setup for low energy implantation of NV centers near to the surface using UHV-conditions. We survey the influence of UHV-implantation and -annealing compared to the usual HV-heating. The usual etching processes with boiling tri-acid to remove graphitic components after the annealing process is unnecessary. In general, the all-UHV-process leads to a cleaner diamond surface and decreases the background intensity in optical characterizations of the samples.

HL 21.33 Mon 15:00 Poster B

Accelerated two dimensional NMR spectroscopy using matrix completion — •Jochen Scheuer[1], Alexander Stark[1], Matthias Kost[2], Boris Naydenov[1], Martin Plenio[2], and Fedor Jelezko[1] — [1]Institut für Quantenoptik, Albert-Einstein-Allee 11, Universität Ulm, Ulm, Germany — [2]Institut für Theoretische Physik, Albert-Einstein Allee 11, Universität Ulm, Ulm, Germany

2D nuclear magnetic resonance (NMR) spectroscopy is one of the major tools for analysing the chemical structure of molecules and proteins. Usually this technique requires quite long measurement times, which limits its application only to stable samples. Here we demonstrate a method which allows to keep the full signal to noise ratio by collecting only a fraction of the experimental data. Our method is based on two dimensional compressed sensing (matrix completion) and with using spectral value decomposition we can recover the full spectral information from randomly sampled data points[1,2]. We experimentally demonstrate the applicability of our technique by performing 2D electron spin echo modulation (ESSEM) experiments on single nitrogen vacancy (NV) centres in diamond. We show that the main peaks in the spectrum can be obtained with only up to 5 % of the total number of the data points. We believe that our results can find an application in all types of two dimensional spectroscopy, as long as the measured matrix has a low rank.

[1] M. Kost, et al., http://arxiv.org/abs/1407.6262, 2014.
[2] Cai, Jian-Feng, et al., SIAM Journal on Optimization 20.4 (2010): 1956-1982.

HL 22: Invited Talk Salvatore Savasta

Time: Tuesday 9:30–10:00 Location: ER 164

Invited Talk HL 22.1 Tue 9:30 ER 164

Ultrastrong coupling regime of excitons interacting with microcavity photons or localized surface plasmons — •Salvatore Savasta — Dipartimento di Fisica e di Scienze della Terra, Università di Messina, Italy

Exciton-polaritons are quasiparticles that arise from the strong coupling of photons and excitons in a semiconductor material [1]. One of the most intriguing extensions of such a light-matter interaction is the so called ultrastrong coupling (USC) regime [2-4]. It is achieved when the Rabi frequency reaches a considerable fraction of the emitter transition frequency. Here we discuss recent experiments in organic semiconductor microcavities where a Rabi splitting up to the 60% of the material band gap was achieved [5]. Strong light matter interaction is also achieved replacing conventional microcavities with metallic micro- or nano-structures supporting surface plasmons [6]. I also analyze the possibility to achieve the USC regime at nanoscale dimensions by exploting localized surface plasmons. I show, by accurate scattering calculations, that this regime can be reached in nanoshells constituted by a core of organic molecules surrounded by a silver or gold shell [7].

[1] Strong Light-Matter Coupling, Edited by: Auffèves et al., World Scientific, (2014). [2] G. Scalari et al., Science **335**, 1323 (2012). [3] Ridolfo et al. Phys. Rev. Lett. **109**, 193602 (2012). [4] Stassi et al. Phys. Rev. Lett. **110**, 243601 (2013). [5] Gambino et al. ACS Photonics **1**, 1042 (2014). [6] Vasa et al. Nat. Photon. **7**, 128 (2013). [7] Cacciola et al., ACS Nano **8**, 11483 (2014).

HL 23: Spintronics: Excitons and local spins (with MA/TT)

Time: Tuesday 9:30–11:30 Location: ER 270

HL 23.1 Tue 9:30 ER 270

Transport and manipulation of indirect exciton spins in GaAs double quantum well structures — Adriano Violante, Serkan Büyükköse, Klaus Biermann, and •Paulo Santos — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

Indirect excitons in double quantum well (DQW) structures are interesting particles for information storage due to the electrically controlled coupling to photons. Here, we report on the coherent control and transport of IX spins in GaAs DQWs using spatially and polarization resolved photoluminescence (PL). We show that optically IXs spins optically excited by a focused, circularly polarized light spot precess around the spin-orbit magnetic field while moving over distances exceeding 20 μm from the excitation spot. The spatial precession frequency depends on the spin transport direction and can be controlled by the bias applied across the DQW structure. From the dependence of the spin dynamics on transport direction, bias, and external magnetic fields we directly determined the Dresselhaus and Rashba electron spin splitting coefficients for the DQW structure. The long *IX* lifetimes, together with the negligible contribution of holes to the spin dynamics, are attributed to spatial separation of the electron and hole wave functions by the electric field, which reduces the electron-hole exchange interaction. If extended to the single exciton regime, the present results imply that IXs can be used as flying spin qubits for application in the quantum information processing.

HL 23.2 Tue 9:45 ER 270

Spin properties of the indirect exciton in indirect band-gap (In,Al)As/AlAs quantum dot ensembles — •Jörg Debus[1], Victor F. Sapega[2], Timur S. Shamirzaev[3], Daniel Dunker[1], Evgeny L. Ivchenko[2], Dmitri R. Yakovlev[1,2], and Manfred Bayer[1,2] — [1]Experimentelle Physik 2, TU Dortmund, Dortmund, Germany — [2]Ioffe Physical-Technical Institute, St. Petersburg, Russia — [3]Institute of Semiconductor Physics, Novosibirsk, Russia

The band structure of type-I (In,Al)As/AlAs quantum dots with band gap energy exceeding 1.63 eV is indirect in momentum space, leading to long-lived exciton states with potential applications in quantum information. Optical access to these excitons is provided by mixing of the Γ- and X-conduction band valleys. We report on spin properties of the indirect exciton studied by time-resolved photoluminescence (TRPL) and resonant spin-flip Raman scattering (SFRS) [1-3]. The SFRS characterizes the Γ-X-valley electron state mixing, provides access to the fine structure of the indirect exciton and enables the preparation of its spin states as well as the determination of the spin-flip mechanisms. From the TRPL we evaluate very long longitudinal spin relaxation times (200 μs at 4 T and 1.8 K) that are rather robust against temperature changes. The temporal evolution of the circular polarization degree of the photoluminescence moreover changes its sign in the μs-range thus hinting at dark and bright indirect excitons contributing by their different spin dynamics. [1] T. S. Shamirzaev et al., Phys. Rev. B **84**, 155318 (2011). [2] D. Dunker et al., Appl. Phys. Lett. **101**, 142108 (2012). [3] J. Debus et al., Phys. Rev. B **90**, 125431 (2014).

HL 23.3 Tue 10:00 ER 270

Coherent control and readout of single spins in silicon carbide — •Matthias Widmann[1], Sang-Yun Lee[1], Torsten Rendler[1], Nguyen Tien-Son[2], Helmut Fedder[1], Erik Janzén[2], and Jörg Wrachtrup[1] — [1]3.Physikalisches Institut, Universität Stuttgart — [2]Department of Physics, Chemistry and Biology, Linköping University

Single spin manipulation is one of the main subjects in research not only for quantum information processing (QIP) but also for quantum metrology. Having isolated spins in solids has advantages of stability and fabrication. Deep level defects in diamond and impurity donors in silicon have been considered as promising candidates and several key steps towards QIP have been achieved. However, there exist disadvantages which have hindered their successful integration into modern electronic devices; cryogenic temperature mandatory for readout of spins in silicon, and difficulty in electrical initialization and readout in diamond. These motivate to investigate other host materials such as silicon carbide (SiC). SiC combines the advantages of silicon and diamond, because electrical detection and optical access of spin ensembles at room temperature (RT) is possible, and it also benefits from modern fabrication techniques. Addressing individual spin states have not been shown yet, however, is highly demanded to set up a base for scalable atomic-scale quantum technologies. By presenting coherent control and readout of single spins in SiC at RT we prove that SiC is a promising platform for the scalable spintronic devices [1]. [1] M. Widmann et al., Coherent control of single spins in silicon carbide at room temperature, to be published in Nature Materials.

HL 23.4 Tue 10:15 ER 270

Nuclear magetic resonance on a single quantum dot — •Gunter Wüst[1], Mathieu Munsch[1], Andreas Kuhlmann[1], Martino Poggio[1], Arne Ludwig[2], Andreas Wieck[2], Dirk Reuter[3], and Richard J Warburton[1] — [1]University of Basel, Switzerland — [2]Ruhr-Universität Bochum, Germany — [3]Universität Paderborn, Germany

The spin coherence of an electron trapped to a GaAs or InGaAs quantum dot is limited by noise in the nuclear spins of the host material [1]. Understanding and controlling the nuclear spins is therefore important for quantum applications. We report here nuclear magnetic resonance (NMR) experiments on the 100,000 nuclear spins that have a contact hyperfine interaction with a quantum dot electron spin [2]. The main technique is to sweep the frequency of an in-plane magnetic field. In this way, all nuclear spins are addressed despite the presence of four main isotopes with different gyromagnetic ratios. The nuclear spins are polarized and read-out via resonant spectroscopy allowing us to reach a sensitivity to about 1,000 nuclear spins. We evidence a plateau in the NMR sweep rate dependence associated to the existence of quadrupole interactions. Detailed analysis allows the quadrupole distributions for each isotope to be determined, along with an effective nuclear spin temperature following polarization (8 mK) and an In concentration (20%). Ongoing experiments determined in addition the Hahn echo coherence times (1 ms) and their dependence on quantum dot charge.

[1] R. J. Warburton et al, Nature Materials 12, 483-493 (2013) [2] M. Munsch, Nature Nanotechnology 9, 671-675 (2014)

HL 23.5 Tue 10:30 ER 270

Distinct Nuclear Spin Signatures in the Spin Noise of Donor Bound Electrons — •Fabian Berski[1], Pavel Sterin[1], Jens Hübner[1], Andreas Wieck[2], and Michael Oestreich[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany — [2]Ruhr-Universität Bochum, Angewandte Festkörperphysik, Universitätsstr. 150, D-44780 Bochum, Germany

The hyperfine interaction acts as a main source of decoherence for localized electron spins in III-V semiconductor material systems and is thus a challenge for quantum information processing [1]. However, this interaction can also serve as a subtle probe of nuclear dynamics, which manifests itself in the spin dynamics of electrons.

Here, we study an ensemble of non-interacting donor bound electrons (D^0X) in a strain-free, high purity Gallium Arsenide host matrix, and find intriguing features of the nuclear spin dynamics in the electronic spin noise. The ideal tool to study such an interplay is spin noise spectroscopy, since it allows to control the dissipated amount of energy in the system and is a potential quantum non-demolition measurement [2]. However, by selecting the detuning between the D^0X transition and the energy of the used laser light, we find strong evidence for a significant nuclear polarization, even at low laser power, linearly polarized light and vanishingly small transversal magnetic fields.

[1] Chekhovich, et al., Nature Mat. **12**, 6 (2013).
[2] Hübner, et al., Phys Status Solidi B **251**, 1824 (2014).

HL 23.6 Tue 10:45 ER 270

Spin Dynamic of Electrons and Holes in Single Quantum Dots — •Ramin Dahbashi[1], Julia Wiegand[1], Jens Hübner[1], Klaus Pierz[2], Arne Ludwig[3], Andreas Wieck[3], and Michael Oestreich[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, Abteilung Nanostrukturen, Appelstr. 2, D-30167 Hannover, Germany — [2]Physikalisch Technische Bundesanstalt, Bundesallee 100, D-38116 Braunschweig, Germany — [3]Ruhr-Universität Bochum, Angewandte Festkörperphysik, Universitätsstr. 150, D-44801 Bochum, Germany

We present new insights into single quantum dot (QD) spin noise spectroscopy (SNS) [1]. We have performed world's first measurements of the single heavy hole spin dynamic in an individual (InGa)As QD by SNS [2]. These measurements reveal (a) very long T_1 hole spin lifetimes of up to 180 μs even in the low magnetic field range of up to 30 mT as well as (b) charge fluctuations in the QD surrounding. In order to suppress the parasitic influence of charge fluctuations, we move to QDs embedded in a Schottky diode structure which yields three main advantages: (i) the charge state of the QD, i.e., electron or hole, can be changed facilitating different coupling strength to the nuclear spin bath, (ii) the sharp single QD resonance can be tuned via the quantum confined Stark shift, and (iii) charge fluctuations are strongly reduced.

[1] J. Hübner, F. Berski, R. Dahbashi, and M. Oestreich, physica status solidi (b) **251**, 1824 (2014).
[2] R. Dahbashi, J. Hübner, F. Berski, K. Pierz, and M. Oestreich, Phys. Rev. Lett **112**, 156601 (2014).

HL 23.7 Tue 11:00 ER 270

Induced nuclear spin polarization in ZnSe:F epilayers — •Johan Erik Kirstein[1], Fabian Heisterkamp[1], Evgeny A. Zhukov[1], Alex Greilich[1], Dmitri R. Yakovlev[1,2], Irina A. Yugova[1,3], Vladimir L. Korenev[2], Alexander Pawlis[4], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Ioffe Physical-Technical Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia — [3]Physical Faculty of St. Petersburg State University, 198504 St. Petersburg, Russia — [4]Department Physik, Universität Paderborn, 33098 Paderborn, Germany

We study the interaction of electron and nuclear spins in fluorine-doped ZnSe epilayers. Using the time-resolved optical pump-probe spectroscopy in the regime of resonant spin amplification we are able to resolve nuclear magnetic resonances (NMR) of ^{77}Se and ^{67}Zn isotopes with non-zero spin. The effective nuclear fields show a dispersive form of its strength around NMR as a function of magnetic field. In the RSA signal this leads a shift of the resonances of the electron spins. Dependences are measured as a function of external parameters, like: pump power, polarization modulation frequency and temperature. In a further experiment an external radio frequency field is applied to investigate the strength of the resulting nuclear field. Theoretical considerations support our findings.

HL 23.8 Tue 11:15 ER 270

Effect of electron spin inertia in II-VI semiconductors — •Fabian Heisterkamp[1], Evgeny A. Zhukov[1], Alex Greilich[1], Vladimir L. Korenev[1,2], Dmitri R. Yakovlev[1,2], Alexander Pawlis[3], Grzegorz Karczewski[4], Tomasz Wojtowicz[4], Jacek Kossut[4], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44227 Dortmund, Germany — [2]Ioffe Physical-Technical Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia — [3]Department Physik, Universität Paderborn, 33098 Paderborn, Germany — [4]Institute of Physics, Polish Academy of Sciences, 02668 Warsaw, Poland

An electron bound to a fluorine donor impurity in ZnSe has been considered as a good candidate for a quantum bit [1]. We study the spin relaxation time (T_1) in fluorine-doped ZnSe epilayers using optical pump-probe spectroscopy. We fix the time-delay between pump and probe pulse and scan the magnetic field in Faraday geometry to measure the polarization recovery curve for different pump helicity modulation frequencies. While the spin polarization is able to reach its steady-state value for low modulation frequencies, the spins cannot be polarized completely, if the pump helicity changes too fast. We present a theoretical model for this effect of electron spin inertia. To test this approach we determine the spin relaxation time also for res-

ident electrons in CdTe QWs. For further information on the optical properties of the samples we refer to Refs. [2] and [3]. [1] Sanaka et al., Phys. Rev. Lett. 103, 053601 (2009). [2] Greilich et al., Phys. Rev. B 85, 121303(R) (2012). [3] Zhukov et al., Phys. Rev. B 76, 205310 (2007).

HL 24: Thermoelectricity

Time: Tuesday 9:30–13:00 Location: EW 202

HL 24.1 Tue 9:30 EW 202

High-throughput exploration of alloying as design strategy for thermoelectrics — •Sandip Bhattacharya and Georg Madsen — ICAMS, Ruhr-Universität Bochum, Germany

The quintessential salient features of a modern thermoelectric material must be, large energy conversion efficiencies and that they must be comprised of economical and innocuous constituents. Along these lines, we will discuss a new materials design strategy based on Vegard's law to optimize the thermoelectric figure of merit, zT, in binary alloys. Using a combinatorial high-throughput formalism we have explored 300 different binary M-X(X') systems, where M is a Group 1-12 element while X (X') is Si, Ge or Sn. We have identified eight promising candidates that are constituted by non-toxic and inexpensive elements and have the potential of a high zT, in addition to being thermodynamically stable. For the candidates, we shall also explore in detail the correlation between their electronic structures and thermoelectric properties, to understand the source of enhancement in their transport characteristics. Furthermore, we will discuss the descriptors used to quantify the improved thermoelectric performance and their ease of alloy formation.

HL 24.2 Tue 9:45 EW 202

Density functional calculations of the thermoelectric properties of ZrNiSn and ZrCoBi — •Gregor Fiedler and Peter Kratzer — Faculty of Physics, University Duisburg-Essen, 47048 Duisburg, Germany

Finding "green", inexpensive and efficient materials combinations for thermoelectric energy harvesting is a challenge. We have conducted a theoretical study of ZrCoBi, ZrNiSn and their heterostructures for thermoelectric applications. We present results from first-principles calculations for all factors contributing to the figure of merit ZT. Using density functional theory, we compute the electronic and phononic spectrum, deformation potentials and elastic constants. From the electronic band structure, the Seebeck coefficient and the electronic conductivity are calculated. For the latter, acoustic intravalley scattering is included using the calculated deformation potentials. Moreover, we show that disordered and off-stoichiometric materials display defects states in the band gap. The unavoidable occurrence of these defects due to their low formation energy is responsible for the very small band gap in ZrNiSn reported experimentally, and the high thermal carrier concentration. In heterostructures of ZrNiSn and ZrCoBi, the thermal conductivity is predicted to be substantially reduced. We estimate this reduction using the diffuse mismatch model based on the calculated phonon spectra, including optical phonons.

HL 24.3 Tue 10:00 EW 202

First principles calculations of point defects to optimize the thermoelectric efficiency of half-Heusler compounds. — •Robin Stern and Georg Madsen — Ruhr-Universität Bochum, ICAMS

In future, thermoelectric materials can play a significant role in enhanced energy efficiency. The thermoelectric performance of a material is determined by the power-factor, $S^2\sigma$ and the thermal conductivity κ. Half-Heusler compounds, consisting of three interpenetrating fcc sublattices, are an interesting class of materials, since they exhibit a relatively large Seebeck coefficient S. Furthermore, each sublattice can be doped independently to increase the power-factor and lower the thermal conductivity. The power-factor is strongly influenced by the carrier concentration. We used DFT point-defect calculations to evaluate the defect formation energies of various dopants and studied the influence on the carrier concentration. Using the example of NiTiSn, we discuss how the growth conditions of the half-Heusler compound influences the intrinsic carrier concentration and how extrinsic doping can significantly increase the latter.

HL 24.4 Tue 10:15 EW 202

Formation and function of vacancies in Si/Ge Clathrates: The importance of broken symmetries — •Amrita Bhattacharya, Christian Carbogno, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

One promising material class for improved thermoelectrics are the clathrates, i.e., semiconducting host lattices encapsulating guest atoms. Even in simple clathrates, such as, Si_{46} and Ge_{46}, the introduction of guests can result in important but not yet understood effects: In Si hosts, the addition of K (or Ba) results in defect-free K_8Si_{46} (Ba_8Si_{46}) phases. In spite of their structural and electronic similitude, Ge hosts behave fundamentally different upon filling: Under addition of K/Ba, the most stable phases are K_8Ge_{44} and Ba_8Ge_{43}, having *two* and *three* tetravalent framework vacancies respectively that completely/ partially balance the electrons donated by the guests. In this work, we use density-functional theory, carefully evaluating the role of exchange correlation functionals, to compute the formation energies of vacancies and vacancy complexes in Si- and Ge-hosts as function of the filling with K/Ba. By taking into account structural disorder, geometric relaxations, and vibrational entropies, we verify and explain the experimentally found vacancy concentration and the thermodynamic stabilities of these compounds. We can trace back the contrasting behavior of Si/Ge clathrates upon filling to a curious, charged vacancy induced break in symmetry that occurs in Si but not in Ge hosts.

HL 24.5 Tue 10:30 EW 202

Chemical ordering in inorganic clathrates and its effect of thermoelectric performance — •Paul Erhart, Mattias Ångqvist, and Daniel Lindroth — Chalmers University of Technology, Gothenburg, Sweden

Inorganic clathrates are of interest due their very good thermoelectric performance at elevated temperatures. Here, we consider type-I clathrates with composition $A_8B_{16}C_{30}$, where A=Ba is the guest species while B=Al/Ga and C=Si/Ge comprise the matrix. Cluster expansions and Monte Carlo simulations are employed to explore chemical ordering in these materials. The cluster expansion models are parametrized with respect to density functional theory calculations using a compressive sampling approach. The calculated site occupancy factors are in very good agreement with experiment. The Al-Al and Ga-Ga nearest neighbor pair interaction is always repulsive, which is in accord with the empirical rule that Al-Al/Ga-Ga pairs are to be avoided. Using Boltzmann transport theory we then quantify the effect of chemical order on the electrical and thermal conductivity as well as the Seebeck coefficient. The results are discussed with respect to their implications on thermoelectric performance and the potential for property modification via controlling the degree of order in the system.

HL 24.6 Tue 10:45 EW 202

Thermoelectric properties of n-doped Silicon and Copper from first-principles — •Mattia Fiorentini and Nicola Bonini — King's College London, Strand, London, United Kingdom

Understanding transport phenomena is a key task to design and engineer materials for thermoelectric and nano-electronic applications. Despite the extensive activity in the field, the state-of-the-art still lacks a comprehensive first-principles numerical framework to tackle the problem. Here we present a computational infrastructure to calculate the electronic transport coefficients of bulk systems within the Boltzmann transport equation (BTE) formalism. The electronic and vibrational properties, including the electron-phonon interaction, are computed using Density Functional theory and Density Functional Perturbation theory. We exploit the Wannier interpolation to efficiently sample fine grids in reciprocal space. The linearized BTE is solved exactly using a Conjugate Gradient algorithm. Our method goes beyond the standard practice, which relies upon various flavors of the relaxation-time approximation and uses semi-empirical models of carriers' dispersions and

interactions. Here we study the thermoelectric properties of n-doped Silicon and Copper in a wide range of temperatures. Our results are in good agreement with the experimental observations and elucidate the relative importance of the various scattering mechanisms in the different regimes. For Copper, we give an explanation for the anomalous behavior of the Seebeck coefficient. As an additional outcome, we assess the accuracy of simplified models and approximations that are commonly used to study transport in semiconductors.

HL 24.7 Tue 11:00 EW 202

Achieving optimum carrier concentrations in p-doped SnS thermoelectrics — •Sandip Bhattacharya[1], Naga Harsha Gunda[1], Robin Stern[1], Gilles Dennler[2], and Georg Madsen[1] — [1]ICAMS, Ruhr-Universität Bochum, Germany — [2]IMRA Europe S.A.S, France

SnS is a commercially viable and environmentally friendly thermoelectric material. Recently [1] it was shown from an intermediate throughput investigation that p-doping in SnS can be achieved effectively with monovalent cations. This improves the itinerant carrier's concentration thereby enhancing its powerfactor. In particular, Ag-doped SnS under Sulphur rich environment showed encouraging transport properties. We shall elaborate upon our previous work and explore the possibility of p-doping SnS with Ag, Li, Cu, Na and K. We will discuss the effects of two ubiquitous effects that can result in decreasing the hole concentration. These undesired phenomena include the formation of coupled defects and oxidation of the dopant. This work serves as a comprehensive guide to achieve an efficient p-doped SnS thermoelectric material. [1] C. Bera, et al, Phys.Chem. Chem. Phys. 16, 19894 (2014).

Coffee break

HL 24.8 Tue 11:30 EW 202

Resistance Fluctuation Spectroscopy on Thermoelectric $CoSb_3$ and Partially Filled $Yb_xCo_4Sb_{12}$ Skutterudites — •Sven Heinz[1], Martin Lonsky[1], Marcus Daniel[2], Manfred Albrecht[2,3], and Jens Müller[1] — [1]Physikalisches Institut, Goethe-Universität, Frankfurt (M), Germany — [2]Institut für Physik, TU Chemnitz, Chemnitz, Germany — [3]Institut für Physik, Universität Augsburg, Augsburg, Germany

Thermoelectric materials can directly convert heat to electricity. For the efficiency of this conversion to be high, materials have to have a high electrical conductivity and a low thermal conductivity. Pure $CoSb_3$ combines these conflicting properties unusually well. Thermal conductivity can be further reduced by introducing so called "rattling atoms" that can move relatively freely at interstitial sites, therefore acting as very efficient scattering centers for phonons. We studied how the introduction of Ytterbium as rattling atoms in $CoSb_3$ alters its electronic transport properties. Besides standard transport measurements, like resistivity and hall-effect measurments, resistance fluctuation spectroscopy has been performed. While $1/f$-type-noise dominates in the unfilled samples, we found unusually strong Lorentzian spectra and random telegraph noise in the Ytterbium-filled samples and determined characteristic activation energies of the underlying switching processes. The activation energies E_a exhibit a characteristic temperature dependence, i.e. E_a increases from values of about 5 meV at low temperatures to values of up to 250 meV near room temperature, which is close to the gap energy for the pure material.

HL 24.9 Tue 11:45 EW 202

Thermoelectrics of mesoscopic transport influenced by an electromagnetic environment — •Michael Mecklenburg, Björn Kubala, and Joachim Ankerhold — University Ulm, Institut for Complex Quantum Systems (ICQ), Albert-Einstein-Allee 11, D-89069 Ulm, Germany

Mesoscopic systems have been considered as interesting candidates for thermoelectric applications. This is due to strong energy-dependent transport features, as shown, for instance, in resonant tunneling through a quantum dot. Transport through such a quantum system is also influenced by the electromagnetic properties of the circuit into which it is embedded. Such effects on thermoelectric properties have, so far, received only scant attention [1].
Here, we apply P(E)-theory to investigate the impact of different types of electromagnetic environment on the thermopower. Introducing a strong asymmetry into the system allows for a controlled tuning of the effective temperature bias. Extensions beyond the single-dot case considered here are possible.

[1] T. Ruokola und T. Ojanen, Phys. Rev. B, **86** (2012), 035454.

HL 24.10 Tue 12:00 EW 202

Bound on Thermoelectric Power in a Magnetic Field — •Kay Brandner and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

Strong numerical evidence for the existence of a so far undiscovered constraint on the Onsager coefficients describing thermoelectric transport in the presence of a magnetic field is presented on the basis of the paradigmatic n-terminal model with n-2 terminals acting as probes mimicking correlations and inelastic scattering. The new constraint implies, inter alia, that power vanishes at least linearly when the maximum efficiency is approached. This result goes beyond the bounds discussed in our previous work [1,2], since, first, it holds for an arbitrarily large number of terminals and, second, power is bounded rather than efficiency. In particular the option of reaching Carnot efficiency at finite power, which, in principle, would be allowed by the bare second law, is finally ruled out for the multi-terminal set-up.

[1] K. Brandner, K. Saito and U. Seifert, Phys. Rev. Lett. **110** 070603 (2013)
[2] K. Brandner and U. Seifert, New J. Phys. **15** 105003 (2013)

HL 24.11 Tue 12:15 EW 202

Quantum Nernst engines — •Björn Sothmann[1], Rafael Sánchez[2], and Andrew N. Jordan[3] — [1]Département de Physique Théorique, Université de Genève, Genève, Switzerland — [2]Instituto de Ciencia de Materiales de Madrid, CSIC, 28049, Madrid, Spain — [3]Department of Physics and Astronomy, University of Rochester, Rochester, USA

Recently, there has been a growing interest in quantum heat engines with broken time-reversal symmetry as such systems in principle allow for increased efficiencies [1]. Here, as a concrete example of such a setup, we consider a quantum Nernst engines based on edge states in the quantum Hall regime [2]. We identify a geometry that exhibits an extreme asymmetry between the off-diagonal Onsager coefficients for heat and charge transports. In terms of thermodynamic efficiency, this engine outperforms a recently proposed classical Nernst engine [3]. A second setup using an antidot is found to be more efficient as energy filtering becomes less strong; a behaviour in stark contrast to other heat engines.

[1] K. Brandner, U. Seifert, New J. Phys. **15**, 105003 (2013).
[1] B. Sothmann, R. Sánchez, A. N. Jordan, EPL **107**, 47003 (2014).
[2] J. Stark, K. Brandner, K. Saito, U. Seifert, Phys. Rev. Lett. **112**, 140601 (2014).

HL 24.12 Tue 12:30 EW 202

Quantum Hall thermoelectrics — •Rafael Sánchez[1], Björn Sothmann[2], and Andrew N. Jordan[3,4] — [1]Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Spain — [2]Département de Physique Théorique, Université de Genève, Switzerland — [3]Department of Physics and Astronomy, University of Rochester, U.S.A. — [4]Institute for Quantum Studies, Chapman University, U.S.A.

In an electronic circuit, current can be generated by the conversion of heat absorbed from a hot region. In the absence of a magnetic field, such thermoelectric response requires broken left-right and particle-hole symmetries. We investigate the thermoelectric properties of a three-terminal quantum Hall conductor. We identify a contribution to the thermoelectric response that relies on the chirality of the carrier motion rather than on spatial asymmetries [1]. The Onsager matrix becomes maximally asymmetric with configurations where either the Seebeck or the Peltier coefficients are zero while the other one remains finite. Reversing the magnetic field direction exchanges these effects. Our results show that thermoelectric measurements are sensitive to the chiral nature of the quantum Hall edge states, opening the way to control quantum coherent heat flows. In particular, powerful and efficient energy harvesters can be proposed [1,2]. The possibility to generate spin-polarized currents in quantum spin Hall samples is also discussed.

[1] R. Sánchez, A. N. Jordan, B. Sothmann, arXiv:1410.6639.
[2] B. Sothmann, R. Sánchez, A. N. Jordan, EPL 107 47003 (2014).

HL 24.13 Tue 12:45 EW 202

Use of resonant tunneling to enhance low dimensional thermoelectric performance — •Bhaskaran Muralidharan and Akshay Agarwal — Department of Electrical Engineering, IIT Bombay, Powai, Mumbai-400076, India

Low-dimensional systems with sharp features in the density of states have been proposed as a means to improving the efficiency of thermoelectric devices. Quantum dot systems, which offer the sharpest density of states achievable, however, suffer from low power outputs while bulk (3-D) thermoelectrics, while displaying high power outputs, offer very low efficiencies. Here, we analyze the use of a resonant tunneling diode structure that combines the best of both aspects, that is, density of states distortion with a finite bandwidth due to confinement that aids the efficiency and a large number of current carrying transverse modes that enhances the total power output [1]. We show that this device can achieve a high power output at efficiencies close to 40% of the Carnot efficiency due to the contribution from these transverse momentum states at a finite bandwidth. We then provide a detailed analysis of the physics of charge and heat transport with insights on parasitic currents that reduce the efficiency.

[1] A. Agarwal and B. Muralidharan, Appl. Phys. Lett., 105, 013104, (2014).

HL 25: Quantum dots: Microcavities and microlaser

Time: Tuesday 9:30–11:00 Location: EW 203

HL 25.1 Tue 9:30 EW 203

Towards a high-cooperativity strong coupling of a quantum-dot in a tunable microcavity — •Sebastian Starosielec, Lukas E. Greuter, Andreas V. Kuhlmann, and Richard J. Warburton — University of Basel, Departement of Physics, Switzerland

An enhanced interaction between photons and quantum emitters offers a rich field of quantum applications, including single photon transistors and emitter-emitter coupling. Tailoring the vacuum properties of high-Q, low mode-volume optical resonators facilitates this enhanced interaction and ultimately allows a coherent and reversal exchange of energy quanta, challenging to achieve at optical frequencies in solid-state system. We investigate this strong coupling regime of an InGaAs/GaAs quantum dot with a high-finesse tunable microcavity [1,2] by means of high resolution laser spectroscopy with a polarization-based dark-field detection [3] under weak resonant excitation. High signal-to-noise spectra show a clear anti-crossing feature with state-of-art exciton/cavity cooperativity ($C = 5.5$). Analyzing the resonance lineshapes, a spurious dispersive contribution to the exciton resonance is identified. In all likelihood a spectral fluctuation rather than a true decoherence process, the dephasing effect reduces the cooperativity from a bare value of $C = 9.1$. Aiming for the high-cooperativity regime, besides a high-Q cavity and low mode-volume, we stress the point that equal efforts need to be taken towards lifetime-limited emitter linewidths.

[1] R. J. Barbour *et al.*, J. Appl. Phys. **110**, 053107 (2011)
[2] L. Greuter *et al.*, Appl. Phys. Lett. **105**, 121105 (2014)
[3] A. V. Kuhlmann *et al.*, Rev. Sci. Instrum. **84**, 073905 (2013)

HL 25.2 Tue 9:45 EW 203

Photon statistics excitation spectroscopy of a quantum dot micropillar laser — •Marc Assmann[1], Tomasz Kazimierczuk[1], Johannes Schmutzler[1], Christian Schneider[2], Martin Kamp[2], Sven Höfling[2,3], and Manfred Bayer[1,4] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Technische Physik, Physikalisches Institut, Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, D-97074 Würzburg, Germany — [3]SUPA, School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, United Kingdom — [4]A. F. Ioffe Physical-Technical Institute, Russian Academy of Sciences, St Petersburg 194021, Russia

We propose photon-statistics excitation spectroscopy as an adequate tool to describe the optical response of a nonlinear system. To this end we suggest to use optical excitation with varying photon statistics as another spectroscopic degree of freedom. We apply photon-statistics excitation spectroscopy to a quantum dot micropillar laser. Both the intensity and the photon number statistics of the emission from the micropillar show a strong dependence on the photon statistics of the light used for excitation of the sample. The results under coherent and pseudothermal excitation reveal that a description of the laser properties in terms of mean input photon numbers is not sufficient. It is demonstrated that the micropillar acts as a superthermal light source when operated close to its threshold. Possible applications for important spectroscopic techniques like two-photon excited fluorescence in biological imaging are discussed.

HL 25.3 Tue 10:00 EW 203

CQED effects in resonantly excited quantum dot-micropillar cavities — •Caspar Hopfmann[1], Micha Strauss[2], Christian Schneider[2], Sven Höfling[2], Martin Kamp[2], and Stephan Reitzenstein[3] — [1]Institute of Solid State Physics, Technische Universität Berlin, D-10623 Berlin, Germany — [2]Technische Physik, Universität Würzburg, D-97074 Würzburg, Germany — [3]present address: University of St Andrews, North Haugh, KY16 9SS UK

Resonance fluorescence of single quantum dots (QDs) as well as cavity quantum electrodynamics (cQED) in high quality QD-microcavities have been subject of extensive research interest in recent years. We employ resonance fluorescence to study cQED effects in high-quality QD-micropillar cavities. An advanced 90 degree excitation/detection scheme as well as spatial filtering is employed to separate excitation and signal. This study of cQED phenomena includes investigation of fundamental cavity effects in the coupled QD-micropillar system in both weak and strong coupling regime as well as their application in non-classical light sources. We investigate strict resonant excitation in the strong coupling regime. In this regime with enhanced light-matter-coupling strength the off-resonant QD-cavity coupling is very efficient and allows us to use the cavity mode emission as a convenient monitor in resonance fluorescence experiments on single QD under variation of the spectral detuning with the cavity mode. Moreover, using resonance fluorescence, dephasing of QD transitions is reduced, which in turn enables the investigation of effects such as higher ranks of the Jaynes-Cummings ladder not accessible in non-resonant excitation schemes.

HL 25.4 Tue 10:15 EW 203

Boosting the photon outcoupling efficiency in deterministic all-epitaxial quantum dot microcavities — •Peter Schnauber, Manuel Gschrey, Arsenty Kaganskiy, Jan-Hindrik Schulze, Alexander Thoma, Sven Rodt, André Strittmatter, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin

Single semiconductor quantum dot (QD) based non-classical light sources have high potential to path the way for future quantum communication networks. In realistic scenarios key requirements are a high photon outcoupling efficiency, strong suppression of multiphoton emission events and a high degree of photon indistinguishability. These strict requirements can be met by integrating single QDs deterministically into microcavities showing acceleration of spontaneous emission and directional outcoupling of light. In this work we present numerical optimization of all-epitaxial QD-microcavities for which a Gaussian shaped photonic defect in the central cavity layer ensures 3D light confinement. Maximizing the outcoupling efficiency η_{ext} of spectrally resonant QDs placed in the center of the photonic defect yields η_{ext} as high as 81% and a Purcell-factor of 9 for such microcavities. The optimized layout is implemented by means of in-situ electron-beam lithography [1] which allows us to achieve spatial and spectral resonance of single pre-registered QDs and the confined mode of all-epitaxial microcavities. Preliminary experimental results show the feasibility and the great potential of this approach.

[1] M. Gschrey et al., APL 102 (25), 251113 (2013)

HL 25.5 Tue 10:30 EW 203

Unconventional Collective Normal-Mode Coupling in Quantum-Dot-based Bimodal Micro-Lasers — •A. Foerster[1], M. Khanbekyan[2], H.A.M. Leymann[1], C. Hopfmann[2], C. Schneider[3], S. Höfling[4], M. Kamp[3], J. Wiersig[1], and S. Reitzenstein[2] — [1]Institut für Theoretische Physik, Universität

Magdeburg, Germany — [2]Institut für Festkörperphysik, Technische Universität Berlin, Germany — [3]Technische Physik, Universität Würzburg, Germany — [4]School of Physics and Astronomy, University of St Andrews, United Kingdom

Collective coupling of multiple emitters and the normal-mode splitting proportional to a generalized coupling strength has been observed in many experiments. We analyze the occurrence of a rather unconventional normal-mode coupling in bimodal micro-lasers. The effect is attributed to the collective interaction of the cavity field with a mesoscopic number of semiconductor quantum dots as the active medium. In contrast to the conventional normal-mode coupling appearing in various schemes in the context of the single-particle or collective strong coupling regime, here we observe a hybridization of the cavity modes that leads to a locking of the frequencies and to a splitting of the linewidths in the coherent regime. Vice versa in the incoherent regime splitting of the frequencies and locking of the linewidths is observed. Our investigations are based on microscopic calculations for a bimodal quantum-dot-laser[1] and experiments that confirm the predictions in the incoherent regime.

[1] H.A.M. Leymann, et al. Phys. Rev. A 87, 053819 (2013)

HL 25.6 Tue 10:45 EW 203

Influence of optical feedback on the characteristics of quantum dot micropillar lasers — •Steffen Holzinger[1], Elisabeth Schlottmann[1], Sören Kreinberg[1], Micha Strauss[2], Christian Schneider[2], Sven Höfling[2,3], Janik Wolters[1], Martin Kamp[2], and Stephan Reitzenstein[1] — [1]Technische Universität Berlin, Germany — [2]Universität Würzburg, Germany — [3]Present address: University of St Andrews, United Kingdom

The chaotic behavior of feedback-coupled semiconductor lasers has been so far mainly experimentally studied in the classical regime. Electrically pumped quantum dot micropillar lasers constitute an advantageous platform for the realization of feedback experiments in the quantum regime, when single photon and single emitter effects become prominent. In these structures two linear, orthogonally polarized lasing modes compete using a common gain medium, resulting in a significant difference between the output power characteristics, especially above the lasing threshold. Using an external cavity, we investigate the influence of the feedback strength and polarization on the output power, photon statistics and coherence times of the lasing modes.

HL 26: Organic electronics and photovoltaics: Transport of charges - from molecules to devices (CPP with HL/TT)

Time: Tuesday 9:30–13:00 Location: C 130

HL 26.1 Tue 9:30 C 130

Electronic properties of biphenylene and the biphenylene carbon sheet — •Johann Lüder, Biplab Sanyal, Olle Eriksson, Carla Puglia, and Barbara Brena — Department of Physics and Astronomy, Uppsala University, Sweden

Biphenylene ($C_{12}H_8$) is a promising candidate for applications in molecular electronics as well as a building block for two dimensional materials such as the biphenylene carbon (BPC) sheet, a possible alternative for graphene in nanoelectronics. The electronic structure of the gas phase biphenylene molecule is measured by core and valence level spectroscopy and detailed insights are revealed in conjunction with Density Functional Theory calculations. Hybrid functional calculations including the recently proposed OT-RSH functional are compared to GW calculations to provide an accurate theoretical description. Using the band structure obtained from GW calculations, we compute the optical adsorption spectrum by solving the Bethe-Salpeter equation of BPC. Typically for two-dimensional materials, a strong excitonic effect is found and bright and dark excitons are determined.

HL 26.2 Tue 9:45 C 130

Dimensionality of excitation transport in sol-gel-derived polymeric carbon nitride photocatalysts — •Christoph Merschjann[1,2], Stefanie Tschierlei[1], Kamalakannan Kailasam[3], Arne Thomas[3], Dirk Hollmann[4], and Stefan Lochbrunner[1] — [1]Institut für Physik, Universität Rostock, D-18051 Rostock, Germany — [2]Freie Universität Berlin, D-14195 Berlin, Germany — [3]Leibniz-Institut für Katalyse, D-18059 Rostock, Germany — [4]Technische Universität Berlin, D-10623 Berlin, Germany

The spectral and temporal development of optically excited states in highly active sol-gel-derived polymeric carbon nitride (SG-CN) photocatalysts is investigated using time-resolved optical spectroscopy. By combining transient absorption results from a femtosecond pump-probe setup and transient photoluminescence using streak-camera investigations, the evolution of a light-emitting species appearing upon UV excitation is obtained. The emission decay reveals a universal power-law behaviour over more than seven decades in time (150 fs to 5 μs), the main difference between samples being the characteristic decay time in the nanosecond range. This finding is consistently described using a random-walk approach for the diffusive transport of light-induced polaron pairs, including both geminate and bimolecular recombination mechanisms. Thus, important features of the light-induced charge transport, namely the dimensionality and the regime of reasonable carrier mobilities, are deduced.

The validity of the approach is shown via comparison to ESR-based carrier-density measurements and photocatalytic activities.

HL 26.3 Tue 10:00 C 130

Simulation of Charge Transport in Organic Self-Assembled Monolayers for Applications in Field-Effect Transistors — •Susanne Leitherer[1], Christof Jäger[2], Marcus Halik[3], Tim Clark[2], and Michael Thoss[1] — [1]Institute for Theoretical Physics, University Erlangen-Nürnberg, Germany — [2]Computer-Chemie-Centrum, University Erlangen-Nürnberg, Germany — [3]Institute of Polymer Materials, University Erlangen-Nürnberg, Germany

We study charge transport through self-assembled monolayers (SAMs), which are used in field-effect transistors [1], employing a combination of molecular-dynamics simulations, semiempirical electronic structure calculations and Landauer transport theory. In particular, we investigate SAMs consisting of multifunctional molecules, where the active π-system is linked to a flexible insulating alkyl-chain. We find a close relation between the transport characteristics and the structural and electronic properties of the SAM [2]. For selected systems, we analyze pathways for efficient charge transport by examining local currents in the molecular layers. The pathways are compared to those obtained using Metropolis Monte Carlo (MC) path searches. In order to study the time-dependence of the preferred electron paths, we consider snapshots of the system selected at different times of a MD simulation. To further examine the influence of fluctuations on the transport properties, we utilize a time-dependent approach of charge transport using time-dependent nonequilibrium Green's function (NEGF) theory.

[1] C. Jäger *et al.*, J. Am. Chem. Soc. **135**, 4893 (2013)
[2] S. Leitherer *et al.*, J. Chem Phys. **140**, 204702 (2014)

HL 26.4 Tue 10:15 C 130

Quantum Molecular Dynamics Studies of Polymer-based Thermoelectric Materials — •Håkan W. Hugosson, Amina Mirsakiyeva, and Anna Delin — Department of Materials och Nano Physics, Royal Institute of Technology KTH, Stockholm, Sweden

Using modern quantum molecular dynamics methods (QMD), where all the interactions are calculated from an electronic structure method (here density functional theory - DFT), we study the polymer-based thermoelectric material PEDOT and its charge carrying polarons. QMD simulations are parameter-free and enable a direct and potentially unbiased simulation of chemical and physical events. Since temperature is taken into account a sampling of the conformational space is made, also making simulations less biased upon choices of e.g. initial conditions and chosen reaction coordinates. Among these studies we will focus on the theoretical modeling of the properties and dynamics of polarons and bipolarons in PEDOT-oligomers and crystals and the effect of novel dopants in PEDOT.

Organic polymer-based thermoelectric materials (like PEDOT), unlike presently used inorganic thermoelectric materials composed of hazardous elements with low natural abundance, though presently being less efficient, can be mass-produced at a low cost using safer abundant elements.

HL 26.5 Tue 10:30 C 130

First-principles based descriptor for intrinsic charge carrier mobility in organic devices — •Christoph Schober, Karsten Reuter, and Harald Oberhofer — Technische Universität München

In organic electronics charge carrier mobility is a key performance parameter. Due to the complex manufacturing processes of e.g. organic field effect transistors (OFETs) measured mobilities are often heavily affected by the device preparation. This masks the intrinsic materials properties and therewith hampers the decision whether further device optimization for a given organic molecule is worthwhile or not. Within hopping models based e.g. on Marcus theory the intrinsic mobility can be reliably calculated from first principles. Using a perturbative approach to this theory we formulate a descriptor that can be efficiently calculated for a wide range of organic molecules. For this descriptor we obtain good correlations to fully calculated mobilities, as well as to highest-quality experimental data where device preparation uncertainties are minimized. This suggests the descriptor as a useful tool for materials screening and quick assessment of device-related influences in measured mobilities.

HL 26.6 Tue 10:45 C 130

Effect of Mesoscale Ordering on the Energy Landscape of a Conjugated Polymer — •Carl Poelking, Patrick Gemünden, Kurt Kremer, Kostas Daoulas, and Denis Andrienko — Max Planck Institute for Polymer Research, Mainz, Germany

A multiscale simulation approach is proposed to study the effect of morphology on charge transport properties of polymeric semiconductors, with poly(3-hexylthiophene) as a test case. The method incorporates both long-range conformational disorder and local ordering, and permits reintroduction of atomistic details into large-scale morphologies generated with a coarse-grained simulation approach. Based on the resulting atomistically resolved mesophases, we investigate how the energy landscape and spatial correlations thereof evolve with increasing degree of structural order in partially ordered systems. We show that a shift towards larger conjugation lengths plays a role in the amplification rather than formation of low-energy states, such that decreased energetic disorder rather than a decreased energetic mean characterize energetics in crystalline domains.

HL 26.7 Tue 11:00 C 130

The role of microstructure on charge transport in semicrystalline polymers — •Riccardo Di Pietro[1], Iyad Nasrallah[2], Joshua Carpenter[3], Lisa Koelln[4], Lars Thomsen[5], Christopher R. McNeill[6], Antonio Facchetti[7], Harald W. Ade[3], Henning Sirringhaus[2], and Dieter Neher[4] — [1]Hitachi Cambridge Laboratory, UK — [2]University of Cambridge, UK — [3]North Carolina State University, Raleigh, USA — [4]University of Potsdam, Germany — [5]Australian Synchrotron, Clayton, Australia — [6]Monash University, Clayton, Australia — [7]Polyera Corporation, Skokie, USA

We present a study on charge transport on two widely used semiconducting polymers, P(NDI2OD-T2) and P3HT. Combining field effect transistor characterization and charge accumulation spectroscopy we provide a consistent and unambiguous correlation between the charge density dependence of mobility and the semicrystalline morphology of the polymer film. This new experimental evidence demonstrates that charge transport in semicrystalline polymers cannot be described using any currently available charge transport model such as multiple trap and release or variable range hopping. A new charge transport model is therefore proposed, which explicitly accounts for the presence of both crystalline and amorphous regions within the polymer film and for the coulobic repulsion between charge carriers accumulated within the same crystallite. It finally provides a coherent picture of charge transport that has important general consequences in regimes that are relevant not only for transistors but also diodes and solar cells.

15 min. break.

HL 26.8 Tue 11:30 C 130

The molecular structure of a high electron mobility n-type copolymer [P(NDI2OD-T2)] as studied by Infrared Transition Moment Orientational Analysis [IR-TMOA] — •Arthur Markus Anton[1], Robert Steyrleuthner[2], Wilhelm Kossack[1], Dieter Neher[3], and Friedrich Kremer[1] — [1]Institut für Experimentelle Physik I, Universität Leipzig, Germany — [2]Fachberich Physik, Freie Universität Berlin, Germany — [3]Institut für Physik und Astronomie, Universität Potsdam, Germany

To investigate the molecular order in thin layers of P(NDI2OD-T2) a novel technique, named Infrared Transition Moment Orientational Analysis (IR-TMOA), is employed. Structure-specific vibrational bands are analyzed in dependence on *polarization and inclination* of the sample film with respect to the optical axis. Making use of IR specificity we deduce the molecular order parameter tensor for the respective moieties with regard to the sample coordinate system and determine separately the orientation of atomistic planes defined through the naphthalenediimide (NDI) and bithiophene (T2) units relative to the substrate, and hence, relative to each other. We observe that chlorobenzene causes the T2 planes to align preferentially parallel to the substrate at an angle of 29°. A chloronaphthalene:xylene mixture, instead, gives rise to a reorientation of the T2 units from a *face on* into an *edge on* arrangement (65 to 70°). In contrast, the NDI part remains basically unaffected. For both solvents, evidence for aggregated chains is observed by UV/vis absorption spectroscopy [Steyrleuthner et al., *J. Am. Chem. Soc.* **136** (2014)].

HL 26.9 Tue 11:45 C 130

Aerosol Jet-Printed Organic Thin Film Transistors - Performance Analysis and Optimization — •Arno John, Hanna Krikcziokat, and Klaus Meerholz — Institut für Physikalische Chemie, Universität Köln

For the success of organic thin film transistors (OTFTs) in industrial applications it is essential to process devices by printing in order to radically lower production costs. Aerosol jet is a direct-write printing method which provides the user great control over material deposition. Along with layout flexibility and material compatibility, this makes this printing technology an excellent tool for fast prototyping devices.

We use aerosol jet technology to fabricate entire p- and n-type OTFTs by printing Ag-ink (source/drain electrodes), PTAA (p-type semiconductor) and N2200 (n-type semiconductor), PMMA (dielectric) and PEDOT:PSS (gate electrode). By varying parameters for individual components and evaluating the resulting transistors we optimize the printing process.

The performance of printed components is compared to evaporated and spin coated transistor components. We show that, with optimized processing parameters, it is possible to print transistors with charge carrier mobility, output current on/off ratio and threshold voltage of nearly equal quality of non-printed transistors.

HL 26.10 Tue 12:00 C 130

Investigation of semiconducting polymers with thermally cleavable side chains for application in multilayer devices I: Morphology and OFET devices. — •Janusz Schinke[1,2], Sabina Hillebrandt[2,3], Milan Alt[2,5], Torben Adermann[2,4], Tobias Glaser[2,3], Annemarie Pucci[2,3], Norman Mechau[2,5], Manuel Hamburger[2,4], Wolfgang Kowalsky[1,2], and Robert Lovrincic[1,2] — [1]TU Braunschweig, IHF, Germany — [2]InnovationLab GmbH, Heidelberg, Germany — [3]U. Heidelberg, KIP, Germany — [4]U. Heidelberg, OCI, Germany — [5]KIT, Germany

Conjugated polymers enable the production of electronic devices from solution at room temperature due to their advantageous combination of their electrical, optical and film-forming properties. A major milestone for this emerging technology consists in achieving printed multi-layer functional devices. A great challenge for printed organic electronics is to deposit the subsequent layer of a multilayer component from the same solvent without destroying the underlying freshly deposited layer. The solubility reduction of semiconducting molecules by the external stimulus of heat is the aim of our work. Novel organic semiconductors bearing thermally cleavable side chains were investigated via AFM, ellipsometry, PE spectroscopy and IR spectroscopy. Their charge transport characteristics were studied using OFETs. These methods allow us to obtain a clear understanding of the pyrolysis process and its influence on the resulting performance. We achieve very homogeneous layers after thermal treatment which exhibit excellent solvent resistance and additionally show an increase in OFET performance.

HL 26.11 Tue 12:15 C 130

Following the evolution of nanomorphology in PEDOT:PSS electrodes in-situ — •Claudia Palumbiny[1], Feng Liu[2], Thomas P. Russell[2], Alexander Hexemer[3], Cheng Wang[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]University of Massachusetts Amherst, Department of Polymer Science and Engineering, 120 Governors Drive, Amherst, MA 01003, USA

— [3]Lawrence Berkeley National Lab, Advanced Light Source, 1 Cyclotron Road, Berkeley, CA 94720, USA

The strongest advantages of organic photovoltaics over classical semiconductors are the possibility of fully flexible devices and easy upscaling, e.g. by slot-die printing. For fully printed and flexible devices there is a strong need for non-brittle and solvent processed electrodes, such as highly conductive PEDOT:PSS. Film properties are strongly correlated to the films nanomorphology and with this strongly depend on the processing technique used. We investigate the film evolution of highly conductive PEDOT:PSS in-situ during the printing process. We monitor the film evolution by in-situ grazing incident wide angle scattering (GIWAXS). Five film formation processes are detected, the crystallization of the polymers is correlated to solvent evaporation and enhanced interchain coupling is induced by the use of high boiling point co-solvents as ethylene glycol. The enhanced conductivity in co-solvent treated PEDOT:PSS films is related to enhanced interchain coupling, change of the PEDOT to PSS ratio and crystallite sizes.

[1] Palumbiny et al., J. Phys. Chem. C 2014, 118, 13598.

HL 26.12 Tue 12:30 C 130

Angle resolved spectroscopy resolving local morphology of organic optoelectronic materials — •Marius van den Berg, Anke Horneber, Kathrin Swider, Martin Meixner, and Dai Zhang — 1Institute of Physical and Theoretical Chemistry, University of Tübingen, Tübingen, Germany

The main component on which organic photovoltaic, transistor and photodetectors rely is the optoelectronic material. Knowledge about the local photophysical and photochemical properties of these materials at nanometer scale is important for improving overall performance and applicability [1]. The crystallinity and domain size of the local donor/acceptor morphology strongly affect the photon-electron conversion efficiencies of organic photovoltaics [2,3]. We aim at understanding the influences of nanometer scale morphology on the photophysical processes between donors and acceptors using a home built parabolic mirror assisted microscope. Using polarized excitation spectroscopy and angle resolved photoluminescence spectroscopy, we determine the relative degree of local structural order and molecular orientation in intact and photo degraded optoelectronic polymers. Furthermore, intensity changes in the angle resolved photoluminescence signals are compared with changes in the local photocurrent, to investigate morphology related photo degradation procedures, as well as the reversible/irreversible degradation steps in pi-conjugated polymers. 1)A. Dupuis et al. Eur. Phys. J. Appl. Phys. 56, 34104 (2011) 2)X. Wanget al. Small, 7, 2793 (2011) 3)R. Noriega et al. Nat. Mater., 12, 1038-1044, (2013)

HL 26.13 Tue 12:45 C 130

Multifunctional SNOM and its Application in Imaging Optoelectric Materials — Anke Horneber, Marius van den Berg, Martin Meixner, Kathrin Swider, and •Dai Zhang — Institute of Physical and Theoretical Chemistry, University of Tübingen

Optoelectronic polymer material is the basic component in photovoltaic, photodetector, or transistor system. In organic photovoltaic, the photon-electron conversion efficiency is strongly influenced by the local donor/acceptor morphology, such as crystalline, or domain size.

To get insight into this topic, we developed multifunctional scanning near-field microscopy allowing simultaneously collecting correlated topographical, optical (Raman scattering and fluorescence), and photocurrent signals with nanometer scale resolutions [1-3]. The distributions and local morphology of donor or acceptor materials are imaged using the Raman fingerprints and scanning probe microscopes. The intensity ratios between the donor photoluminescence and the local photocurrent will be discussed, with respect to the charge transfer processes in films of different morphologies. Furthermore, photodegradation will be compared, especially in the aspects of local morphology, and optical properties. References: [1] Zhang, D. et al, Phys. Rev. Lett., 2010, 104, 056601. [2] Wang, X., Azimi, H., Zhang, D., et al, Small, 2011, 7, 2793. [3] Wang, X., Egelhaaf, H., Zhang, D., Adv. En. Mater, 2014, 1400497. [4] Wang, X., Broch K., Zhang, D. et al., J. Phys. Chem. Lett., 2014, 5, 1048.

HL 27: Doped Si nanostructures (DS with HL/TT)

Time: Tuesday 9:30–13:00 Location: H 2032

Invited Talk HL 27.1 Tue 9:30 H 2032

Electronic doping of crystalline silicon nanoparticles — •Rui N. Pereira — Walter Schottky Institut and Physik-Department, Technische Universitaet Muenchen, Germany — Department of Physics and I3N, University of Aveiro, 3810-193 Aveiro, Portugal

Crystalline silicon nanoparticles (NPs) have been attracting much research interest due to their remarkable electronic, optical, and chemical properties. Si NPs combine the processing advantages enabled by nanoparticles with the unique features of Si at the nanoscale such as wavelength tunable light emission and multiple exciton generation. The natural abundance of silicon and its dominant role in microelectronics industry may also facilitate the introduction of Si NPs in commercial products such as solar cells and light emitting devices. The essential role played by doping in semiconductor technology has in recent years triggered the study of doping of Si NPs with n- and p-type dopants. In this presentation a review of the current knowledge of doping in Si NPs will be given. Particular focus will be given to NPs synthesized from gas-phase in silane plasmas, with which most of the investigations reported so far have been carried out.

HL 27.2 Tue 10:00 H 2032

Silicon nanocrystal thin films for solution-cast electronics — •Willi Aigner[1], Markus Wiesinger[1], Stanislav Abramov[1], Hartmut Wiggers[2], Rui N. Pereira[1,3], and Martin Stutzmann[1] — [1]Walter Schottky Institut and Physics Department, Technische Universität München, Garching, Germany — [2]Institute for Combustion and Gasdynamics - Reactive Fluids, Universität Duisburg-Essen, Duisburg, Germany — [3]Institute for Nanostructures, Nanomodelling and Nanofabrication, University of Aveiro, Aveiro, Portugal

In the last years, high-performance thin-film field-effect transistors (FETs) with an active layer of solution-processed semiconductor nanocrystals (NCs) films were demonstrated. However, few studies apply Si NCs, which are environmentally favorable and offer controlled n- and p-type doping. Recently, FETs using intrinsic Si NCs [1], as well as Si NC films doped with an electronic coupling agent [2] have been reported. In this work, we carried out a comprehensive study on the morphology and its influence on the electrical properties of Si NC thin films deposited by spray-coating. The effect of film thickness and NC size was investigated studying the electrical characteristics of FETs such as current-voltage behavior, hysteresis and ambipolar conduction under illumination. As we observe a strong dependence on morphology, we optimized our deposition parameters and achieved FETs with field-effect mobilities one order of magnitude higher than reported in the literature so far [1,2].

[1] Z. C. Holman, *et al.* Nano Lett. **10**, 2661 (2010) [2] R. N. Pereira, *et al.* Nano Lett. **14**, 3817 (2014)

Invited Talk HL 27.3 Tue 10:15 H 2032

Impurity doping of Si nanocrystals studied by single-quantum-dot spectroscopy — •Jan Valenta[1], Ilya Sychugov[2], Jan Linnros[2], and Minoru Fujii[3] — [1]Department of Chemical Physics & Optics, Charles University, Prague, Czechia — [2]Materials and Nano Physics, Royal Institute of Technology, Kista-Stockholm, Sweden — [3]Department of Electrical & Electronic Engineering, Kobe University, Nada, Japan

Recent research effort proved that doping of nanostructured semiconductors is much more complicated than in bulk due to the self-purification effect, increasing formation energy of substitutional doping sites etc. In order to get a deeper insight on impurity effects in Si nanocrystals (NCs) we applied single NC spectroscopy to study luminescence of two types of samples: (i) random quantum dots prepared by etching of highly doped (B, P, As, Sb) SOI wafers, (ii) highly B and P co-doped Si NCs formed by sputtering, annealing and etching. The effect of B, P, As, and Sb impurities on individual emission spectra are determined by comparison with the undoped NCs. From the statistical analysis of the luminescence spectra, the donor ionization energies for NCs emitting in the range of 1.5-2 eV are estimated to be 140-200 meV, while the exciton-impurity binding energy for As and Sb-doped NCs is

found to be about 40-45 meV. It means that both the donor ionization energy and the excitonic binding energy are increased by an order of magnitude compared to bulk Si. The luminescence spectra of heavily B,P co-doped Si NCs are characterized by a very broad emission band (>0.2eV) even at low temperature (10 K).

Invited Talk HL 27.4 Tue 10:45 H 2032

Active Silicon Nanovolume Doping: Failure and Alternatives — •Dirk König — University of New South Wales, Sydney, Australia

We report on phosphorous (P) doping of SiNC/SiO2 systems [1]. Relevant P configurations within SiNCs, at SiNC surfaces, within the sub-oxide interface shell and in the SiO2 matrix were evaluated by hybrid (h-) DFT. Atom probe tomography (APT) and its statistical evaluation provide detailed spatial P distributions. We obtain ionisation states of P atoms in SiNC/SiO2 systems at room temperature using X-ray absorption near edge structure (XANES) spectroscopy. P K shell energies were confirmed by h-DFT. While P diffuses into SiNCs and predominantly resides on interstitial sites, its ionization probability is extremely low; free localized electrons to SiNCs are not provided.

As alternative, SiO2 and Si3N4 create substantial energy offsets of electronic states in SiNCs [2]. h-DFT, interface charge transfer and experimental verifications arrive at the same NC size below which the embedding dielectric dominates their electronic properties. An increased energy gap was found for Si NCs in Si3N4 vs. SiO2 by h-DFT and confirmed in experiment. We describe the interface impact as nanoscopic field effect and show that the energy offset is very robust and controllable. As application example, we propose an undoped CMOS-able and CMOS technology-compatible Si-Nanowire MISFET.

[1] D. König, S. Gutsch, H. Gnaser et al., Nature Sci. Rep., accepted for publication (2014)

[2] D. König, D. Hiller, S. Gutsch et al., Adv. Mater. Interf. (2014); http://onlinelibrary.wiley.com/doi/10.1002/admi.201400359/abstract

15 min. break.

Invited Talk HL 27.5 Tue 11:30 H 2032

Doping issues in semiconductor field-effect transistors — •Joachim Knoch — Institute of Semiconductor Electronics, RWTH Aachen University, Aachen, Germany

The functionality of silicon devices such as transistors, solar cells etc. rely on the ability to create doping profiles. However, due to the continued downscaling of device dimensions doping becomes increasingly difficult due to a number of fundamental reasons. First, dopants will be statistically distributed within the silicon nanostructures leading to a dopant fingerprint that results in fluctuations of e.g. electronic transistor characteristics from device to device. Second, studying the resistivity of in-situ doped, VLS-grown nanowires we were able to show that with decreasing nanowire diameter the resistivity increases due to a deactivation of dopants. The reason for the deactivation was shown to be the modified effective dielectric environment if the nanowire diameter is scaled down. In turn, the deactivation results in larger parasitic resistances of the contacts of e.g. transistors, substantially deteriorating their performance. Third, ultimately scaled conventional field-effect transistors (FETs) and in particular novel device architectures such as band-to-band tunnel FETs require extremely small nanowire diameters and eventually lead to one-dimensional (1D) electronic transport. While 1D transport is beneficial to conventional FETs, in the case of tunnel FETs the 1D density of states leads to an inability of appropriate doping (even if deactivation and the statistical dopant distribution could be avoided). The effects will be discussed particularly with respect to their impact on device functionality.

Invited Talk HL 27.6 Tue 12:00 H 2032

Probing composition and conductivity in 3D-structures and confined volumes. — •Wilfried Vandervorst — Imec, Kapeldreef 75, B-3001 Leuven, Belgium

Developing and implementing next technology nodes is a complex task involving innovation in materials engineering, process development and device design. The down scaling of devices into non-planar structures has led to physical phenomena which can only been seen in 3D-structures and confined volumes such that the metrology is now pushed into dealing with analysis on a scale commensurate with device dimensions. Concepts like Atomprobe tomography with its inherent 3D-resolution are obviously a potential solution although its routine application is still hampered by localization problems, reconstruction artifacts due to inhomogeneous evaporation, sensitivity due to the limited statistics, poor tip yield, etc. On the other hand concepts like scanning probe microscopy are inherently 2D can be extended towards 3D appear either by the design of dedicated tests structures or by novel approaches such as mechanical scalping. Recent applications of Scalpel SPM have unraveled the filament formation in RRAM-devices and highlighted the conduction paths in NAND devices. Despite the apparent 1D-nature of Secondary Ion Mass Spectrometry, novel concepts like Self-focusing SIMS enable to probe layer composition within trenches as narrow as 20 nm.

Invited Talk HL 27.7 Tue 12:30 H 2032

Silicon Nanowire Devices and Applications — •Thomas Mikolajick[1,2,3] and Walter Weber[1,3] — [1]NaMLab gGmbH, Nöthnitzer Str. 64, 01187 Dresden — [2]Institut für Halbleiter und Mikrosystemtechnik, TU Dresden, 01062 Dresden — [3]Center for Advancing Electronics Dresden (CfAED), TU Dresden, 01062 Dresden

Due to the quasi 1-dimensional nature of nanowires the controlability of elctrical fileds and currents are significantly enhanced. Therfore silicon nanowires are in development in the semiconductor industry as a very promision option for end of roadmap CMOS devices. Additionally new device concepts that are hard to realize in planar structures are enabled [1]. In this talk, first the fabrication of silicon nanowires and related device structures are explained. In the second part interesting transport properties that enable new device options will be shown. Based on these observations the most important nanowire device concepts will be deduced. The reconfigurable field effect transistor (RFET) will be explained as one interesting example that makes use of the specific advantage of the nanowire geometry. Finally an outlook to other applications of silicon nanowires like chemical sensing will be given.

[1] T. Mikolajick et al., Silicon nanowires - a versatile technology platform, Phys. Status Solidi RRL 7, No. 1, p. 793-799 (2013)

HL 28: Transport: Topological insulators 2 (TT with HL/DS)

Time: Tuesday 9:30–13:00 Location: H 3005

HL 28.1 Tue 9:30 H 3005

How electron-electron interactions may lead to a spontaneous time reversal symmetry breaking in (fractional) topological insulators — •Tobias Meng[1,2] and Eran Sela[3] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland — [3]Raymond and Beverly Sackler School of Physics and Astronomy, Tel-Aviv University, Tel Aviv, 69978, Israel

We analyze the consequences of strong electron-electron interactions in topological insulators. Naively, topological insulators can be thought of as two copies of quantum Hall states for spin up and spin down electrons at opposite magnetic field, hence maintaining time reversal symmetry. Using an extension of the coupled-wire construction of quantum Hall states to systems with zero magnetic field, we find that interactions between electrons of spin up and spin down can stabilize a large family of fractional topological phases with broken time reversal invariance. The latter is manifest by a spontaneous spin polarization, a finite Hall conductivity, or by both. This suggests the possibility that strongly correlated fractional topological insulators may be unstable to spontaneous symmetry breaking.

HL 28.2 Tue 9:45 H 3005

Emergence of surface conductivity at low temperatures in FeSi — •Michael Wagner, Ralf Korntner, Andreas Bauer, and Christian Pfleiderer — Physik-Department, Technische Universität München, D-85748 Garching, Germany

We report a comprehensive study of the influence of the sample quality on the Hall-conductivity in the correlated semiconductor FeSi. For our study three high-quality $Fe_{1+x}Si$ single crystals with slightly dif-

ferent Fe concentrations x were grown by optical float zoning under ultra-high vacuum compatible conditions. While the magnetic properties vary sensitively for the samples studied, the transport properties display several key features that are independent of the Fe concentration. As our main result we find, that the Hall-conductivity of FeSi can be described in terms of a Drude-model. For low temperatures a second transport channel emerges besides bulk conductivity, which can be assigned unambiguously to the sample surface. Remarkably, the mobility of this surface conduction is extraordinarily high as compared to similar effects in conventional semiconductors, being quantitatively consistent with topological insulators such as Bi_2Te_3 where they are viewed as the signature of topologically protected transport channels.

HL 28.3 Tue 10:00 H 3005

Spin transport in 3d-topological insulator nanostructures — •Matthias Stosiek, Sven Essert, Cosimo Gorini, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

The spin-momentum locking for charge carriers on the surface of three-dimensional topological insulators holds promising prospects for spintronics applications. In this predominantly numerical study, we investigate the transport properties of nanostructures of 3d-TIs with ferromagnetic leads using model Hamiltonians. We also explore the influence of external electric and magnetic fields.

HL 28.4 Tue 10:15 H 3005

Tunnel Magnetoresistance scan of surface states of 3D topological insulators — •Sthitadhi Roy — Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany

The Fermi-surface of surface states of a 3D topological insulator (TI) has zero magnetization owing to time reversal symmetry, but an arbitrary segment of the full Fermi surface has a unique magnetic moment consistent with the type of spin-momentum locking. A three-terminal set up is proposed which directly couples to the magnetization of a chosen segment of a Fermi surface, hence leading to a finite tunnel magnetoresistance (TMR) response of the non-magnetic TI surface states, when coupled to spin polarized STM probe. This multi-terminal TMR reconstructs the in-plane momentum locked spin texture and also the out-of-plane spin polarization of hexagonally warped Fermi surfaces relevant for materials like Bi_2Te_3. This proposal is further extended to surfaces exposed by cleaving crystals at arbitrary angles to the crystal growth axis, and it shown that the TMR response not only probes and distinguishes these surfaces uniquely but the study of the spin textures for different surfaces put together acts like a hologram of the bulk band structure of the material.

HL 28.5 Tue 10:30 H 3005

Weak Antilocalization of 3DTI Surface States in the Presence of Spin-Orbit Impurities — •Pierre Adroguer[1], Weizhe Liu[2], Dimitrie Culcer[2] und Ewelina Hankiewicz[1] — [1]Institut füt Theoretische Physik und Astrophysik, Universität Würzburg, Deutschland — [2]School of Physics, The University of New South Wales, Sydney, Australia

The recent realization of three dimensional topological insulators (3DTIs) allows to probe the coherent transport of Dirac systems. In the presence of scalar disorder, weak antilocalization (WAL) is observed. However, TIs are materials where spin-orbit plays a crucial role, and the effect of spin-orbit impurities on coherent transport had not be studied yet.

In conventional electron gases where electrons have a parabolic dispersion, the concentration of spin-orbit impurities is of significative importance. Indeed, when the concentration of spin-orbit impurities is increased, the sign of the quantum correction to conductivity changes, going from weak localization to weak antilocalization (WAL).

In this work, we derive with the standard diagrammatic technique the quantum correction to conductivity when we add spin-orbit impurities to the diffusion of Dirac fermions in a disordered potential. We show that for every concentration of the spin-orbit impurities we remain in the symplectic class of WAL. We also derive the value of this quantum correction to conductivity in the presence of a transverse magnetic field, and we show that fits with the conventional theory have to be revisited in the view of our results.

HL 28.6 Tue 10:45 H 3005

SmO thin films: a flexible route to correlated flat bands with nontrivial topology — •Deepa Kasinathan[1], Klaus Koepernik[2], Liu Hao Tjeng[1], and Maurits Haverkort[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Using density functional theory based calculations, we show that the correlated mixed-valent compound SmO is a 3D strongly topological semi-metal as a result of a $4f$-$5d$ band inversion at the X point. We also show that the topological non-triviality in SmO is very robust and prevails for a wide range of lattice parameters, making it an ideal candidate to investigate topological nontrivial correlated flat bands in thin-film form. Moreover, the electron filling is tunable by strain. In addition, we find conditions for which the inversion is of the $4f$-$6s$ type, making SmO to be a rather unique system. The similarities of the crystal symmetry and the lattice constant of SmO to the well studied ferromagnetic semiconductor EuO, makes SmO/EuO thin film interfaces an excellent contender towards realizing the quantum anomalous Hall effect in a strongly correlated electron system.

15 min. break.

Invited Talk HL 28.7 Tue 11:15 H 3005

Interacting Topological Insulators — •Stephan Rachel — Institut für Theoretische Physik, Technische Universität Dresden

The physics of electronic correlations in systems with topological band structures is a young and exciting field. In this talk, I will give an overview of the most relevant and interesting interaction effects in 2D and 3D topological insulators. Specifically, I will address the physics of the Kane-Mele-Hubbard model, the prototypical model of a correlated topological insulator, and its descendants in 2D as well as topological Mott insulators emerging in 3D topological band structures. Eventually, I will explain how strong interactions can affect the surface states of strong topological insulators and lead to even more exotic phases.

HL 28.8 Tue 11:45 H 3005

Interplay of topology and interactions in the quantum Hall regime of two-dimensional topological insulators — •Stefan Jürgens, Maxim Kharitonov, and Björn Trauzettel — Institute of Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany

We study a class of two-dimensional topological insulators, in which the single-particle edge states are preserved in the presence of the magnetic field by a symmetry (e.g., crystalline) other than time-reversal. We focus on the vicinity of the crossing point between the zero-mode Landau levels. At half-filling, Coulomb interactions become particularly strong and lead to the formation of the quantum Hall "ferromagnetic" state with gapped charge excitations in the bulk. We identify the phases of this state that have gapped or gapless collective charge edge excitations and are characterized by the presence or absence of spontaneous symmetry breaking. The transitions between these phases can occur either continuously (via second order) or abruptly (via first order), depending on the parameters of the system. These transitions are accompanied by the corresponding behavior of the egde gap, which could be detected in transport measurements. Our findings provide an example of the interplay of topological and interaction-induced (spontaneous symmetry breaking) phenomena in the strong coupling regime.

HL 28.9 Tue 12:00 H 3005

Superconducting proximity effect in three-dimensional topological insulators in the presence of external magnetic fields — •Pablo Burset, Grigory Tkachov, Ewelina Hankiewicz, and Björn Trauzettel — Institute for Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany

The proximity induced pair potential in a topological insulator-superconductor hybrid features an interesting superposition of conventional spin-singlet potential from the superconductor and spin-triplet pairing induced by the surface state of the topological insulator. We theoretically describe ballistic junctions between superconductors and topological insulators under external magnetic fields. We use Green functions techniques to calculate experimentally relevant transport signatures like normal-superconductor tunnel spectroscopy, local density of states, and Josephson current. Additionally, we consider the effect of both topological order and an external magnetic field in the superconducting correlations. We associate the unconventional transport signatures with the symmetry of the singlet and triplet components of the pair potential.

HL 28.10 Tue 12:15 H 3005

Non-universal conductance fluctuations in 3D topological insulator nanowires. — •Emmanouil Xypakis[1], Jens H Bardarson[1], Louis Veyrat[2], Joseph Dufouleur[2], and Romain Giraud[2] — [1]Max-Planck-Institut fuer Physik Komplexer Systeme, Noethnitzer Straße 38, D-01187 Dresden, Germany — [2]Leibniz Institute for Solid State and Materials Research, IFW Dresden, D-01069 Dresden, Germany

The topic of this talk is a joint theoretical and experimental study of conductance fluctuations in 3D strong topological insulator nanowires. Specifically, when a nanowire is subjected to a magnetic field and disorder weak enough to be away from the universal diffusive limit, the amplitude of the conductance fluctuations oscillates with respect to the magnetic field along the wire. We explain this oscillatory behaviour by the Dirac nature of the topologically protected surface quasiparticles of the topological insulator. We further demonstrate the robustness of this quasi-ballistic transport regime by a direct comparison with experimental data obtained for Bi_2Se_3 nanowires.

HL 28.11 Tue 12:30 H 3005

How dephasing and charge puddles affect the edge transport in 2d-topological insulators — •Sven Essert, Viktor Krueckl, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

State of the art 2d-TI material systems show a length dependent non-quantized conductance for sample sizes larger than one micron. This feature is so far not well understood: Coherent elastic backscattering is symmetry forbidden and the observed weak temperature dependence does not seem to match the predictions for inelastic backscattering. We analytically and numerically investigate the effects of a third mechanism which was proposed to play a major role for the edge resistance: The combined effect of dephasing and elastic backscattering in charge puddles which are known to exist in the experimental samples.

We extract a range of dephasing times which are consistent with the experimental results. In addition, we make predictions for experiments on artificial charge puddles from which the real dephasing time scale could be determined.

HL 28.12 Tue 12:45 H 3005

Anderson localization at the edge of a 2D topological insulator — •Eslam Khalaf and Pavel Ostrovsky — Max Planck institute for solid state research, Stuttgart, Germany

We study transport via edge modes in a 2D topological insulator. Topological protection prevents complete localization of the edge states; however, quantum interference effects are still relevant for the transport properties at finite length scales. We mainly focus on the two most experimentally relevant cases: (i) a junction between two quantum Hall insulators with different filling factors and hence an imbalance in the number of right- and left-propagating modes (symmetry class A) and (ii) a relatively thick HgTe quantum well in the insulating state with an arbitrary number of edge modes (symmetry class AII). We derive the distribution of transmission probabilities as a function of the distance between leads. This allows us to demonstrate topological effects in the average conductance and the shot noise of the setup. We also consider mesoscopic fluctuations and compute the variance of conductance. This quantity is strongly influenced by topology in the quantum Hall case. All the calculations are carried out assuming localization effects are weak, i.e., in the short length limit. Technically, this amounts to studying 1D non-linear sigma model with a proper topological term and source fields on the semiclassical level. Remarkably, the semiclassical limit of the 1D sigma model can be exactly mapped onto a fully quantum 0D sigma model of a different symmetry class. This allows us to identify the distribution of transmission probabilities with the spectrum of a certain random matrix.

HL 29: Transport: Graphene (TT with CPP/DS/DY/HL/O)

Time: Tuesday 9:30–12:15 Location: A 053

HL 29.1 Tue 9:30 A 053

Observation of supercurrent in graphene-based Josephson junction — •Libin Wang[1], Chuan Xu[2], Sen Li[1], Wencai Ren[2], and Ning Kang[1] — [1]Key Laboratory for the Physics and Chemistry of Nanodevices and Department of Electronics, Peking University, Beijing 100871, China — [2]Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China

Josephon junctions with a normal metal region sandwiched between two superconductors (S) are known as superconductor- normal-superconductor (SNS) structures. It has attracted significant attention especially when changing the normal metal with graphene, which allow for high tunability with the gate voltage and to study the proximity effect of the massless Dirac fermions. Here we report our work on graphene-based Josephon junction with a new two dimensional superconductor crystal, which grown directly on graphene, as superconducting electrodes. At low temperature, we observer proximity effect induced supercurrent flowing through the junction. The temperature and the magnetic field dependences of the critical current characteristics of the junction are also studied. The critical current exhibits a Fraunhofer-type diffraction pattern against magnetic field. Our experiments provided a new route of fabrication of graphene-based Josephon junction.

HL 29.2 Tue 9:45 A 053

Magnetoresistance of nanocrystalline and ion-irradiated graphene — •Paul Linsmaier[1], Lorenz Weiss[1], Armin Shaukat[1], Christian Bäuml[1], Daniel Steininger[1], Ina Schneider[1], Matthias Büenfeld[2], Nils-Eike Weber[2], Andrey Turchanin[2], Miriam Grothe[3], Thomas Weimann[3], Ferdinand Kisslinger[4], Heiko B. Weber[4], and Christoph Strunk[1] — [1]Inst. f. Exp. and Appl. Physics, University of Regensburg — [2]Fac. of Physics, University of Bielefeld — [3]Physikalisch-Technische Bundesanstalt, Braunschweig — [4]Fac. of Physics, F.-A. University Erlangen-Nürnberg

We investigate the magnetotransport in Hall bar structures of nanocrystalline graphene [1] compared to Ar^+-bombarded epitaxial graphene [2]. We measured the resistance $R(T)$ and $R(B)$ for samples with different sheet resistance (10-40 kΩ/sq at T = 300K). The I-V characteristics of both types show strong non-linear behavior at low temperatures. Low resistive samples of nanocrystalline graphene show positive magnetoresistance (MR) with values up to + 60 % in perpendicular magnetic field for temperatures below a crossover temperature. Above this temperature the MR becomes negative. The perpendicular MR in the ion-bombarded graphene was always negative. In parallel magnetic field the MR exhibits large positive values up to + 700 % in the nanocrystalline graphene. Strongly non-monotonic behavior of the MR was observed in the ion-bombarded sample in parallel field.

[1] A. Turchanin et al., ACS Nano 5 (2011).
[2] K. V. Emtsev et al., Nat. Mat. 8, 203 - 207 (2009).

HL 29.3 Tue 10:00 A 053

Aharonov-Bohm effect in a graphene ring encapsulated in hexagonal boron nitride — •Jan Dauber[1,2], Martin Oellers[1], Alexander Epping[1,2], Kenji Watanabe[3], Takashi Taniguchi[3], Fabian Hassler[4], and Christoph Stampfer[1,2] — [1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, Aachen, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, Jülich, Germany — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba, Japan — [4]JARA-Institute for Quantum Information at RWTH Aachen University, Aachen, Germany

Recent developments in the van der Waals assembly of heterostructures of two-dimensional materials enable the fabrication of graphene on substrate with very high quality. Outstanding charge carrier mobility and mean free path have been reported for micrometer sized samples of graphene encapsulated in hexagonal boron nitride (hBN). These unique electronic properties offer opportunities for the observation of rich mesoscopic transport phenomena in sub-micron sized graphene-hBN devices. Here, we present low-temperature magnetotransport measurements on a high mobility graphene ring encapsulated in hexagonal boron nitride. We observe the co-existence of weak localization, Aharonov-Bohm (AB) oscillations and universal conductance fluctuations. We investigate the periodicity of the AB oscillations as a function of charge carrier density and find clear evidence of the AB effect even at very low carrier densities. Finally, we report on the in-

vestigation of the AB oscillations in the cross over regime of emerging quantum Hall effect at reasonable magnetic fields.

HL 29.4 Tue 10:15 A 053

Ab-initio simulations of local current flows in functionalized graphene flakes and ribbons — •Michael Walz[1], Jan Wilhelm[2], Alexei Bagrets[1], and Ferdinand Evers[3] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany — [2]Institute of Physical Chemistry, University of Zürich, CH-8057 Zürich, Switzerland — [3]Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

Using our DFT-based transport framework AITRANSS [1], we calculate the transmission and the local current density in graphene flakes functionalized by adsorbed atoms, such as nitrogen or hydrogen. We find that even a single nitrogen atom can almost completely suppress the conductance of a (gated) graphene armchair nano-ribbon. In this situation local ring currents emerge that result in local (orbital) magnetic moments.

In addition, the current flow shows a highly inhomogeneous structure. In the absence of any scatters, the current flows along parallel streamlines that exhibit a strong lateral modulation [2]. In the presence of scattering centers, such as 20% hydrogen absorbants, we observe a filamentary pattern of streamlines. It exhibits local ring currents ("eddies") that go along with sizeable local magnetic fields, $\mathbf{B}(\mathbf{r})$. [3]

In the future, we plan to study the statistics of local currents of such large flakes and its dependency on the impurity concentration.

[1] A. Arnold, F. Weigend, F. Evers, J. Chem. Phys. 126 (2007)
[2] J. Wilhelm, M. Walz, F. Evers, Phys. Rev. B 89 (2014)
[3] M. Walz, J. Wilhelm, F. Evers, Phys. Rev. Lett. 113 (2014)

HL 29.5 Tue 10:30 A 053

Fabry-Pérot interference in monolayer and bilayer graphene devices — •Ming-Hao Liu and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany

Recent progress on high-quality graphene device fabrications has made submicron- or even micron-scale phase-coherent phenomena in graphene experimentally observable. Hence reliable quantum transport simulations for ballistic graphene devices are nowadays highly demanded. In this talk we give an overview on how such simulations can be accurately and efficiently performed. Concrete examples of Fabry-Pérot interference in single pn junctions in suspended monolayer graphene [1], multiple pn junctions in monolayer graphene on substrate [2], and pnp junctions in bilayer graphene encapsulated by hexagonal boron nitrite [3] will be briefly shown, as well as further studies of "electron optics" in graphene.

[1] P. Rickhaus, R. Maurand, M.-H. Liu, M. Weiss, K. Richter, and C. Schönenberger, Nature Comm. **4**, 2342 (2013); M.-H. Liu, et. al., arXiv:1407.5620 (2014).
[2] M. Drienovsky, F.-X. Schrettenbrunner, A. Sandner, D. Weiss, J. Eroms, M.-H. Liu, F. Tkatschenko, and K. Richter, Phys. Rev. B **89**, 115421 (2014).
[3] A. Varlet, M.-H. Liu, V. Krueckl, D. Bischoff, P. Simonet, K. Watanabe, T. Taniguchi, K. Richter, K. Ensslin, and T. Ihn, Phys. Rev. Lett. **113**, 116601 (2014).

HL 29.6 Tue 10:45 A 053

Substrate-Induced doping of supported graphene: an ab initio study — •Arezoo Dianat[1], Rafael Gutierrez[1], Zhongquan Liao[2], Martin Gall[2], Ehrenfried Zschech[2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science, Technische Universität Dresden, D-01062 Dresden, Germany — [2]Fraunhofer Institute for Ceramic Technologies and Systems, D-01109 Dresden, Germany

A major challenge for applications of graphene in nanoelectronics is the absence of a band gap in its low energy spectrum. One possibility of gap opening is doping and there are various methods to achieve it: evaporation, thermal treatment, and plasma doping. In this study, using ab initio molecular dynamics, we investigate graphene doping mediated by substrate-induced mechanisms. More specifically, we address graphene on a B-doped Si(100) surface. Our ab initio total energy calculations show that B atoms prefer to locate on the surface layer of Si(100). Further, intercalation of B atoms into vacancy positions of graphene is only found for temperatures larger than 700 K. In a second step, the electrical transport properties of B-doped graphene are studied using the non-equilibrium Green's function approach.

15 min. break.

HL 29.7 Tue 11:15 A 053

Density of states of graphene with vacancies — •Soumya Bera — MPI-PKS, Dresden

We numerically calculate the density of states (DOS) of graphene in the presence of compensated vacancy disorder. The model belongs to the BDI class of Atland-Zirnbauer symmetry classification of disordered metals, where the non-linear Sigma model predicts a Gade-type singularity in the DOS $\rho(E) \sim E^{-1}\exp(-|\log(E)|^{-1/2})$. We show that in the pre-asymptotic regime this is indeed true, however, at even lower energies the Gade-type behavior gives away to a stronger singularity of the form $\rho(E) \sim E^{-1}|\log(E)|^{-x}$ with $2 > x \geq 1$ in agreement with recent analytical work (Ostrovsky et al., PRL 113, 186803). We conclude that the generic Sigma model of the BDI class does not apply for strong (unitary) scatterers; the nature of disorder is of important to determine the low energy behaviour of disordered graphene.

[1] PRL 113, 186802 (2014).

HL 29.8 Tue 11:30 A 053

Nonlocal optical excitations and dynamic shear viscosity of graphene — •Julia Link, Peter P. Orth, and Jörg Schmalian — Institute for Theoretical Condensed Matter physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe

We study the dynamic shear viscosity of the interacting electronic fluid of graphene in the finite frequency, collision-less regime, relevant for nonlocal optical properties. We determine the frequency dependence of the dynamic shear viscosity for non-interacting graphene and study the influence of the long-range Coulomb interaction. Finally we discuss a setup where the viscosity can be spectroscopically measured.

HL 29.9 Tue 11:45 A 053

Transport phenomena in deformed graphene: Magnetic field versus curvature — Thomas Stegmann[1,2] and •Nikodem Szpak[1] — [1]Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Germany — [2]Instituto de Ciencias Fisicas, Universidad Nacional Autonoma de Mexico, Cuernavaca, Mexico

The current flow in deformed graphene nanoribbons is studied theoretically. Using a tight-binding model, we apply the nonequilibrium Green's function (NEGF) method to investigate how a localized deformation and a perpendicular magnetic field affect the current flow. At long wavelengths, the eikonal approximation applied to the effective Dirac equation leads to the Mathisson-Papapetrou equations describing trajectories of a spinning point-like particle in a curved space. We show that these trajectories are compatible with the current flow paths of the NEGF calculations. The deformation has two-fold effect on them: First, via a pseudo-magnetic field, with sixfold symmetry of attractive and repulsive regions, which acts differently on electrons and holes, but changes its sign when going from the K to the K' point. Second, via an attractive force due to the curvature of the ribbon, which treats electrons and holes equivalently. We conclude with an outlook on how to use deformed graphene ribbons for geometrical focusing of the current flow.

HL 29.10 Tue 12:00 A 053

Merging of the Dirac points in electronic artificial graphene — •Juraj Feilhauer[1,2], Walter Apel[1], and Ludwig Schweitzer[1] — [1]Physikalisch-Technische Bundesanstalt (PTB), Braunschweig, Germany — [2]Institute of Electrical Engineering, Slovak Academy of Sciences, Bratislava, Slovakia

Artificial graphene (AG) is a man-made electron system which has a similar bandstructure as normal graphene, i.e. in the low-energy part of the electronic spectrum, two bands touch and form a pair of Dirac cones. We study analytically and numerically the bandstructure of electronic AG under uniaxial strain. Here, AG is created from the two-dimensional electron gas by applying a repulsive triangular potential and the effect of strain is modeled by tuning the distance between the repulsive potentials along the armchair direction. In normal graphene, the theory based on nearest-neighbour tight-binding approximation predicts that due to the change of the hopping integrals by applying uniaxial strain, both Dirac cones are shifted away from the corners of the Brillouin zone and also becomes elliptical instead of circular. With increasing compressive strain, the Dirac cones move along the edge of Brillouin zone towards each other until they merge. We show that such a merging of the Dirac cones also exists in uniaxially compressed AG. With applied strain, we find the Dirac cones are also tilted and that

can be simulated by the presence of a next-nearest-neighbour hopping in the tight-binding hamiltonian. We discuss a possible realization of our theoretical results in a recent experiment with molecular graphene.

HL 30: Photovoltaics: Nanostructured materials

Time: Tuesday 10:15–11:45 Location: ER 164

HL 30.1 Tue 10:15 ER 164

Theoretical Study of Frenkel to Wannier-Mott Exciton Transition in a Molecular Dye Aggregate-CdSe Nanocrystal Arrangement — •Thomas Plehn[1], Dirk Ziemann[1], Jörg Megow[2], and Volkhard May[1] — [1]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, D-12489 Berlin, Germany — [2]Institut für Chemie, Universität Potsdam, Karl-Liebknecht-Straße 24-25, D-14476 Potsdam, Germany

Transfer processes at hybrid organic-inorganic interfaces have become one of the key research topics. Theoretical studies are presented which give insight into the nature of energy transfer in a realistic molecular-semiconductor hybrid system. Transitions are described from Frenkel excitons in a gigantic tubular cyanin dye aggregate (about 60 nm length and 15 nm diameter) to Wannier-Mott excitons in a nearby placed CdTe nanocrystal (4.5 nm diameter). Despite the size of the system the whole investigation is based on a full atomistic picture. The structure of the tube and the nanocrystal are obtained by molecular dynamics simulations and a tight-binding model, respectively. The Frenkel excitons are described by coupled single molecular excited states and the Wannier-Mott excitons in terms of Coulomb correlated electron-hole pairs. FRET-type rates have been calculated for diverse spatial set-ups. Even brought into contact, the transfer stays incoherent (rates of about 1/k=1 ns). The suggested creation of hybrid excitons does not occur due to only weak coupling across the interface.

HL 30.2 Tue 10:30 ER 164

Investigation of the Spatial-Dependent Charge Carrier Collection Probability in $CuInS_2$/ZnO Colloidal Quantum Dot Solar Cells — •Dorothea Scheunemann, Sebastian Wilken, Jürgen Parisi, and Holger Borchert — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, 26111 Oldenburg

Colloidal quantum dot (CQD) solar cells with solution-producible absorber layers have made rapid progress in the last few years. In particular, the so-called depleted-heterojunction concept, consisting of a wide band gap n-type semiconductor and a p-type CQD film as absorber, appears promising. As an alternative to the commonly used but highly toxic Pb chalcogenide materials, we recently reported on the successful utilization of $CuInS_2$ nanocrystals as absorber layer in $CuInS_2$/ZnO heterojunction solar cells [1]. However, to date, the efficiency of these devices remained limited compared to state-of-the-art Pb-based CQD solar cells. To investigate possible limitations of the $CuInS_2$/ZnO system, we modeled the spatially and spectrally resolved absorption in the individual layers of the device stack using the transfer-matrix method. Here, we present a simple method to extract a spatial-dependent charge carrier collection efficiency based on the reconstruction of external quantum efficiency measurements using the modeled absorption profiles. With the help of this analysis, we identified a substantial "dead zone" in our devices, where the collection probability of excess carriers is dramatically reduced.

[1] D. Scheunemann *et al.*, Appl. Phys. Lett. **103**, 133902 (2013).

HL 30.3 Tue 10:45 ER 164

Patterned growth of ZnO nanorods as light scatterers for photovoltaic application — •Nivedita Yumnam and Veit Wagner — Jacobs University, Campus Ring 1, 28759 Bremen, Germany

One of the major loss mechanisms in solar cells is due to inefficient absorption in active semiconductor layer. The absorption can be enhanced by incorporating ZnO nanorods. They can act as scattering centers of light and hence, they increase the optical path length of light. To grow ZnO, electrochemical deposition is employed since it can be done at relatively low temperature and hence, it is compatible for flexible substrates like PET (Polyethylene terephthalate). ZnO nanorods are grown on Au coated PET. Direct electrochemical deposition on Au/PET yields a very dense ZnO nanorod distribution, which is cumbersome for infiltration of semiconductor polymer. In order to tune the density of ZnO nanorods, self-assembled monolayer (SAM) of 1-octadecanethiol is applied on top of the Au surface. By doing so, the ZnO nanorods grow through the pinholes of the SAM layer, whilst creating gaps between them. The size of the ZnO nanorods is systematically varied by changing the parameters of electrochemical deposition such as temperature, growth time, concentration and voltage. An ultrathin layer of Au is sputter coated on top of the nanorods to improve the reflection characteristics. Angle resolved light scattering measurements are carried out to document the beneficial impact of these nanorods on the light scattering properties.

HL 30.4 Tue 11:00 ER 164

Enhanced photoelectrochemical activity of vertically aligned ZnO-coated TiO2 nanotubes — •Hua Cai[1,2], Qin Yang[2], Zhigao Hu[3], Zhihua Duan[3], Qinghu You[2], Jian Sun[2], and Jiada Wu[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Fudan University, Shanghai, China — [3]East China Normal University, Shanghai, China

Vertically aligned ZnO-TiO2 hetero-nanostructures constructed of anatase TiO2 nanotubes (NTs) and wurtzite ZnO coatings are fabricated by atomic layer deposition of ZnO coatings on electrochemical anodization formed TiO2 NTs, and their photoelectrochemical activities are studied through photoelectrochemical and electrochemical characterization. Compared with bare TiO2 NTs, the transient photocurrent increases to over 1.5-fold for the annealed ZnO-coated TiO2 NTs under visible illumination. The ZnO-coated TiO2 NTs also show a longer electron lifetime, a lower charge-transfer resistance and a more negative flat-band potential than the bare TiO2 NTs, confirming the improved photoelectrochemical activity due to the enhanced charge separation.

HL 30.5 Tue 11:15 ER 164

Black Silicon Prepared by Maskless Plasma Etching at High Temperatures Above 0 °C for PV Applications — •Maria Gaudig[1,2], Jens Hirsch[1,3], Johannes Ziegler[2], Thomas Schneider[2], Martina Werner[3], Alexander Sprafke[2], Norbert Bernhard[1,3], and Ralf Wehrspohn[3,4] — [1]Anhalt University of Applied Sciences, Technologies of Photovoltaics Group, Bernburger Str. 55, 06366 Köthen — [2]Martin Luther University Halle-Wittenberg, Institute of Physics, Group microMD, Heinrich-Damerow-Str. 4, 06120 Halle (Saale) — [3]Fraunhofer Center for Silicon Photovoltaics, Otto-Eißfeldt-Straße 12, 06120 Halle (Saale) — [4]Fraunhofer Institute for Mechanics of Materials, Walter-Hülse-Str. 1, 06120 Halle (Saale)

In this work, black silicon prepared by plasma etching at temperatures above 0 °C is demonstrated. The microtexturing is realised with a maskless dry plasma etch process with capacitive and additionally inductive plasma generation. Randomly distributed, parabolic shaped pits are created on the surface with dimensions in the micrometer range and an aspect ratio of the averaged vertical against the lateral dimension of about 2:1. After passivation of the textured samples with a thin aluminium oxide layer deposited by thermal atomic layer deposition, effective charge carrier lifetimes above 1 ms could be reached. Additionally, the absorption, weighted on the AM1.5g spectrum from 300-1150 nm, is slightly increased with the aluminium oxide layer to values about 95 %. In conclusion, a black silicon process at etch temperatures above 0 °C is introduced which could be an option for photovoltaic applications.

HL 30.6 Tue 11:30 ER 164

Maskless Inductively Coupled Plasma (ICP) Generated Black-Silicon as Alternative Technique to Wet Chemical Textures for Crystalline Silicon Solar Cells — •Jens Hirsch[1,2], Maria Gaudig[1], Marcus Gläser[2], and Dominik Lausch[1,2] — [1]Anhalt University of Applied Sciences, Faculty EMW, Bernburger Str. 55 DE-06336 Köthen — [2]Fraunhofer Center for Silicon Photovoltaics CSP, Otto-Eißfeld-Str. 12, DE-06120 Halle

The current standard for the frontside texturing of crystalline silicon wafers for photovoltaic applications is the wet chemical etching. An alternative technique to this standard process is the maskless in-

ductively coupled plasma (ICP) nanotexturing of the front surface. Plasma technology allows the specifically texturing of mono and multicrystalline silicon, hence parabolic like surface nano structures can be generated on multicrystalline silicon of every orientation too. In this contribution, the results of industrial standard wet and dry SF6/O2-ICP textures will be compared. In contrast to wet chemical textures, the optical properties of ICP-Nanotextures are based on the so-called Moth-Eye-Effect. This effect is the reason for the excellent optical properties of ICP-Textures under a normal and oblique angle of incidence. In particular, in this contribution the surface morphology, reflection and formation of dry ICP-Nanotextures will be investigated and compared to wet chemical standard textures. In this context, intense attention is given to the surface recombination velocity (SVR). Finally, a first attempt for simulating the influence on the reflection through the geometric of the surface structure will be given.

HL 31: Invited Talk in honor of Bruno K. Meyer: Axel Hoffman

Time: Tuesday 10:30–11:00 Location: EW 201

Invited Talk HL 31.1 Tue 10:30 EW 201

Bruno K. Meyer: Excitons, defects and impurities in nitrides and oxides — •Axel Hoffmann — TU Berlin, Institut für Festkörperphysik, Berlin, Germany

In this talk the contribution of Bruno K. Meyer to the field of nitrides and oxides will be highlighted and reviewed.

HL 32: Graphene: Growth & intercalation (O with HL/TT)

Time: Tuesday 10:30–13:00 Location: MA 041

HL 32.1 Tue 10:30 MA 041

First-principles Study of the Origin of a Rippled Graphene Phase on Ir(001) — •Mighfar Imam[1], Natasa Stojic[1,2], and Nadia Binggeli[1,2] — [1]The Abdus Salam International Centre for Theoretical Physics Strada Costiera 11, 34151 Trieste, Italy — [2]IOM-CNR Democritos, Trieste, I-34151, Italy

An interesting graphene phase on Ir(001) comprising ordered one-dimensional ripples of nanometer periodicity with exceptionally large buckling has recently been observed experimentally [1]. In this phase, chemisorbed lines of graphene, only a few nanometers wide, strongly bind to the substrate along Ir[010], while the whole graphene film markedly buckles between these periodic lines, resulting in graphene ripples along Ir[100]. We have performed a density functional theory study including the long range van der Waals interactions to investigate the microscopic mechanisms responsible for the formation of this new graphene phase on Ir(001). With our calculated trends of the chemisorption and rippling energies, we explain the appearance of a buckled chemisorbed phase with a specific nanometer periodicity. We have also analyzed the effect of changing graphene curvature on its electronic structure and chemisorption energy, finding a new feature in the conduction band close to the Fermi energy. This new feature in the conduction states is identified as the one largely responsible for the strong local chemisorption of graphene.

[1] A. Locatelli et al., ACS Nano, 7, 6955 (2013)

HL 32.2 Tue 10:45 MA 041

Graphene induced faceting of Ir(557) — Christian Witt, Michael Horn-von Hoegen, and •Frank-J. Meyer zu Heringdorf — University Duisburg-Essen, Faculty for Physics and CENIDE, Lotharstrasse 1, 47057 Duisburg

With its great application potential due to the unique electronic structure and the mechanical properties, graphene holds promise for future carbon-based device architectures. Lately, a lot of effort has been invested into the growth of graphene on metal surfaces, due to the possibility to separate the graphene from the surface after growth. In some cases, however the interaction between graphene and the substrate, in conjunction with the elevated sample temperatures, results in a modification of the substrate surface morphology during growth. Here we investigate the modification of a regularily stepped Ir(557) surface during catalytic growth of graphene at various ethylene pressures and temperatures with low energy electron microscopy. Ir(557) is a vicinal (111) surface with a miscut of 9.45° in [001] direction. We find simultaneous growth of graphene flakes and nano-ribbons, depending on ethylene pressure and sample temperature. The nano-ribbons grow exclusively along the steps. Both, flakes and nano-ribbons, induce a faceting of the surface during growth. An intercalation of oxygen between the graphene and the faceted surface does not affect the already present facets. The orientation of the facets were determined by reciprocal space mapping and (ex-situ) AFM measurements.

HL 32.3 Tue 11:00 MA 041

Comparing graphene growth on Cu(111) vs. oxidized Cu(111) — Stefano Gottardi[1], Kathrin Müller[1], Luca Bignardi[1], Juan Carlos Moreno Lopez[1], Tuan Anh Pham[1], Alexei Barinov[2], Jonas Björk[3], Petra Rudolf[1], and •Meike Stöhr[1] — [1]University of Groningen — [2]Sincrotrone Trieste — [3]Linköping University

The epitaxial growth of graphene on catalytically active metallic surfaces via chemical vapor deposition (CVD) is known to be one of the most reliable routes towards high quality large-area graphene. This CVD-grown graphene is generally coupled to its metallic support resulting in a modification of its intrinsic properties. Growth on oxides is a promising alternative that might lead to a decoupled graphene layer. Here, we compare graphene on a pure metallic to graphene on an oxidized copper surface, in both cases grown by a single step CVD process under similar conditions. Remarkably, the growth on copper oxide - a high-k dielectric material - preserves the intrinsic properties of graphene; it is not doped and a linear dispersion is observed close to the Fermi energy. Density functional theory calculations give additional insight into the reaction processes and help explaining the catalytic activity of the copper oxide surface.

HL 32.4 Tue 11:15 MA 041

Ir(111) surface state stability against Li adsorption: role of graphene — •Petar Pervan[1], Ivo Pletikosić[2], Marin Petrović[1], Iva Šrut Rakić[1], Marko Kralj[1], Milorad Milun[1], Tonica Valla[2], and Predrag Lazić[3] — [1]Institut za fiziku, Bijenička 46, 10000 Zagreb, Croatia — [2]Department of Condensed Matter Physics & Materials Science, Brookhaven National Lab, Upton — [3]Institut Rudjer Bošković, Bijenička 54, 10000 Zagreb, Croatia

Surface states (SS) are known to be extremely sensitive to the presence of defects or adsorbates with the effect that any surface state would disappear in response to submonolayer coverage of adsorbates. Moreover, adsorbates can induce a change of the surface potential which in turn may strongly affect its binding energy. In this work we report on the Li intercalation of graphene on Ir(111) and its influence on the Ir surface state at the K point studied by means of the Low Energy Electron Diffraction (LEED), the Angle Resolved Photoemission Spectroscopy (ARPES) and the Density Functional Theory (DFT). We have found that at all stages of the Li intercalation the integrity of the surface state at the K point has been preserved. Despite the increase of the SS binding energy its spectral intensity and the width were constant at all Li concentrations. This finding suggests an unperturbed surface state coherence at the K point. Away from the K point the surface state exhibits strong hybridization with graphene pi bands which is accompanied by the opening of the band gap at higher binding energy with respect to the hybridisation point.

HL 32.5 Tue 11:30 MA 041

Chemical Functionalization of Graphene via Hyperthermal Molecular Reaction — Girjesh Dubey[1], Roberto Urcuyo[1], Sabine Abb[1], Gordon Rinke[1], Marko Burghard[1], •Stephan

Rauschenbach[1], and Klaus Kern[1,2] — [1]Max-Planck-Institute for Solid State Research, Stuttgart, Germany — [2]Institut de Physique de la Matière Condensée, EPFL, Lausanne, Switzerland

Covalent functionalization represents a viable pathway for tailoring graphene's electronic properties, for instance to open a band-gap. It furthermore enables subsequent chemical coupling for applications in molecular diagnostics and molecular electronics. In this study, chemical vapor deposited (CVD) graphene is covalently functionalized though electrospray ion beam deposition (ES-IBD) of hyperthermal molecular cation beams of 4,4-azobis(pyridine). The one-step, room temperature ion-surface reaction process takes place in high vacuum (10^{-7} mbar), and requires a threshold kinetic energy of 165 eV of the molecular ions. The covalent attachment of the molecules is proven by the effect of thermal annealing, which removes the intense D peak in the Raman spectrum of the functionalized graphene. Based up X-ray photoelectron spectroscopy data, we conclude that the attached species are azopyridinium groups. A high functionalization degree of 3% of the carbon atoms of graphene is attained after 3-5 hours of ion exposure of 2×10^{14} azopyridinium/cm^2 of which 50% bind covalently.

G. Dubey et al.: *J. Am. Chem. Soc.* **136**, 13482-13485 (2014)

HL 32.6 Tue 11:45 MA 041

Quantum interference on the doped graphene/SiC systems — •Mykola Telychko[1], Pablo Merino[2], Pingo Mutombo[1], Martin Ondračeк[1], Prokop Hapala[1], Oleksandr Stetsovych[1], Martin Švec[1], and Pavel Jelínek[1] — [1]Institute of Physics ASCR, Cukrovarnicka 10, Praha, Czech Republic — [2]Max Planck Institute for Solid State Research, Heisenberg Strasse 1, 705669 Stuttgart

We report methodology for co-doping of epitaxial graphene grown on the SiC(0001) substrate by boron and nitrogen atoms. Nitrogen doping was achieved using direct nitrogen ion implantation into the graphene lattice and subsequent thermal stabilization. Boron doping was achieved by introducing the additional source of boron atoms during growth process of the graphene/SiC(0001).

Atomically-resolved low-temperature STM/AFM measurements of well-defined single substitutional nitrogen and boron dopants reveal that nitrogen dopants in graphene lattice feature a strong destructive quantum interference effect, tunable by changing the tip-sample separation. The current dependence on the tip position is successfully modelled by DFT and STM simulations for the both types of dopants. Absence of the destructive interference over the boron dopants allows clear chemical discrimination between the N and B atoms.

HL 32.7 Tue 12:00 MA 041

Scanning Tunneling Microscopy of epitaxial Graphene with single ion-implanted Boron, Nitrogen and Carbon atoms — •Philip Willke[1], Anna Sinterhauf[1], Julian Amani[2], Sangeeta Thakur[3], Thomas Kotzott[1], Steffen Weikert[2], Kalobaran Maiti[3], Hans Hofsäss[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Universität Göttingen, Germany — [2]II. Physikalisches Institut, Universität Göttingen, Germany — [3]Department of Condensed Matter Physics and Materials' Science, TIFR, Mumbai, India

Using scanning tunneling microscopy and spectroscopy we investigate the structural and electronic properties of single substitutional atoms in SiC-graphene. These are prepared by low-energy ion implantation, which we use as a suitable method for boron and nitrogen incorporation in graphene [1,2]. We find, that boron and nitrogen atoms lead to an effective doping of the graphene sheet and allow to reduce or raise the position of the Fermi level, respectively. The electronic properties of the doping atoms are additionally addressed. To reveal the defect creation in the doping process $^{12}C^+$ carbon ions, that only introduce defects and no impurity atoms, are studied as a reference. Moreover, we perform magnetotransport measurements to investigate the influence of the microscopic structure on the graphene transport properties. This work was supported by DFG priority program 1459 "Graphene".

[1] P. Willke et al., Appl. Phys. Lett. 105, 111605 (2014)

[2] U. Bangert et al., Nano Lett. 13(10) (2013)

HL 32.8 Tue 12:15 MA 041

Reversible Hydrogenation of Graphene on Ni(111) - Synthesis of 'Graphone' — •Julian Gebhardt[1], Wei Zhao[2], Florian Späth[2], Karin Gotterbarm[2], Christoph Gleichweit[2], Hans-Peter Steinrück[2], and Andreas Görling[1] — [1]Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — [2]Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Understanding the adsorption and reaction between hydrogen and graphene is of fundamental importance for developing graphene-based concepts for hydrogen storage and for the chemical functionalization of graphene by hydrogenation. Recently, theoretical studies of single-sided hydrogenated graphene, so called graphone, predicted it to be a promising semiconductor for applications in graphene-based electronics. Here, we report on the synthesis of graphone bound to a Ni(111) surface. We investigate the formation process by X-ray photoelectron spectroscopy (XPS), temperature-programmed desorption (TPD), and density-functional theory calculations, showing that the hydrogenation of graphene with atomic hydrogen indeed leads to graphone, i.e., a hydrogen coverage of 1 ML (4.2 wt%). In addition, the dehydrogenation of graphone was shown to be possible by XPS and TPD measurements. The complex desorption process was attributed to coverage-dependent changes in the activation energies for the associative desorption of hydrogen as molecular H_2.

HL 32.9 Tue 12:30 MA 041

Towards Understanding the Wetting of Nanostructured Surfaces — •Mausumi Chattopadhyaya and Alexandre Tkatchenko — Fritz Haber Institut der MPG, Berlin, Germany

Water is arguably the most important liquid. Understanding how water interacts with nanostructures leads to many fundamental questions both in theory and experiment. On the experimental side, it has been widely quoted that the contact angle of water on graphite is in the range of 90°-95°. However, careful measurements using ultra high vacuum techniques lead to drastically different values of 35±4°. From theory point of view, a precise description of water interacting with nanostructured surfaces seems to require the highest levels of correlated quantum-chemical methods. Here, we study the interaction of water with layered materials with the aim to determine the contact angle of water on different nanostructured surfaces. This demands a precise calculation of the surface energy of the nanostructure and the interaction energy between water and the surface. We have carried out systematic calculations of water interacting with few-layer graphene and h-BN surfaces. These calculations have been done using pairwise Tkatchenko-Scheffler(TS) scheme and many-body dispersion (MBD) method within density functional theory (DFT). Remarkably, our results suggest that the binding energy of a water molecule does not depend on the number of graphene or h-BN layers. We finally discuss the current work aiming to understand the contact angle of water on a range of nanostructured surfaces.

HL 32.10 Tue 12:45 MA 041

Fingerprinting graphene: self-assembly by breaking the rules of surface science — •Samuel Grandthyll[1], Stefan Gsell[2], Michael Weinl[2], Matthias Schreck[2], Karin Jacobs[1], and Frank Müller[1] — [1]Saarland University, Experimental Physics, 66041 Saarbruecken, Germany — [2]University of Augsburg, Experimental Physics 4, 86135 Augsburg, Germany

Epitaxial graphene is expected to be the only synthesis route to obtain large-area sheets of this silicon substitute for the engineering of future nano electronic devices on an industrial scale. So far, there are different recipes to obtain epitaxial graphene, using either intrinsic carbon, as released by the selective desorption of silicon from a SiC surface, or using extrinsic carbon, as via the chemical vapor deposition (CVD) of simple hydrocarbons on transition metal surfaces. In addition, even ex-situ deposition of liquid precursors (LPD) provides well-ordered graphene monolayers. In order to explore the limits of self-assembly in LPD synthesis, we show that graphene formation on transition metal surfaces is an extraordinarily robust mechanism that also works when carbon is provided in the maximal undefined way, namely by using a human fingerprint as a precursor. Our results show that "fingerprinting" graphene provides well-ordered monolayers of the same quality as in case of using ultrapure synthetic single precursors. The unique directedness of the self-assembly process of graphene on transition metals by liquid precursor deposition therefore offers a simple synthesis route for epitaxial graphene [1].

[1] F. Müller et al., Langmuir 30 (2014), 6114-6119

HL 33: Frontiers of Electronic Structure Theory: Nuclear Dynamics, Methods

Time: Tuesday 10:30–13:30 Location: MA 004

Invited Talk HL 33.1 Tue 10:30 MA 004

Electronic structure in the vicinity of strong non-adiabatic couplings — •Eberhard K.U. Gross — Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

The Born-Oppenheimer (BO) approximation is among the most fundamental ingredients of modern Condensed-Matter Theroy. Yet, some of the most fascinating phenomena such as the process of vision or phonon-driven superconductivity occur in the regime where the BO approximation breaks down. To tackle such situations one has to face the Hamiltonian of the complete system of interacting electrons and nuclei. We deduce an exact factorization [1] of the full electron-nuclear wavefunction into a purely nuclear part and a many-electron wavefunction which parametrically depends on the nuclear configuration. The resulting equations of motion for the nuclear and electronic wavefunctions lead to a unique definition of exact potential energy surfaces as well as exact geometric phases. We show an example [2] where the geometric phase associated with the conical intersection of BO surfaces has no counterpart in the true electron-nuclear wavefunction. In the time-domain, whenever there is a splitting of the nuclear wavepacket in the vicinity of an avoided crossing, the exact time-dependent surface shows a nearly discontinuous step [3], reminiscent of Tully surface hopping algorithms. Based on this observation we propose novel mixed-quantum-classical algorithms.

[1] Abedi, Maitra, Gross, PRL 105, 123002 (2010).
[2] Min, Abedi, Kim, Gross, PRL 113, 263004 (2014).
[3] Abedi, Agostini,Suzuki, Gross, PRL 110, 263001 (2013).

HL 33.2 Tue 11:00 MA 004

Towards First-Principles Modeling of Electrolytic Solvent Effects in Photo-Catalytic Water Splitting — •Stefan Ringe[1], Sebastian Matera[2], Harald Oberhofer[1], and Karsten Reuter[1] — [1]Technische Universität München — [2]Freie Universität Berlin

Due to the complexity of the physical processes underlying photocatalytic surface reactions, ab-initio computational approaches have to overcome major challenges concerning accuracy and computational costs. In particular, an efficient description of electrolytic solvent effects—which are crucial for charge driven reactions—is highly necessary.

We present an implementation of the modified Poisson-Boltzmann (MPB) model in the highly parallel and numerically efficient all-electron DFT code FHI-aims. In contrast to most implicit solvent models, this technique combines nonlinear dielectric solvent response with a statistical description of solvated finite-sized ions. This has been shown to capture a majority of electrochemical solvent effects appearing in heterogeneous photo-catalysis.[1]

We developed a self-consistent function-space oriented solution scheme for Poisson-Boltzmann-like equations which in contrast to common multi-grid solvers is able to exploit the specialized grids and optimized integration schemes of FHI-aims. We demonstrate the approach and its efficiency for the linearized Poisson-Boltzmann equation and a range of molecular systems. Finally, we discuss how the methodology can be employed for the solution of non-linear problems. [1] Kilic,M.S., Bazant, M.Z., *Phys. Rev. E*, *75*, **2007**, 021502.

HL 33.3 Tue 11:15 MA 004

Phonons in Molecular Crystals: The Role of Collective van der Waals Interactions — •Johannes Hoja and Alexandre Tkatchenko — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

By now, it is well established that dispersive van der Waals (vdW) interactions are crucial for the structure and stability of molecular crystals [1]. However, complete understanding of functionality of molecular crystals also requires a predictive description of response to external perturbations. Here we study the role of vdW interactions on phonons in molecular crystals. This subject is important since such low-frequency vibrations can be used to identify for instance drugs, explosives, and different polymorphic forms of molecular crystals. We studied the vibrational spectra of several molecular crystals with density-functional theory, including many-body dispersion interactions (DFT+MBD method). We find that long-range MBD effects can give rise to novel peaks in the phonon density of states [2], which can not be observed with a simple pairwise treatment of vdW interactions. We further discuss the nature of these vibrations and demonstrate a non-trivial connection between collective vdW interactions and entropy of molecular crystals.

[1] L. Kronik, A. Tkatchenko, Acc. Chem. Res. 47, 3208 (2014).
[2] A. M. Reilly, A. Tkatchenko, Phys. Rev. Lett. 113, 055701 (2014).

HL 33.4 Tue 11:30 MA 004

Converged Nuclear Quantum Statistics from Semi-Classical Path Integrals — •Igor Poltavskyi and Alexandre Tkatchenko — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

The quantum nature of nuclear motions plays a vital role in the structure, stability, and thermodynamics of molecular systems. The standard approach to take nuclear quantum effects (NQE) into account is the Feynman-Kac imaginary-time path-integral molecular dynamics (PIMD). Conventional PIMD simulations require exceedingly large number of classical subsystems (beads) to accurately capture NQE, resulting in considerable computational cost even at room temperature due to the rather high internal vibrational frequencies of many molecules of interest.

We propose a novel parameter-free form for the PI partition function and estimators to calculate converged thermodynamic averages. Our approach requires the same ingredients as the conventional PIMD simulations, but decreases the number of required beads by roughly an order of magnitude. This greatly extends the applicability of *ab initio* PIMD for realistic molecular systems. The developed method has been applied to study the thermodynamics of N_2, H_2O, CO_2, and C_6H_6 molecules. For all of the considered systems at room temperature, 4 to 8 beads are enough to recover the NQE contribution to the total energy within 2% of the fully converged quantum result.

HL 33.5 Tue 11:45 MA 004

Can we get reliable quantum dynamics simulations for vibrational spectra in the condensed phase? — •Mariana Rossi[1], David Manolopoulos[1], and Michele Ceriotti[2] — [1]University of Oxford, Oxford, UK — [2]EPFL, Lausanne, Switzerland

At the level of accuracy we can now achieve in first-principles calculations, the inclusion of more subtle nuclear quantum effects (NQE) in simulations become more relevant. However, their inclusion is challenging for anharmonic and dynamical processes, in particular in the condensed phase. We show a new method to approximate quantum corrections in time-dependent properties based on a path integral framework, called thermostatted ring polymer molecular dynamics (TRPMD) [1], which is immune to pathological problems of previously proposed methods. We perform a systematic comparison of TRPMD with other approaches that rely on different approximations to quantum dynamics, to assess their performance for the IR spectrum of HOD in D_2O and water at different phases/temperatures [2]. Using an empirical potential energy surface (q-TIP4P/f), we find that the different techniques are largely consistent with one another, within a few tens of cm^{-1}. Comparison with classical molecular dynamics demonstrates the importance of NQE even up to 600K. The cross validation between these different approaches provides clues to limitations of their underlying approximations and paves the way for more reliable approaches to nuclear quantum dynamics that are feasible together with electronic structure methods. [1] M. Rossi, M. Ceriotti, D. Manolopoulos, JCP 140, 234116 (2014); [2] M. Rossi, et al., JCP 141, 181101 (2014)

HL 33.6 Tue 12:00 MA 004

Ultra-high temperature properties of ZrC: a fully-anharmonic ab-initio approach — •Andrew Duff[1], Dominique Korbmacher[2], Albert Glensk[2], Blazej Grabowski[2], Joerg Neugebauer[2], and Mike Finnis[1] — [1]Department of Physics and Department of Materials, Thomas Young Centre, Imperial College London, Exhibition Road, London SW7 2AZ, UK — [2]Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, Düsseldorf 40237, Germany

As a binary end-member of many of the technologically highly interesting MAX phases, as well a useful refractory material in its own right, there is much to be gained from achieving a more accurate first-principles assessment of the behaviour of ZrC at ultra-high temper-

atures. Exploiting recent developments in finite-temperature density functional theory (DFT) calculations, we provide valuable data at temperatures where the available experimental data is of low accuracy. Within the framework of the UP-TILD approach [Grabowski 2007], the thermal expansion and heat-capacity of ZrC are calculated up to the melting-point. These fully anharmonic results are compared to calculations performed within the widely used quasi-harmonic approximation (QHA), which treats anharmonic effects in only an approximate manner. Sizeable deviations are found close to the melting point, consistent with the strongly anharmonic lattice vibrations present at such temperatures.

HL 33.7 Tue 12:15 MA 004

Quo vadis electronic friction? Assessing vibrational lifetimes beyond the independent atom approximation — •Simon P. Rittmeyer[1], J. Iñaki Juaristi[2], Jörg Meyer[3], and Karsten Reuter[1] — [1]Technische Universität München, Germany — [2]Depto. & Centro de Física de Materiales (CSIC-UPV/EHU), San Sebastián, Spain — [3]Leiden University, Leiden, The Netherlands

The quest for a both accurate and numerically efficient first-principles-based treatment of electronically non-adiabatic adsorbate dynamics on metal surfaces is still ongoing. A promising candidate in this regard is the concept of electronic friction within the local density friction approximation (LDFA). The numerical efficiency of this approach stems from an intrinsic decomposition and mapping of the interacting system to independent atoms individually embedded in a free electron gas. This inherent simplicity has raised serious conceptual concerns about the accuracy of this theory. On the other hand, it is not clear how much these approximations actually affect the description of "real" observables. In this regard, vibrational lifetimes of high-frequency adsorbate modes on metal surfaces provide a sensitive measure to gauge a non-adiabatic theory. We thus target this observable applying the LDFA for several well-studied systems and discuss it by comparing the results to other theoretical approaches as well as experimental data. Moreover, we present a simple and computationally efficient strategy to extend the LDFA beyond the yet indispensable frozen-surface and independent-atom approximation.

HL 33.8 Tue 12:30 MA 004

Polynomial-oriented linear least squares fits of potential energy surfaces for quantum dynamics — •Florian Habecker and Thorsten Klüner — Universität Oldenburg, Germany

The field TD-QM Molecular Dynamics is facing two major problems within the BO-approximation: I. Solution of the TISE for the electrons and II. Solution of the TDSE for the nuclei. Electronic structure calculations result in a K-dimensional PES (K: number of d.f. for the nuclei) on which the motion of the nuclei is simulated, subsequently.

For economical reasons, the number of sampling points calculated by QC methods is generally smaller than those needed in the QD calculation. Hence, an interface is required to link the two major tasks. Taking the scalar energies E with the corresponding geometry parameters as input, the output of such an interface is a function to calculate any points of the PES, i.e. interpolated and extrapolated values.

Following classical papers on H_3^+ [1 and refs. therein], the linear model function was chosen as a K-dimensional polynomial in this study. The lack of flexibility in this uniform ansatz was restored using appropriate non-linear variable transformations. Applying the method of LLS, precise fits can be calculated in a single non-iterative step. The capability of this approach was validated with a set of 7942 ab initio data points from a 3-D PES of a $CO/Ti_9O_{18}Mg_7^{14+}$-system [2]. Precise fits with chemical accuracy and better have been obtained for moderate expansions of the model function.

[1] W. Meyer, P. Botschwina, P. Burton, *J. Chem. Phys.* **84**, 891 (1986).
[2] H. Spieker, T. Klüner, *Phys. Chem. Chem. Phys.* **16**, 18743 (2014).

HL 33.9 Tue 12:45 MA 004

Representing Complex Potential Energy Surfaces by Artificial Neural Networks — •Christopher Handley and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universit*at Bochum, D-44780 Bochum, Germany

Computer simulations of large systems are computationally costly, and in many cases intractable, when using ab initio methods. More efficient potentials are typically based on approximations specific for particular atomic interactions, and the fitting of these potentials is not straightforward. Neural Networks (NNs) can provide interatomic potentials that are comparable to the accuracy of quantum mechanical calculations [1,2]. They are flexible enough to fit complex functions to quantum mechanical training data and yield accurate energies and forces. Here, we present our recent work towards more transferable NN potentials. [1] C. M. Handley and P. L. A. Poplier, J. Phys. Chem. A, 114, 3371- 3383, (2010). [2] J. Behler, PCCP, 13, 17901-18232 (2011).

HL 33.10 Tue 13:00 MA 004

Kinetic Monte Carlo simulations of thin film growth with anisotropic particles — •Miriam Klopotek, Martin Oettel, and Frank Schreiber — Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen

Thin film growth is a topic of fundamental experimental research, in particular for organic molecules with semiconducting properties. Thin films of organic molecules are composed of multiple 'imperfect' layers of the molecules, and the structures formed are of fundamental interest for various applications. Organic molecules are mostly highly anisotropic, rendering complex ordering at various length- and timescales within the growing film that is not seen in the case of isotropic molecular/atomistic films [1]. We explore how this particle anisotropy affects the growth dynamics by means of computer simulations. We have developed a novel algorithm to simulate large-scale thin film growth with rod-like particles using an accelerated Monte Carlo technique called *kinetic Monte Carlo* [2]. We disuss the simulations and the most relevant findings arising from statistical observables related to the orientational order of the rods. To relate the non-equilibrium growth structures to equilibrium we performed equilibrium calculations of a single layer of rods, as well. [1] S. Kowarik, A. Gerlach, S. Sellner, F. Schreiber, L. Cavalcanti, and O. Konovalov. Real-time observation of structural and orientational transitions during growth of organic thin films. *Phys. Rev. Lett.*, 96:125504, March 2006. [2] Andrea C. Levi and Miroslav Kotrla. Theory and simulation of crystal growth. *Journal of Physics: Condensed Matter*, 9(2):299, 1997.

HL 33.11 Tue 13:15 MA 004

Ti and N adatom diffusion on, and N_2 desorption from TiN(001) surfaces via *ab initio* and classical molecular dynamics — •Davide G. Sangiovanni[1], Daniel Edström[1], Lars Hultman[1], Ivan Petrov[1,2], Valeriu Chirita[1], and Joe E. Greene[1,2] — [1]Thin Film Physics, IFM, Linköping University, Sweden — [2]University of Illinois, Urbana-Champaign, Illinois, USA

We use classical and *ab initio* molecular dynamics to investigate fundamental atomistic processes and surface properties responsible for TiN surface evolution during thin film growth. The rate of adatom migration and N_2 desorption events are determined as a function of temperature to extract activation energies, attempt frequencies, and diffusion coefficients. Ti adatoms (Ti_{ad}), highly mobile on TiN(001) terraces, diffuse among fourfold hollow sites, primarily along <100> channels via single and long jumps. Ti_{ad} jumps on TiN(001) are highly correlated; an effect which leads to smaller diffusion coefficients than those determined via adatom random walks. Due to strong bonds formed with underlying N surface (N_{surf}) atoms, N adatoms (N_{ad}) are considerably less mobile on TiN(001) than Ti adatoms. After several N_{ad}/N_{surf}-pair exchange reactions, with very few N_{ad} jumps among neighboring stable surface sites, the N_{ad}/N_{surf} pair desorbs, leaving an anion surface vacancy which acts, in turn, as a catalyst for N_2 dissociative chemisorption. This pathway for N_2 desorption from TiN(001) is considerably more probable than N adatom recombination, which is kinetically hindered due to short-range N_{ad}/N_{ad} repulsive interactions.

HL 34: Nitrides: Dots, rods, and structures

Time: Tuesday 11:15–13:00 Location: EW 201

HL 34.1 Tue 11:15 EW 201

Direct evidence of quantum dot emission from GaN islands nucleated at threading dislocations — •G. Schmidt[1], S. Metzner[1], C. Berger[1], P. Veit[1], G. Callsen[2], J. Bläsing[1], F. Bertram[1], A. Dadgar[1], A. Hoffmann[2], A. Strittmatter[1], and J. Christen[1] — [1]Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Germany — [2]Institute of Solid State Physics, Technical University Berlin, Germany

We give direct evidence of quantum dot (QD) emission from nanometer-sized GaN islands nucleated in close proximity of threading dislocations (TDs) using cathodoluminescence spectroscopy performed in a scanning transmission electron microscope (STEM-CL).

The islands result from a GaN quantum well (QW) layer growth by metal-organic vapor phase epitaxy on AlN/sapphire templates. After deposition of few monolayers of GaN forming the QW layer a growth interruption without ammonia supply was applied prior to 40 nm of AlN cap layer growth.

We are able to spatially resolve cathodoluminescence between 220 nm and 300 nm from the nanometer-sized GaN islands nucleated in the close proximity of AlN TDs, which do not inhibit the luminescence. Very sharp emission lines with line widths below 500 μeV are measured confirming quantum dot like electronic properties within these islands. This full width at half maximum represents a state-of-the-art line width compared to Stranski-Krastanov grown wurtzite polar, non-polar, and zinc-blende GaN QDs as well as GaN QDs embedded in nanowires.

HL 34.2 Tue 11:30 EW 201

Temperature dependence of the luminescence dynamics of InGaN/GaN MQW microrod structures — •Angelina Vogt[1], Linus Krieg[2], Matin Sadat Mohajerani[1], Xue Wang[1,3], Jana Hartmann[1], Martin Strassburg[3], Tilman Schimpke[3], Hergo-Heinrich Wehmann[1], Andreas Waag[1], Jürgen Gutowski[2], and Tobias Voss[1] — [1]Institute of Semiconductor Technology and LENA, TU Braunschweig — [2]Institute of Solid State Physics, University of Bremen — [3]Osram Opto Semiconductors GmbH

Three-dimensional core-shell GaN-based microrods with embedded InGaN multi-quantum-well structures (MQW) are promising candidates for sensors and light-emitting diodes in the green to ultraviolet spectral region. The large area of active layers in relation to the surface area of the substrate is one of the advantages of the microrod structures. Here, we study the temperature dependence of the luminescence dynamics of microrod LED structures with a picosecond time resolution. Their luminescence dynamics were studied in order to characterise the fundamental optical properties and to investigate the influence of varying sample compositions. We compare and discuss the luminescence dynamics of different InGaN/GaN microrod LEDs with regard to the variation of the decay time for different sample positions and temperatures. All samples show a characteristic decay time of the InGaN PL between 50 and 300 ps. In particular, the luminescence on the high energy side typically exhibits a faster decay than that on the low energy side. This is attributed to relaxation and recombination processes of the charge carriers in that energy range.

HL 34.3 Tue 11:45 EW 201

Nano-scale-characterization of ordered core-shell GaN micropillars — •Marcus Müller[1,2], Gordon Schmidt[1], Eduardo Mayolo[1], Peter Veit[1], Frank Bertram[1], Sergiy Krylyuk[2,3], Ratan Debnath[2,4], Matthew King[5], Jong-Yoon Ha[2,3], Baomei Wen[2,4], Abhishek Motayed[2,3,4], Albert Davydov[2], and Jürgen Christen[1] — [1]Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Germany — [2]Materials Science and Engineering Division, National Institute of Standards and Technology, USA — [3]Institute for Research in Electronics and Applied Physics, University of Maryland, USA — [4]N5 Sensors Inc., USA — [5]Northrop Grumman ES, USA

In this study we report on the approach of combining top-down principle and the bottom-up processes to fabricate ordered core-shell GaN micropillars. The overgrowth of inductively coupled plasma etched GaN pillars by hydride vapor phase epitaxy produces hexagonally shaped micropillars with vertical non-polar sidewalls and top facet truncated by highly vicinal facets. Scanning electron microscopy measurements of the samples reveal a homogeneous growth. The strain tensors at selected regions of micropillars were analysed, using electron-backscattered-diffraction. Direct correlation of the optical and structural properties of the core-shell GaN micropillars has been achieved using highly spatially resolved cathodoluminescence spectroscopy. CL mappings of the MOVPE grown GaN-bulk template, and the etched core-shell GaN heterostructures reveal a distinct blue-shift of the donor-bound exciton emission due to a strain relaxation.

HL 34.4 Tue 12:00 EW 201

Highly reflective distributed Bragg reflectors for LEDs by modulation doped GaN:Ge — •Christoph Berger, Armin Dadgar, Jürgen Bläsing, Peter Veit, and André Strittmatter — Otto-von-Guericke-Universität Magdeburg

We report on the growth of strain-free, vertically conductive nitride-based Bragg reflectors for LED applications by taking advantage of the Burstein-Moss-effect in highly Ge-doped GaN. The Burstein-Moss-effect describes an increase of the effective bandgap for high carrier concentrations leading to a reduction of the refractive index of the layer. Significant changes of the refractive index can be achieved for carrier concentrations of the order of 1020 cm-3 which is possible in GaN using Ge-doping. For such doping levels, the refractive index of GaN:Ge is reduced to GaN:uid by more than 2 % at a wavelength of 430 nm . We have grown reflectors with 60 periods of GaN:Ge/GaN:uid. Layer growth was monitored by in-situ metrology and no degradation of the layer structure was observed. Close to the targeted wavelength at 430 nm, a stopband centered at 426 nm wavelength with a maximum reflectivity of 60 % was found, which is below the expected reflectivity of 90 %. The reasons for this are under investigation. An InGaN/GaN multiple quantum well grown on top of a 100-pair GaN:Ge/GaN:uid DBR shows significantly altered photoluminescence spectra compared to MQWs grown on an undoped GaN buffer. The spectra of MQW grown on the GaN:Ge/GaN:uid DBR exhibits a drastically reduced linewidth and doubled emission intensity.

HL 34.5 Tue 12:15 EW 201

High-reflectivity, crack-free AlN/AlGaN Bragg mirrors for deep UV micro-cavity structures — •Christoph Berger, Gordon Schmidt, Peter Veit, Armin Dadgar, Jürgen Bläsing, 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 have recently demonstrated narrow emission lines from single GaN quantum dots grown on AlN/sapphire templates by employing the Stranski-Krastanov regime in a MOVPE growth environment. From uPL measurements we find single emission lines with one of the smallest ever reported line width of only 450 ueV for GaN. Maximizing the emission into a distinct direction generally requires the use of mirrors which may also allow for enhanced spontaneous emission rates if such QDs were integrated inside in a resonant cavity structure. Therefore, we have developed highly reflecting, epitaxially grown distributed Bragg reflectors consisting of 50 periods of AlN/Al0.7Ga0.3N. Since these materials have a strong lattice-mismatch, in general these DBRs are subject of distinct crack-formation. Growing the DBR on a thin AlN buffer with a thickness of about 200 nm, smooth DBRs nearly free of cracks could be realized. These DBRs exhibit very high-reflectivities above 98 % at a wavelength around 270 nm. Optical and structural results from GaN quantum dots grown on top of such reflectors will be presented.

HL 34.6 Tue 12:30 EW 201

Structural and optical properties of a GaN-bulk semi-microcavity structure — •Alexander Reuper, Gordon Schmidt, Peter Veit, Frank Bertram, Silke Petzold, Christoph Berger, Armin Dadgar, Alois Krost, André Strittmatter, and Jürgen Christen — Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Germany

Using transmission electron microscopy combined with cathodoluminescence spectroscopy (STEM-CL) we analyze structural and spatially resolved optical properties of a GaN-based bulk semi-microcavity structure.

The sample has been grown by metal-organic vapor phase epitaxy on a c-plane Al_2O_3 substrate. A lattice matched 45 pair AlInN/AlGaN distributed Bragg reflector (DBR) serves as bottom mirror for the GaN emission. As active medium consists the whole GaN-bulk cavity which ensures the complete overlap with the cavity mode.
Within the buffer structure, dislocation reduction by a SiN mask is found, whereas low temperature AlN layers, intended for stress control, generate new threading dislocations. In the DBR structure high resolution TEM images show the formations of thin AlN interlayers located at AlInN-AlGaN interfaces, indicating In desorption. Highly spatially resolved STEM-CL at 15 K exhibits GaN-NBE emission at 356 nm, corresponding to compressive strain of about 0.3 GPa. Furthermore, we observe a continuous redshift of GaN-NBE luminescence in growth direction from 356.5 nm at the cavity/DBR interface to 356.9 nm at the surface, indicating elastic relaxation of the GaN cavity.

HL 34.7 Tue 12:45 EW 201

Direct correlation of structural properties and luminescence of an AlInN/AlGaN based microcavity structure — •Max Trippel, Gordon Schmidt, Peter Veit, Frank Bertram, Christoph Berger, Armin Dadgar, André Strittmatter, and Jürgen Christen — Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Germany

Using transmission electron microscopy combined with cathodoluminescence spectroscopy (STEM-CL) we present the spatially resolved optical properties of a microcavity structure (MC) on nanometer scale at 15 K.

The MC structure was grown by metal-organic vapor phase epitaxy (MOVPE) on a c-plane sapphire substrate with optimized AlGaN buffer. A lattice matched 45 pairs $Al_{0.85}In_{0.15}N/Al_{0.17}Ga_{0.83}N$ distributed Bragg reflector (DBR) operates as the bottom mirror. The active medium consists of two InGaN/AlGaN multiple quantum well stacks (MQW), which are separated by a 50 nm thick AlGaN barrier.

STEM-CL images clearly resolve the complete stacking sequence of the MC structure. At 15 K the integrated STEM-CL spectrum is dominated by the MQW emission at about 360 nm. Highly spatially resolved STEM-CL linescans reveal a constant MQW peak position along growth direction indicating spectrally identical QWs. Both MQW stacks show distinct luminescence and can be resolved separately. The capture length of both MQWs was calculated to 15 nm.

HL 35: Semiconductor laser

Time: Tuesday 11:15–12:45 Location: EW 203

HL 35.1 Tue 11:15 EW 203

InP-based narrow-linewidth widely tunable QD-DFB-lasers — •Annette Becker[1], Marko Bjelica[2], Vitalii Sichkovskyi[1], Anna Rippien[1], Florian Schnabel[1], Philipp Baum[1], Bernd Witzigmann[2], and Johann Peter Reithmaier[1] — [1]Technische Physik, Institute of Nanostructure Technologies and Analytics (INA), CINSaT, University of Kassel — [2]Computational Electronics and Photonics, CINSaT, University of Kassel

For high-capacitance coherent optical communication narrow-linewidth widely tunable DFB lasers as reference lasers are needed.InP based quantum dot (QD) material developed for 1.55 μm enables tailoring of device properties, like gain bandwidth and low linewidth enhancement factor (α-factor) favorable for such an application. Theoretical considerations taking into account the quasi zero-dimensional nature of the active zone, clearly predict a strong reduction of the laser linewidth by appropriate tailoring the QD material design. QD lasers with 2 and 5 QD layers were grown and distributed feedback (DFB) lasers fabricated with integrated micro-heaters. A continuous single-mode thermal tuning range up-to 10 nm and a linewidth considerably below 1 MHz could be obtained with DFB lasers consisting of 5 QD layers. A comparison of the two designs confirms the theoretically predicted trend of reduced linewidth for the high-gain design with 5 QD layers, which can be related to a reduction of the α-factor.

HL 35.2 Tue 11:30 EW 203

High UV-Power by a frequency doubled AlGaInP-VECSEL — •Stefan Baumgärtner, Hermann Kahle, Roman Bek, Thomas Schwarzbäck, Michael Jetter, and Peter Michler — Universität Stuttgart, Institut für Halbleiteroptik und Funktionelle Grenzflächen and Research Center SCoPE, Allmandring 3, 70569 Stuttgart

We present a frequency-doubled, optically pumped vertical-external-cavity surface-emitting laser (VECSEL), exceeding continuous-wave output power of 400 mW in the ultraviolet spectral region at 332 nm which is a huge improvement to earlier publications [1]. The VECSEL structure was grown by metal-organic vapor-phase epitaxy with an inhomogeneous quantum well (QW) distribution optimized due to the absorption of the pump laser [2].
The ultraviolet light was generated in a v-shaped cavity by intra-cavity frequency-doubling using β-Bariumborate as a nonlinear crystal. Using a birefringent filter inside the cavity the emission wavelength can be tuned totally 14.9 nm in the ultraviolet spectral region. Also power transfer measurements were performed with a maximum output power of 429 mW at 332 nm. The intensity of the second harmonic beam can be simulated with the theory of Boyd and Kleinman. Current work is focusing on the usage of other nonlinear crystals, namely Bismuthborate and Lithiumtriborate.

[1] Kahle, Bek, et al. J. of appl. Phys. Ex., 7, 092705, (2014) [2] Baumgärtner, Kahle, et al. J. of Crystal Growth, DOI: 10.1016/j.jcrysgro.2014.10.016

HL 35.3 Tue 11:45 EW 203

Mode-locked QD-VECSEL emitting picosecond pulses at 650 nm — •Roman Bek, Grizelda Kersteen, Stefan Baumgärtner, Fabian Sauter, Hermann Kahle, Thomas Schwarzbäck, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen and Research Center SCoPE, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

We present a SESAM mode-locked VECSEL emitting at 650 nm with a FWHM pulse duration in the order of a picosecond. A v-shaped cavity with the semiconductor samples as end mirrors and a highly reflective output coupler as folding mirror was used to tightly focus onto the absorber region. As active material, both the gain chip and the absorber contain InP-QDs embedded in $Al_{0.1}GaInP$ and $Al_{0.55}GaInP$. The semiconductor structures were grown by MOVPE in an anti-resonant design. In order to increase the field enhancement and therefore reduce the saturation fluence, SESAM samples were additionally coated with fused silica layers of different thicknesses. For an overall resonant design, the mode locking operation is found to be more stable, but with an increased pulse duration. Therefore we were able to use an output coupler with a slightly reduced reflectivity (99.7 %), resulting in an average output power of more than 10 mW. Current research is made towards intra-cavity frequency doubling of the mode-locked VECSEL.

HL 35.4 Tue 12:00 EW 203

Impact of nanomechanical resonances on the lasing of electrically pumped quantum dot micropillars — •Thomas Czerniuk[1], Andrey Akimov[2,5], Jan Tepper[1], Sebastian Unsleber[3], Christian Schneider[3], Martin Kamp[3], Sven Höfling[4], Dmitri Yakovlev[1,5], and Manfred Bayer[1,5] — [1]TU Dortmund, Dortmund, Germany — [2]University of Nottingham, Nottingham, United Kingdom — [3]University of Würzburg, Würzburg, Germany — [4]University of St Andrews, St Andrews, United Kingdom — [5]Ioffe Physical-Technical Institute, St. Petersburg, Russia

We use a picosecond acoustics technique to modulate the laser output of electrically pumped GaAs/AlAs micropillar lasers with InGaAs quantum dots. The modulation of the emission wavelength takes place on the frequencies of the nanomechanical extensional and breathing (radial) modes of the micropillars. The amplitude of the modulation for various nanomechanical modes is different for every micropillar which is explained by a various elastic contact between the micropillar walls and polymer environment.

HL 35.5 Tue 12:15 EW 203

Metal grating based Interband Cascade Lasers from 3-6 microns — •Julian Scheuermann[1], Michael von Edlinger[1], Robert Weih[2], Lars Nähle[1], Marc Fischer[1], Johannes Koeth[1],

Sven Höfling[2], and Martin Kamp[2] — [1]nanoplus GmbH, Oberer Kirschberg 4, 97218 Gerbrunn, Germany — [2]Technische Physik Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

The wavelength region from 3 to 6 microns is of great interest for gas sensing, since many gases have their strongest absorption features in this range. A common approach for highly accurate detection is the so called tunable laser spectroscopy, using distributed feedback (DFB) lasers. Monomode DFB type interband cascade lasers (ICLs) can address the spectral range of interest with superior performance and show low threshold currents as well as low power consumption, which is essential for the application in modern gas sensing systems.

We will report on the fabrication and characterization of novel ICL DFB lasers with lateral metal grating structure. The performance characteristics of fabricated devices are discussed. The definition of the ridge waveguide structure by dry etching and the metal grating structure by electron beam lithography are particular critical processing steps having a high influence on mono mode performance and tuning behavior. Single mode continuous wave emission at room temperature was obtained for various laser structures emitting in the 3-6 μm region with current tuning range up to 22 nm and (noise limited) side mode suppression ratios in excess of 30 dB. Threshold currents below 10 mA and output powers above 20 mW have been observed.

HL 35.6 Tue 12:30 EW 203

Microscopic model for intersubband gain from electrically pumped quantum-dot structures — •Stephan Michael[1], Weng Wah Chow[2], and Hans Christian Schneider[1] — [1]Department of Physics, University of Kaiserslautern, P.O. Box 3049, 67653 Kaiserslautern, Germany — [2]Sandia National Laboratories, Albuquerque, NM 87185-1086, USA

Quantum cascade lasers (QCLs) based on quantum wells (QWs) has been an exciting topic of research for decades. QCLs can operate up to and above room temperature and can produce a high output power. An alternative would be QCLs consisting of self-assembled quantum dots (QDs). Steps in this direction are midinfrared photodetectors using QDs, which include the demonstration of midinfrared electroluminescence at low and more recently also in room temperature. In this contribution, we investigate theoretically the performance of electrically pumped self-organized QDs as gain material in the mid-IR range at room temperature. Therefore, we analyze a comprehensive model based on an AlGaAs structure composed of dots-in a-well sandwiched between two QWs. We find that steady-state gain requires an efficient extraction process, that prevents an accumulation of electrons in the continuum states of the QDs. However, comparing the modal gain to a standard QW structure as used in QCLs, our calculation predict reduced threshold current densities of the QD structure for comparable modal gain. But this is only possible for an inhomogeneous broadening of a QD ensemble that is close to the lower limit achievable today using self-organized growth.

HL 36: Organic electronics and photovoltaics: OPV I (CPP with HL/TT)

Time: Tuesday 14:00–16:00 Location: C 130

Invited Talk HL 36.1 Tue 14:00 C 130

Ultrafast Coherent Charge Transfer in Solar Cells and Artificial Light Harvesting Systems — •Christoph Lienau[1], Ephraim Sommer[1], Antonietta de Sio[1], Ralf Vogelgesang[1], Margherita Maiuri[2], Giulio Cerullo[2], Angel Rubio[3], Carlo A. Rozzi[4], and Elisa Molinari[4] — [1]Carl von Ossietzky University, Oldenburg, Germany — [2]Politecnico di Milano, Milano, Italy — [3]Universidad del País Vasco, San Sebastian, Spain — [4]Dipartimento di Scienze Fisiche, Modena, Italy

To elucidate the fundamental microscopic processes in solar energy conversion, we have recently combined coherent femtosecond spectroscopy and first-principles quantum dynamics simulations [1,2] and have used this approach to explore the primary photoinduced electronic charge transfer in two prototypical structures: (i) a carotene-porphyrin-fullerene triad, an elementary component for an artificial light harvesting system [2] and (ii) a polymer:fullerene blend as a model for an organic solar cell [1].

Our results provide strong evidence that in both systems, at room temperature, the driving mechanism of the primary step within the current generation cycle is a quantum-correlated wavelike motion of electrons and nuclei on a timescale of few tens of femtoseconds. They suggest that the strong coupling between electronic and vibrational degrees of freedom is of key importance for the dynamics and yield of the charge separation process. Here, I will discuss our most recent experimental and theoretical findings. [1] S. M. Falke et al., Science 344, 6187 (2014). [2] C. A. Rozzi et al., Nature Comm. 4, 1602 (2013)

HL 36.2 Tue 14:30 C 130

Calculation of exciton dissociation rates in ordered and disordered 2D model organic photovoltaic interfaces — •Hector Vazquez[1] and Alessandro Troisi[2] — [1]Inst. of Physics, Academy of Sciences of the Czech Rep., CZ — [2]Dept. of Chemistry and Centre of Scientific Computing, University of Warwick, UK

The efficient generation of free charges from incident light in organic photovoltaic cells has been studied extensively but is not yet well understood. In order to separate, electron and hole have to overcome the Coulomb attraction and several mechanisms have been proposed. In particular, 'hot' excitons having excess energy have received a lot of attention but no consensus yet exists [1].

In this talk, I will introduce a method to calculate exciton dissociation rates [2] and will describe its application to 2-Dimensional model organic photovoltaic interfaces. The method uses Green's functions within a widely applicable model Hamiltonian of donor/acceptor interfaces with and without disorder. Initial states are Frenkel excitons while final states are Charge-Transfer (CT) states. I will present results for the generation rates of CT states where I will highlight the importance of disorder and the delocalization of the excitonic wavefunctions. Excitons dissociate into 'hot' CT states with partially separated charges, where electron and hole are located far from the interface.

1) A. A. Bakulin et al., Science 335, 1340 (2012), A. E. Jailaubekov et al., Nat. Mater. 12 66 (2013), G. Grancini et al., Nat. Mater. 12 29 (2013), K. Vandewal et al., Nat. Mater. 13 63 (2013).

2) H. Vazquez, A. Troisi, Phys. Rev. B 88, 205304 (2013).

HL 36.3 Tue 14:45 C 130

Charge separation at C_{60}/P3HT and P3HT/ZnO interfaces probed by femtosecond time-resolved second harmonic generation measurements — •Marc Hänsel[1], Michael Schulze[1], Yunus Sevinchan[2], Yana Vaynzof[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut, Heidelberg, Germany — [2]Centre of Advanced Materials, Heidelberg, Germany

A deeper understanding of the process of ultrafast charge transfer and separation at donor/acceptor interfaces is a prerequisite for improvement of organic and hybrid solar cells. Time-resolved second harmonic generation (TR-SHG) with femtosecond temporal resolution was used to investigate different donor/acceptor interfaces. With this intrinsically interface sensitive technique we were able to monitor the charge transfer dynamics of the well-defined single heterojunctions C_{60}/P3HT and P3HT/ZnO. In addition some modifications via cesium doping were made to the ZnO/P3HT interface. At the C_{60}/P3HT interface a pump energy dependent ultrafast charge transfer state with a population time of 320fs has been observed.

HL 36.4 Tue 15:00 C 130

Modelling charge transfer in Polymer/SWNT/PCMB hybrid systems — •Livia Glanzmann, Duncan Mowbray, and Angel Rubio — Nano-bio Spectroscopy Group and ETSF Scientific Development Centre, Universidad del Pais Vasco UPV/EHU, Av. Tolosa 72, E-20018 San Sebastian, Spain

One way to increase power conversion efficiencies of organic photovoltaic devices (OPVs) is to optimize the electron donor (D) acceptor (A) materials. The level alignment of the frontier orbitals at the D-A heterojunction interface is important for an efficient charge transfer. Since the first heterojunction OPV, consisting of 3-alkylpolythiophene (P3HT) and Fullerene, several combinations of D-A materials were tested. As well, carbon nanotubes were introduced, which increased the efficiency of such multi-component systems. Still, the electronic processes within such systems are not well understood. To shed light on this subject, we simulate photovoltaic processes occuring in selected

sets of P3HT-based-Polymer/SWNT or PCBM heterojunctions. As a first step, we create the excited states within the donor materials by performing TDDFT calculations and extract the electron density of the exciton. Then, we use the delta SCF approach to study the D-A electron transfer. On top, we calculate the probability of an electron passing the D-A interface and being transported through a nanotube by performing G0W0 calculations. All these results show the effect of certain types of D-A material, as well of their level alignment, on the efficiency of OPVs.

HL 36.5 Tue 15:15 C 130

Photoinduced Dynamics of Charge Separation: from Photosynthesis to Polymer-Fullerene Bulk-Heterojunctions — •Andreas Sperlich[1], Oleg G. Poluektov[2], Jens Niklas[2], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Chemical Sciences and Engineering Division, ANL, Argonne, Illinois 60439, USA — [3]ZAE Bayern, 97074 Würzburg

Understanding charge separation and charge transport is crucial for improving the efficiency of organic solar cells. This is due to the excitonic nature of their active media, based on organic molecules, serving as both a light absorbing and transport layer. Charge transfer (CT) states play an important role, being intermediate for free carrier generation and charge recombination. Here, we use light-induced electron paramagnetic resonance (EPR) spectroscopy to study the charge transfer dynamics in composites of the polymers P3HT, PCDTBT, and PTB7 with the fullerene derivative $PC_{60}BM$. Transient EPR measurements show strong spin-polarization patterns for all polymer-fullerene blends, confirming predominant generation of singlet CT states. These observations allow a comparison with charge separation processes in molecular donor-acceptor systems, as found in natural and artificial molecular photosynthetic systems and clarification of the initial steps of sequential charge transfer in organic photovoltaic (OPV) materials. The detection of strong electron spin-polarization in OPV materials points out to the significance of spin dynamics for the efficient functioning of solar cell devices.

HL 36.6 Tue 15:30 C 130

Sub-ns Triplet State Formation in PSBTBT:PC70BM and PCPDTBT:PC60BM Photovoltaic Blends — Fabian Etzold[1], Ian Howard[1,2], and •Frédéric Laquai[1] — [1]Max Planck Research Group for Organic Optoelectronics, Max Planck Institute for Polymer Research, D-55128 Mainz, Germany — [2]Institute of Microstructure Technology (IMT), Karlsruhe Institute of Technology (KIT), D-76344 Eggenstein-Leopoldshafen, Germany

The excited state dynamics in low-bandgap polymer:fullerene blends using the donor-acceptor copolymers PCPDTBT and its silicon-substituted analogue PSBTBT are investigated by femto- to microsecond broadband Vis-NIR transient absorption (TA) pump-probe spectroscopy. The TA experiments and analysis of the TA data by multivariate curve resolution (MCR-ALS) reveal that after exciton dissociation and free charge formation is completed, fast sub-nanosecond nongeminate recombination occurs and leads to a substantial population of the polymer's triplet state. The extent to which triplet states are formed depends on the initial concentration of free charges, which itself is controlled by the microstructure of the blend, especially in case of PCPDTBT:PC60BM. Interestingly, PSBTBT:PC70BM blends show a higher charge generation efficiency, but less triplet state formation at similar free charge carrier concentrations. This indicates that the solid-state morphology and interfacial structure of PSBTBT:PC70BM blends reduce non-geminate recombination and thus triplet state formation, leading to increased device performance compared to optimized PCPDTBT:PC60BM blends.

HL 36.7 Tue 15:45 C 130

Triplet Exciton Formation in High-Efficiency Donor-Acceptor Photovoltaic Blends — •Stefan Väth[1], Hannes Kraus[1], Andreas Baumann[2], Kristofer Tvingstedt[1], Andreas Sperlich[1], Vladimir Dyakonov[1,2], John Love[3], and Thuc-Quyen Nguyen[3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg — [3]University of Santa Barbara, Santa Barbara, CA 93106, USA

In donor-acceptor based bulk-heterojunction solar cells, the splitting of singlet excitons at the donor and acceptor interface is of crucial importance for charge generation. The reversed process, in which two initially free charge carriers meet at the interface to form an exciton with singlet or triplet multiplicity is rather beneficial for light emission in OLEDs but considered as one of the loss factors in OPV.

In our experiments, the occurrence of triplet excitons and CT states was probed by using spin sensitive detection of the photo- and electroluminescence. A substantial generation of molecular triplet excitons was found in high efficiency donor-acceptor OPV systems based on the low bandgap copolymer PTB7 and in the soluble small molecule p-DTS(FBTTh2)2, both blended with PC70BM as acceptor. We ascribe these findings to an electron back transfer from the CT state to the triplet state on the donor material. In summary, the fundamental understanding of the transformation processes involving the CT states, triplet excitons, as well as free electrons and holes and their dependence on nanoscale morphology and energetics of blends is essential for the optimization of OPV devices.

HL 37: Transport: Topological insulators 3 (TT with HL/DS)

Time: Tuesday 14:00–16:00 Location: H 0110

HL 37.1 Tue 14:00 H 0110

Helical Surface States In Strained HgTe — •Jan Boettcher and Ewelina M. Hankiewicz — Universität Würzburg, Faculty for Physics and Astronomy, TP IV

Strained HgTe is a 3D topological insulator with negligible bulk conductivity, where the transport is dominated by the surface states for a wide density range [1]. We analytically show the existence of a topologically protected surface state within the framework of a simplified 6x6 Kane Hamiltonian defined on the half-space. Strained HgTe is different from other 3D TIs due to an additional coupling of the surface states, forming between the light-hole and electron-like (S) bands, to the heavy-hole bands. This coupling causes an avoided crossing between these bands and, therefore, opens a large gap in the surface state spectrum by which the topological protection is not affected. Furthermore, we investigate the spin texture of the surface states. In the presence of an external magnetic field, we study the Landau level spectrum and discuss the experimental signatures which would be a consequence of our model.

We acknowledge grant HA 5893/4-1 within SPP 1666.

[1] Brüne et al., arXiv:1407.6537 (to be published in PRX 2014).

HL 37.2 Tue 14:15 H 0110

Trasport signatures of a Zeeman-split quantum dot coupled to a helical edge state — •Benedikt Probst[1], Pauli Virtanen[2], and Patrik Recher[1] — [1]Institut für Mathematische Physik, TU Braunschweig, 38106 Braunschweig, Germany — [2]O.V. Lounasmaa Laboratory, Aalto University School of Science, Finland

We investigate the transport signatures of a Zeeman-split quantum dot (QD) containing a single spin 1/2 weakly coupled to a helical Luttinger liquid (HLL) within a generalized master equation approach. The HLL induces a tunable magnetization direction on the QD controlled by an applied bias voltage when the quantization axes of the QD and the HLL are noncollinear. This tunability allows to extract characteristic signatures of a HLL and the spin dynamics of the QD via the backscattering conductance and the current noise.

HL 37.3 Tue 14:30 H 0110

Effects of random Rashba spin-orbit coupling and magnetic impurities on edge state transport in topological insulators — Lukas Kimme[1], •Bernd Rosenow[1], and Arne Brataas[2] — [1]Institut für Theoretische Physik, Universität Leipzig, D-04103, Leipzig, Germany — [2]Department of Physics, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway

CdTe/HgTe quantum-wells that exceed a critical thickness host topologically protected edge states, which give rise to a quantized conductance. Despite the topolgical protection, experimentally a mean free path of a few microns is found [1]. The experimentally observed weak temperature dependence of the mean free path challenges proposed

theoretical explanations, many of which predict power law behaviors. We here consider a model where edge electrons experience spatially random Rashba spin-orbit coupling, and are also coupled to a magnetic impurity. Using a rate equation model, we determine the steady state of the impurity spin in the finite bias regime, and compute both linear and nonlinear resistances. For a finite density of impurity spins, we obtain a weak temperature dependence of the mean free path, in agreement with experimental findings.

[1] M. König, S. Wiedmann, C. Brüne, A. Roth, H. Buhmann, L. W. Molenkamp, X.-L. Qi, and S.-C. Zhang, Science 318, 766 (2007).

HL 37.4 Tue 14:45 H 0110

Spin-based Mach-Zehnder interferometry in topological insulator p-n junctions — •Fernando de Juan[1,2], Roni Ilan[1], and Joel E. Moore[1] — [1]University of California, Berkeley — [2]Freie Universität Berlin

A p-n junction, an interface between two regions of a material populated with carriers of opposite charge, is a basic building block of solid state electronic devices. From the fundamental physics perspective, it often serves as a tool to reveal the unconventional transport behavior of novel materials. In this work, we show that a p-n junction made from a three dimensional topological insulator (3DTI) in a magnetic field realizes an electronic Mach-Zehnder interferometer with virtually perfect visibility. This is owed to the confinement of the topological Dirac fermion state to a closed two-dimensional surface, which offers the unprecedented possibility of utilizing external fields to design networks of chiral modes wrapping around the bulk in closed trajectories, without the need of complex constrictions or etching. Remarkably, this junction also acts as a spin filter, where the path of the particle is tied to the direction of spin propagation. It therefore constitutes a novel and highly tunable spintronic device where spin polarized input and output currents are naturally formed and could be accessed and manipulated separately.

HL 37.5 Tue 15:00 H 0110

Broken-gap topological insulators in magnetic fields — Rafał Skolasinski[1], Dimitry Pikulin[2], and •Michael Wimmer[1] — [1]Delft University of Technology, The Netherlands — [2]University of British Columbia, Canada

Two-dimensional topological insulators have helical edge channels protected by time-reversal symmetry, leading to a quantized conductance within the topological gap. A magnetic field breaks time-reversal symmetry, and thus is expected to break the quantization of conductance. Yet, recent experiments on topological insulators in broken-gap InAs/GaSb quantum wells have found very little dependence on magnetic field [1]. We discuss the effects of the orbital and the Zeeman part of the magnetic field on broken-gap quantum wells, and consider in which regime quantized conductance can be preserved.

[1] L. Du et al., arXiv:1306.1925

HL 37.6 Tue 15:15 H 0110

Cherenkov effect in topological insulators — •Sergey Smirnov — Institute for theoretical physics, Regensburg University, 93040 Regensburg, Germany

The Cherenkov radiation discovered experimentally by Cherenkov in optics of transparent media and theoretically explained later by Tamm and Frank reappears in solids where particles move faster than sound and, as a result, excite lattice vibrations or phonons. In both cases the photons or phonons are distributed within a forward cone centered around the momentum of the particle producing the Cherenkov light or sound.

Here we demonstrate that at high energies helical particles on surfaces of topological insulators excite anomalous Cherenkov sound outside the forward cone when the anisotropy of the surface states exceeds a critical value. The sound features many outstanding properties. In particular, at strong anisotropy it localizes into a few forward and backward beams propagating along specific directions [1].

At low energies we predict that an in-plane magnetic field applied to a surface of a topological insulator will asymmetrically reverse the Cherenkov sound. This asymmetric Cherenkov acoustic reverse may be of practical relevance in design of low energy electronic devices such as acoustic ratchets or, in general, in low power design of electronic circuits with an external control of the Cherenkov dissipation [2].

[1] S. Smirnov, Phys. Rev. B 88, 205301 (2013).
[2] S. Smirnov, Phys. Rev. B 90, 125305 (2014).

HL 37.7 Tue 15:30 H 0110

One-dimensional Dirac electrons on the surface of weak topological insulators — •Alexander Lau[1], Carmine Ortix[1], and Jeroen van den Brink[1,2] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, Germany — [2]Department of Physics, TU Dresden, Germany

We show that a class of weak three-dimensional topological insulators feature one-dimensional Dirac electrons on their surfaces. Their hallmark is a line-like energy dispersion along certain directions of the surface Brillouin zone. Interestingly, these one-dimensional Dirac line degeneracies are topologically protected by a symmetry that we refer to as in-plane time-reversal invariance. As an example, we demonstrate how this invariance leads to Dirac lines in the surface spectrum of stacked Kane-Mele systems.

HL 37.8 Tue 15:45 H 0110

Fractional quantization of the topological charge pumped in a 1D superlattice — •Pasquale Marra[1], Roberta Citro[1,2], and Carmine Ortix[3] — [1]CNR-SPIN, I-84084 Fisciano (Salerno), Italy — [2]Dipartimento di Fisica "E. R. Caianiello", Universitá di Salerno, I-84084 Fisciano (Salerno), Italy — [3]Institute for Theoretical Solid State Physics, IFW Dresden, D-01069 Dresden, Germany

A one-dimensional quantum charge pump transfers a quantized charge in each pumping cycle. This quantization is topologically robust being analogous to the quantum Hall effect. The charge transferred in a fraction of the pumping period is instead generally not quantized. We show, however, that with specific symmetries in parameter space the charge transferred at well-defined fractions of the pumping period is quantized as integer fractions of the Chern number. We illustrate in details this fractional quantization in a one-dimensional Harper-Hofstadter model for both periodic and open boundary conditions, and discuss its relevance for cold atomic gases in optical superlattices.

[1] arxiv:1408.4457 [cond-mat]

HL 38: Frontiers of electronic structure theory: Charge and spin dynamics

Time: Tuesday 14:00–15:45 Location: MA 004

Invited Talk HL 38.1 Tue 14:00 MA 004

First-principles theories of electron-plasmon and electron-spin fluctuation interactions in nanomaterials — •Johannes Lischner — Imperial College, London, United Kingdom

The GW method includes an accurate treatment of many-electron interaction effects beyond density-functional theory and is the state-of-the-art approach for computing spectral functions and quasiparticle energies in nanomaterials. These quantities are measured in photoemission and tunneling experiments. Despite its great success, the GW approach has certain shortcomings and I will discuss two topics that require going beyond GW: i) plasmon satellites in spectral functions and ii) the coupling of quasiparticles to spin fluctuations.

Plasmon satellites in recent photoemission experiments on doped graphene have been interpreted in terms of novel plasmaron excitations, strongly coupled plasmon-hole states, predicted by GW theory. Using a cumulant expansion of the Green's function to include higher-order electron-electron interaction effects and an accurate description of the substrate, I will demonstrate that no plasmaron states need to be invoked to explain the experiments. Similar conclusions are drawn for tunneling spectra of semiconductor quantum-well two-dimensional electron gases. I will also discuss the interaction of quasiparticles with spin fluctuations in iron selenide and demonstrate that significant coupling constants can give rise to superconducting transition temperatures consistent with experimental findings.

HL 38.2 Tue 14:30 MA 004

Charge separation dynamics and opto-electronic properties of a diaminoterephthalate-C60 dyad — •Stefano Pittalis[1], Alain

Delgado[1], Jörg Robin[2], Lena Freimuth[3], Jens Christoffers[3], Christoph Lienau[2], and Carlo Andrea Rozzi[1] — [1]Istituto Nanoscienze - CNR, Modena, Italy — [2]Institut fuer Physik and Center of Interface Science, Carl von Ossietzky Universität, Oldenburg, Germany — [3]Institut fuer Chemie and Center of Interface Science, Carl von Ossietzky Universität, Oldenburg, Germany

A novel dyad composed of a diaminoterephthalate scaffold, covalently linked to a Fullerene derivative, is explored as a nanosized charge separation unit powered by solar energy. Its opto-electronic properties are studied and the charge separation rate is determined. Simulations of the coupled electronic and nuclear dynamics in the Ehrenfest approximation are carried out on a sub 100 fs time scale after photoexcitation in order to gain insights about the mechanisms driving the the charge separation. In particular, the role of vibronic coupling and of the detailed morphology are highlighted.

HL 38.3 Tue 14:45 MA 004

Transfering spin into an extended π-orbital of a large molecule – ab-initio study of Au-PTCDA:Au(111) — •T. Deilmann[1], T. Esat[2], B. Lechtenberg[3], P. Krüger[1], C. Wagner[2], R. Temirov[2], F.B. Anders[3], F.S. Tautz[2], and M. Rohlfing[1] — [1]Institut für Festkörpertheorie, Universität Münster, Germany — [2]Peter Grünberg Institute (PGI-3), FZ Jülich, Germany — [3]Lehrstuhl für Theoretische Physik II, TU Dortmund, Germany

The combination of an organic molecule with an unpaired spin offers a large variety of interplay between spins and orbitals, with high sensitivity to structural and environmental details. Recently, a single Au atom on a PTCDA monolayer physisorbed on Au(111) has been investigated experimentally; it exhibits a Kondo peak in the STS spectrum.

In this talk we discuss ab-initio mean-field electronic spectra (which will then serve as input data for a subsequent NRG calculation to describe the Kondo effect). Based on ab-initio structural data (in agreement with observed STM images) we evaluate the electronic spectra by many-body perturbation theory within the *GW* approximation, as well as, a simplified LDA+*GdW* approach [1]. For gas-phase PTCDA and Au-PTCDA, both methods agree well with one another and with available measurements. For Au-PTCDA on Au(111), a full *GW* calculation is too expensive due to the substrate. LDA+*GdW*, on the other hand, fully allows to incorporate the substrate polarizability in the self energy inside the molecule and leads to good agreement with the experimental data.

[1] M. Rohlfing, *Phys. Rev. B* **82**, 205127 (2010).

HL 38.4 Tue 15:00 MA 004

Quasi-particle band structure of the transition-metal-based zero-gap semiconductors — •Murat Tas[1], Ersoy Sasioglu[2], Iosif Galanakis[3], Christoph Friedrich[2], and Stefan Blügel[2] — [1]Department of Basic Sciences, İstanbul Kemerburgaz University, 34217 İstanbul, Turkey — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [3]Department of Materials Science, School of Natural Sciences, University of Patras, GR-26504 Patra, Greece

Zero-gap semiconductors (SCs) are promising materials for a variety of applications ranging from spintronics to thermoelectricity. Using the *GW* approximation within the framework of the FLAPW method, we study the quasi-particle band structure of a number of transition-metal-based zero-gap SCs XX′YZ, where X, X′ and Y are the transition metal elements, and Z is an *sp* element. We find that, in contrast to *sp*-electron based SCs such as Si and GaAs, the many-body renormalization has a minimal effect on the electronic band structure of these systems. It turns out that for many compounds the change of the band gap is less than 0.2 eV, which makes the starting point PBE a good approximation for the description of the electronic properties of these materials. Furthermore, the band gap can be tuned either by the variation of the lattice parameter or by the substitution of the Z element.

HL 38.5 Tue 15:15 MA 004

Keldysh nonequilibrium Green's function vs. Feshbach projection operator approach for plasmon-assisted photoemission — •Yaroslav Pavlyukh, Michael Schüler, and Jamal Berakdar — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany

A unified theoretical treatment of the single and double electron emission is achieved by using the Feshbach projection method. In this formalism the final target's state fixes the projection operator which subsequently determines the effective Hamiltonian and the optical potential for emitted electrons. The method of non-equilibrium Green's functions is a complementary approach which also allows to treat such processes diagrammatically. We explicitly establish a correspondence between these two approaches and illustrate the diagrammatic technique by calculations of the two-electron emission from C_{60} assisted by the excitation of plasmons.

HL 38.6 Tue 15:30 MA 004

Inclusion of thermal lattice vibrations and spin fluctuations within transport calculations — •Sergiy Mankovsky, Kristina Chadova, Diemo Ködderitzsch, Svitlana Polesya, and Hubert Ebert — Dept. Chemie/Physikalische Chemie, Universität München, Butenandtstr. 5-13, D-81377 München, Deutschland

We present an approach for the calculation of response quantities, e.g. Gilbert damping and electrical conductivity, accounting for temperature induced effects of lattice vibrations and spin fluctuations. The approach is based on the alloy analogy model with thermal vibrations and spin fluctuations modeled by random atomic displacements or magnetic moments deviations, respectively. We discuss various models to deal with spin fluctuations, determining their impact on the temperature dependent behaviour of conductivity and Gilbert damping parameter. We demonstrate the non-additivity of the separate contributions to the conductivity. The results of the calculations are compared to experimental data demonstrating a rather good agreement for the systems under consideration.

HL 39: Posters II (Topological insulators; Graphene; Spintronics and spin physics; Quantum information science)

Presenters are kindly requested to be near their poster for at least one hour in the time between 14:00-16:00 or to leave a note about their availability for discussions.

Time: Tuesday 14:00–20:00 Location: Poster F

HL 39.1 Tue 14:00 Poster F

Magnetic and structural stability of topological-insulator / ferromagnet hybrid structures during thermal annealing procedures — •Michal Vališka[1], Martin Vondráček[2], Hubert Steiner[3], Gunther Springholz[3], Václav Holý[1], Vladimír Sechovský[1], and Jan Honolka[2] — [1]DCMP, Charles University, Prague, Czech Republic — [2]IoP, Academy of Sciences of the Czech Republic, Prague, Czech Republic — [3]HFP, Johannes Kepler Universität, Linz, Austria

Magnetic atoms in the vicinity of the topologically protected surface states (TTS) of 3D topological insulators could break time-reversal symmetry and open efficient spin-flip channels for backscattering processes. We have shown earlier that single magnetic adatom spins situated on Bi_2Se_3 surfaces randomly fluctuate at temperatures T∼4 K[1]. In order to achieve stable exchange fields, our present work focuses on MBE-grown heterostructures consisting of thin surface layers of pure Bi_2Se_3 and a buried, remanently magnetized Mn-doped layer. The heterostructure is sealed by a protective Se capping. We present an optimized Se capping and decapping procedure of Mn-doped samples under UHV conditions. Surface properties after decapping are controlled by PEEM and XPS measurements, and the TSS state is monitored in situ by k-PEEM. The important question of potential changes of the magnetic properties of Mn-doped layers (1-10%) due to diffusion effects during decapping at elevated temperatures is addressed via measurements of the bulk magnetization using SQUID.

[1] J. Honolka, et al., Physical Review Letters 108, 256811 (2012)

HL 39.2 Tue 14:00 Poster F

Strain-tuning of Dirac states at the SnTe (001) surface — •Matthias Drüppel, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

The topological crystalline insulator SnTe belongs to the recently discovered class of materials in which a crystalline symmetry ensures the existence of topologically protected Dirac like surface states. In contrast to topological insulators, this symmetry can be broken via deformations of the crystal. This opens up new possibilities of manipulating the Dirac states and inducing a controllable gap. Here, we have employed density-functional theory to investigate the response of the Dirac states to lattice deformations [1].

The (001) surface exhibits four Dirac cones which lie at non-time-reversal-invariant points close to $\overline{\mathrm{X}}$, along the projection of the $(\bar{1}10)$ and (110) mirror planes. Our calculations show that a gap of up to $\approx$ 30 meV can be introduced via lattice deformations that break at least one of these mirror symmetries. Remarkably, distortions at the *surface only* can already open up the gap, even though bulk properties are not changed.

The gap is formed at either all four or just two cones, depending on the direction of the displacement vector, making it possible to create a state where gaped and non-gaped Dirac cones coexist. Notably, if the whole slab is distorted, bulk bands are being pushed into the gap making the whole system metallic.

[1] M. Drüppel *et al.*, Phys. Rev. B 90, 155312 (2014)

HL 39.3 Tue 14:00 Poster F

Vapor phase deposition of bismuth selenide on hexagonal boron nitride — •Shaham Jafarpisheh[1], Regine Ockelmann[1], Kenji Watanabe[2], Takashi Taniguchi[2], Bernd Beschoten[1], and Christoph Stampfer[1,3] — [1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — [2]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan — [3]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany

Three dimensional topological insulators (TIs) have shown unique electronic band structures making them promising materials for future spintronic devices. Topological insulators are materials with electrically insulating bulk while having gapless spin-polarized surface states with a linear dispersion relation which are topologically protected against backscattering resulting in a spin-polarized current on the surface of these materials. Among various materials predicted to show topological insulating properties, Bi2Se3 is in particular interesting because of its band structure and its relatively large bulk band gap of 0.3 eV which is much larger than the room temperature energy scale. In this study we report the vapor phase deposition of large area Bi2Se3 thin flakes on atomically flat surface of hexagonal boron nitride (hBN). Atomic force microscopy (AFM) and Raman spectroscopy were used to characterize the synthesized flakes. Finally, e-beam lithography and metallization is used to make electrical contacts on the as-grown Bi2Se3 flakes for further characterization by electron transport measurements.

HL 39.4 Tue 14:00 Poster F

Cd_3As_2 Nanowires by Chemical Vapour Deposition — •Piet Schönherr and Thorsten Hesjedal — Department of Physics, Clarendon Laboratory, University of Oxford, Oxford OX1 3PU, United Kingdom

Cd_3As_2 has been well known for its very high mobility. Recently, it was discovered that the material displays two Dirac points with linearly dispersing states that are stabilized by crystal symmetry (three-dimensional Dirac semimetal). The Dirac cones live in three-dimensional k-space unlike topological insulators that only have two-dimensional Dirac cones on their surface. This makes Cd_3As_2 a three-dimensional analogue of graphene.

We present the growth and characterisation of Cd_3As_2 nanowires including results from electric transport measurements. Nanowires with a diameter as small as 10 nm were grown in a self-catalysed vapour-liquid-solid process using chemical vapour deposition. We analyse the growth mechanism and compare the vibrational modes of Cd_3As_2 nanostructures with bulk samples.

HL 39.5 Tue 14:00 Poster F

Heteroepitaxial $YBiO_3$ thin films grown by pulsed laser depostion — •Marcus Jenderka, Marius Grundmann, and Michael Lorenz — Institut für Experimentelle Physik II, Universität Leipzig, Linnéstraße 5, D-04103 Leipzig. Germany

The cubic perovskite $YBiO_3$ (YBO) has recently been predicted to be a novel oxide topological insulator candidate by first-principles calculations [1]. In the past, YBO was used as a buffer layer for the high-temperature superconductor $YBa_2Cu_3O_{7-y}$. [2] Its large bulk band gap and high bulk resistivity distinguishes YBO from conventional TIs such as Bi_2Te_3. [3,4] Thus, room-temperature operation and the separation of surface from bulk degrees of freedom promise better TI-based devices.

Here, we report on heteroepitaxy of YBO thin films grown by pulsed laser deposition (PLD) on $LaAlO_3$ single crystalline substrates. Resistivity dependent on magnetic field and film thickness is measured from 300 to 15 K to find signatures of a topological insulator phase.

[1] H. Jin *et al.*, Scientific Reports **3**, 1651 (2013).
[2] G. Li *et al.*, J. Mater. Res. **22**, 2398-2403 (2007).
[3] Y. Xia, Y. *et al.*, Nat. Phys. **5**, 398-402 (2009).
[4] H. Zhang *et al.*, Nat. Phys. **5**, 438-442 (2009).

HL 39.6 Tue 14:00 Poster F

Comprehensive study of undoped Bi_2Se_3 microflakes via structural, chemical and transport investigations — •Dominic Lawrenz[1], Christian Riha[1], Franz Herling[1], Olivio Chiatti[1], Srujana Dusari[1], Jaime Sanchez-Barriga[2], Anna Mogilatenko[3], Lada Yashina[4], Sergio Valencia[2], Ahmet Ünal[2], Oliver Rader[2], and Saskia Fischer[1] — [1]Neue Materialien, Institut für Physik, Humboldt Universität zu Berlin, 12489 Berlin, Germany — [2]Helmholtz-Zentrum-Berlin für Materialien und Energie, 12489 Berlin, Germany — [3]Ferdinand-Braun-Institut, 12489 Berlin, Germany — [4]Department of Chemistry, Moscow State University, 119992 Moscow, Russia

Surface states of topological insulators are expected to show peculiar electrical transport properties [1]. The remaining bulk conductivity, however, renders these elusive in transport measurements so far.

A combined investigation of single-crystalline Bi_2Se_3 was undertaken to obtain a comprehensive picture. The band structure of the bulk material was investigated via ARPES. Flakes from the bulk to the thin-film range (thicknesses from 270 nm to 70 nm) were then exfoliated. Their crystal structure was investigated by HRTEM and the chemical composition by EDX and X-PEEM. Hall measurements of the conductivity were undertaken to determine the charge carrier mobility and density. Our results confirm the high quality of the material. The temperature dependence of the conductivity and magnetoresistance down to 0.3 K are presented and discussed.

[1] Hasan, Kane, *Rev. Mod. Phys.* **82**, 3045 (2010)

HL 39.7 Tue 14:00 Poster F

Electron dynamics of the topological insulator Sb_2Te_2S — •Anna Sophia Ketterl[1], Thomas Kunze[1], Daniel Przyrembel[1], Dominic Lawrenz[1,3], Evgeny Chulkov[2], and Martin Weinelt[1] — [1]Freie Universität Berlin, Germany — [2]UPV/EHU San Sebastian, Spain — [3]Humbold Universität Berlin, Germany

We investigate the electron dynamics of the topological insulator Sb_2Te_2S by means of time-resolved two-photon photoemission measurements with an angle-resolving time-of-flight spectrometer.

Sb_2Te_2S is p-doped and exhibits a Dirac cone 0.3 eV above the Fermi energy at the center of the Brillouin zone. In our experiment, the Dirac cone is populated by an infrared pump-pulse *via* direct absorption and interband scattering from the conduction band. In the Dirac cone we observe picosecond lifetimes. The spectra hint at a stepwise relaxation *via* small-energy transfer processes and strong surface-to-bulk coupling. Cooling of the system leads to faster electron dynamics.
The observed dynamics are governed by electron-phonon and defect scattering. Thus our measurements confirm the supercollision model which was proposed for graphene.[1]

Quality and component stoichiometries of the samples were studied by XPS after different preparation methods. We find that Sb_2Te_2S is rather inert and only slowly oxidizes after cleaving under ambient conditions.

[1] J. C. W. Song *et. al.*, *Phys. Rev. Let.* **109**, 106602 (2012).

HL 39.8 Tue 14:00 Poster F

Fabrication and characterization of InAs/GaSb compound quantum wells for electrically tunable topological insulator devices — •Georg Knebl, Pierre Pfeffer, and Martin Kamp — Technische Physik, Universität Würzburg, Deutschland

InAs/GaSb compound quantum wells (CQW) sandwiched between two AlSb barrier layers were proposed by Liu et al. [1] to show a topological phase similar to the one realized in HgTe/CdTe [2]. While in the

HgTe/CdTe system the transition from the normal to the topical insulator state can only be tuned by a variation of the quantum well thickness, for InAs/GaSb CQWs this is predicted to be tunable by the gate voltage. Our structures are fabricated by molecular beam epitaxy on GaSb and GaAs substrates, with an additional buffer structure on the latter ones. We will present results on the growth and fabrication of gated CQW structures for quantum spin Hall field effect transistors. Transport data and reversible light induced switching of majority carriers from electrons to holes will be shown.

[1] C. Liu, T. Hughes, X.-L. Qi, K. Wang, and S.-C. Zhang, Quantum Spin Hall Effect in Inverted Type-II Semiconductors, Phys. Rev. Lett., vol. 100, no. 23, p. 236601, Jun. 2008.

[2] M. König, S. Wiedmann, C. Brüne, A. Roth, H. Buhmann, L. W. Molenkamp, X.-L. Qi, and S.-C. Zhang, Quantum spin hall insulator state in HgTe quantum wells., Science, vol. 318, no. 5851, pp. 766-70, Nov. 2007.

HL 39.9 Tue 14:00 Poster F

Suspended graphene nanoribbons fabricated by electron beam-induced nano-etching — •Alessio Miranda, Jens Sonntag, Benedikt Sommer, Daniel Braam, Günther Prinz, Martin Geller, and Axel Lorke — Faculty of Physics, Universität Duisburg-Essen, Lotharstraße 1 Duisburg, 47058 Germany

Suspended graphene without any contact to a substrate is the ultimate two-dimensional system based on the honeycomb lattice structure of carbon atoms. However, the fabrication of nanodevices in suspended graphene needs a processing technique that preserves ideally its lattice structure or should be at least minimally invasive. We use here a fabrication technique based on electron beam induced nano-etching, which can cut suspended graphene with a resolution down to 7 nm. We show its use for the fabrication of suspended nanoribbons (GNR) and nanoribbons with asymmetric width (nanoconstrictions). The structural quality of suspended graphene after the cut is investigated using both 2D Raman spectroscopy and electrical characterization. Comparison of Raman maps taken on the same area before and after cutting confirm that the lattice structure still has a high quality. The electrical measurements of graphene nanoribbons show the characteristic conductance diamond as a function of drain and backgate voltage. Asymmetric nanoribbons show current rectification as a function of the drain voltage. The dependence of the rectification ratio on the back gate voltage is also studied.

References: [1] C. Thiele, et al. Carbon 64, 84 (2013). [2] B. Sommer, et al., Scientific Reports, submitted (2014).

HL 39.10 Tue 14:00 Poster F

Optical spectroscopy on ultrathin $NbSe_2$ and $NbSe_2$-semiconductor heterostructures — •Sven Gelfert[1], Nicola Paradiso[1], Gerd Plechinger[1], Philipp Nagler[1], Philipp Tonndorf[2], Steffen Michaelis de Vasconcellos[2], Rudolf Bratschitsch[2], Christoph Strunk[1], Christian Schüller[1], and Tobias Korn[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany — [2]Physikalisches Institut, Westphälische Wilhelms-Universität Münster, 48149, Münster, Germany

$NbSe_2$ is a layered transition metal dichalcogenide with a superconducting transition. By applying an exfoliation method, it can be thinned down to a few molecular layers and be transfered onto a Si/SiO_2 substrate. We have produced $NbSe_2$ flakes with "terraces" of different thickness down to the nanometer scale. In Raman measurements we observed a layer-dependent frequency shift in the characteristic phonon modes.

Furthermore, we have produced heterostructures by combining singlelayer WSe_2 and $MoSe_2$ with ultrathin $NbSe_2$. In time-resolved photoluminescence experiments on these heterostructures we observed a dynamic charge transfer between the semiconducting layer and the adjacent $NbSe_2$. We have analysed the photocarrier dynamics of both, isolated $WSe_2/MoSe_2$ single layers, and heterostructures, as a function of temperature.

HL 39.11 Tue 14:00 Poster F

Stacked Graphene nanostructures produced from transfered layers — •Christopher Belke, Dmitri Smirnov, Johannes C. Rode, Hennrik Schmidt, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, D-30167 Hannover, Germany

Here we report on graphene sheets, stacked by a transfer method [1] to produce novel complex layersystems.

Graphene is exfoliated on a thin PMMA layer, which can be detached from the silicon wafer. This layer is then placed on other graphene mono- or bilayer flakes.

The samples were characterized at low temperatures and in dependence of a magnetic field. Measurements show interesting novel effects, e. g. high resistance extrema near the charge neutrality point and magnetic field independent oscillations.

[1] C. Dean et al. Nature Nanotechnology **5**, 722 (2010)

HL 39.12 Tue 14:00 Poster F

Hartree-Fock theory in the full Brillouin zone of graphene — •Prakash Parida[1], Maxim Trushin[2], Tobias Stauber[3], and John Schliemann[1] — [1]Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany — [2]Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — [3]Departamento de Teoría y Simulación de Materiales, Instituto de Ciencia de Materiales de Madrid, CSIC, E-28049 Madrid, Spain

Within the Hartree-Fock approximation, we explore how pseudospin texture and conductivity in the full Brillouin zone of graphene can be tuned by the electron-electron interactions. The pseudospin texture in the in-plane phase remains same as that of the non-interacting case. In the out-of-plane phase, the exchange interaction lifts the singularity of the pseudospin vector field at the Dirac point and the z-component of pseudospin orientation becomes maximum at the Dirac point. We find a semimetal-insulator transition at a critical value of $\alpha = \alpha_c$ (α = effective fine structure constant). The exchange interaction breaks the parity and the broken symmetry state in turn becomes the ground state in the pseudospin out-of-plane phase for $\alpha > \alpha_c$. While the renormalization of the Fermi velocity occurs in the in-plane gapless phase, a gap is generated in the broken symmetry out-of-plane phase. Finally, the out-of-plane pseudospin component shows optical valley Hall effect and polarization sensitive interband optical absorption.

HL 39.13 Tue 14:00 Poster F

Quantitative transmission electron microscopy of two-dimensional transition metal dichalcogenides — •Florian Winkler[1], Amir H. Tavabi[1], Emrah Yucelen[2], Beata E. Kardynal[3], and Rafal E. Dunin-Borkowski[1] — [1]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons and Peter Grünberg Institute 5, Research Centre Jülich, Germany — [2]FEI Company, Achtseweg Noord 5, 5600 KA Eindhoven, The Netherlands — [3]Peter Grünberg Institute 9, Research Centre Jülich, Germany

Layered transition metal dichalcogenides (TMDs) have been the subject of intense research for applications in nanoelectronics. Strong spin-orbit interactions combined with a direct bandgap in monolayers of MX_2 (M: Mo, W; X: S, Se) have been shown to make TMDs very attractive for spintronics and valleytronics. The layered structures of TMDs make them ideal for quantitative studies using transmission electron microscopy (TEM), which can further be compared with device performance. Here, we study WSe_2 samples with thicknesses of between 1 and 4 monolayers using several quantitative TEM techniques, including off-axis electron holography and high-angle annular dark-field scanning TEM. We show that challenges associated with sample contamination, sample stability and and electron-beam-induced charging can be minimised through experimental design and a careful choice of imaging parameters. We perform statistical analyses of phase shifts measured using medium-resolution and high-resolution off-axis holography to measure the mean inner potentials of the samples and the numbers of S or Se atoms in individual atomic columns, respectively.

HL 39.14 Tue 14:00 Poster F

Bend Resistance in Nanoscale Epitaxial Bilayer Graphene Cross Junctions — •Epaminondas Karaissaridis[1], Claudia Bock[1], Florian Speck[2], Thomas Seyller[2], and Ulrich Kunze[1] — [1]Werkstoffe und Nanoelektronik, Ruhr-Universität Bochum — [2]Technische Physik, Technische Universität Chemnitz

We investigated inertial-ballistic transport in nanoscale orthogonal cross junctions prepared on epitaxial bilayer graphene on SiC(0001) [1]. The average film thickness of 1.8 layers was determined by XPS measurements. Hall bars were used to characterize the graphene bilayer by Hall measurements in a temperature range of 1.5 K $\leq T \leq$ 300 K. At low temperatures ($T \leq 50$ K) a mobility of $\mu \approx 1400$ cm^2/(Vs) and an electron density of $n \approx 4 \cdot 10^{12}$ cm^{-2} were determined. 50 nm wide cross junctions were studied in bend resistance geometry by DC measurements. We obtained a negative bend resistance of $R = -525\ \Omega$ at $T = 4.2$ K indicating ballistic transport. The measured bend resis-

tance is three times higher than the value obtained from similar devices on monolayer graphene [2, 3]. Even at $T = 100$ K, we determined a negative bend resistance of $R = -110\ \Omega$ which promises ballistic transport well above 100 K. We suppose that the enhanced bend resistance in bilayer graphene is a consequence of its bandgap. This results in a depletion region that reduces scattering at the edges which is an important scattering mechanism in narrow graphene channels.

[1] T. Ohta *et al.*, Science **313**, 951 (2006).
[2] S. Weingart *et al.*, Appl. Phys. Lett. **95**, 262101 (2009).
[3] C. Bock *et al.*, Nanotechnology **23**, 395203 (2012).

HL 39.15 Tue 14:00 Poster F

Correlation between structural and electrical properties of transition metal dichalcogenide transistors — •Florian Winkler[1], Sven Borghardt[2], Martial Duchamp[1], Rafal E. Dunin-Borkowski[1], and Beata E. Kardynal[2] — [1]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons and Peter Grünberg Institute 5, Research Centre Jülich, Germany — [2]Peter Grünberg Institute 9, Research Centre Jülich, Germany

Layered transition metal dichalcogenides (TMDs) have been researched intensively as materials for low power transistors. Strong spin orbit interactions combined with a direct bandgap in monolayers of MX_2 (M: Mo, W; X: S, Se) make them very attractive for spintronics and valleytronics. The realization of the promise offered by these materials depends on the ability to access their intrinsic properties, rather than measuring the effect of the environment.

In this work, we compare the electrical conductance of TMD field effect transistors with the structural properties of TMD films that were prepared in the same way. We study several combinations of channel materials (WSe_2 and MoS_2) and metals (Sc, Ti/Au, Pd) prepared using different techniques and measured under different conditions. We show clear correlations between the level of contamination of the films and their measured electrical characteristics. We discuss the effect of metal deposition on the compositions and properties of the TMD films. The results strongly suggest that the performance of TMD transistors is limited by the contamination of the channel material, as well as by interactions of metals with the TMD during metal deposition.

HL 39.16 Tue 14:00 Poster F

Scanning Tunneling Microscopy And Spectroscopy of Metallic Islands on Graphene/Cu and Graphene/SiO_2 — •Anne Holtsch, Tobias Euwens, and Uwe Hartmann — Institut für Experimentalphysik, Universität des Saarlandes, Saarbrücken

Using scanning probe techniques we investigate how graphene interacts electronically with various types of substrates in the presence of metallic islands. In the case of transition metals, due to the hybridization of their d orbital the p_z orbital of graphene, the band structure is significantly altered with respect to graphene [1]. By contrast, the interaction is expected to be much weaker for insulating SiO_2. Using scanning tunneling spectroscopy (STS) the different effects of the two substrates Cu and SiO_2 are investigated for absent and present metallic islands. The islands made from gold, nickel, or cobalt are put onto graphene by in-situ evaporation. Afterwards their relative orientation with respect to the graphene lattice was observed by scanning tunneling microscopy (STM). We further heat the system to induce intercalation of the metallic islands, resulting in a second change of the band structure of the sample. Due to specific Moiré patterns the intercalation processes are observable in STM images. Our goal is to evaluate how strongly the band structure measured via STS depends on the material properties of both the substrate and the metallic islands.

[1] E. N. Voloshina and Yu. S. Dedkov, Mater. Res. Express 1, 035603 (2014), arXiv:1405.2556.

HL 39.17 Tue 14:00 Poster F

Electrostatic induced graphene superlattice — •Nicolas Kurz — Institute of Nanotechnology, Karlsruhe Institute of Technology, Hermann-von-Helmholtz Platz 1, D- 76021 Karlsruhe, Germany

Graphene exhibits extraordinary transport properties such as extremly high electron mobility or outstanding thermal conductivity. What is maybe the most fascinating aspect of graphene is its linear dispersion in the vicinity of the K point, which is, hence, called Dirac point. It was predicted that by applying a periodic potential to graphene, the band structure can reveal extra Dirac points. So far the emergence of additional dirac points has been observed experimentally when graphene was put on top of hexagonal boron nitride, having same lattice structure and similar lattice constant. Due to the Van- der Waals interaction, a Moiré pattern is created which induces a superlattice.
However, this method lacks of tunability of the superlattice potential. We try to overcome this problem by using a special patterned metal gate which generates a 1D periodic potential. We use electron beam lithography and graphene encapsulated between hexagonal boron nitride in order to enhance the graphene's transport properties. These type of heterostructure has been become known as 'Van der Waals heterostructures' recently. We use a home-made transfer set-up and mechanical exfoliated material for the assembly of the heterostructure.

HL 39.18 Tue 14:00 Poster F

Graphene Ruthenium Complex Phototransistors — •Nicolai Walter — Institute of Nanotechnology, Karlsruhe Institute of Technology, Hermann-von-Helmholtz Platz 1, D- 76021 Karlsruhe, Germany

Graphene exhibits interesting electronic, optical, and mechanical properties, e.g. ultrahigh charge carrier mobility, broad spectra transmission, and superior strain resistance. These features make graphene a promising material in a variety of fields, i.a. flexible electronics.

However, due to the negligible thickness (atomic monolayer) and therefore small optical absorption together with short recombination times an efficient photodetection is not possible with bare graphene. This issue can be addressed by using graphene heterostructures where other materials or structures make up for those shortcomings.

We investigate graphene heterostructure phototransistors, consisting of a layer of photoactive ruthenium complex molecules imbedded between two cvd graphene sheets. The molecules are functionalized by pyrene moieties which enable them to attach to the graphene surface by π-π-stacking. In order to apply a defined amount of molecules a nanoimprint technique is applied using PDMS stamps aiming towards a monolayer of molecules. After the fabrication of test samples, the interaction between the ruthenium complex molecules and the graphene is to be investigated by measuring the change in electronic properties with illumination. In order to further determine the type of photoresponse, a temperature dependence measurement shall be conducted within a cryostat down to 4 K.

HL 39.19 Tue 14:00 Poster F

Thermal induced lattice distortion of diluted magnetic semiconductors — •Holger Göhring, Michael Paulus, Thomas Büning, Simon Wulle, Karin Esch, Christian Sternemann, Manfred Bayer, and Metin Tolan — Fakultät Physik/DELTA, Technische Universität Dortmund, 44221, Germany

Diluted magnetic semiconductors, which combine the properties of semiconductors and ferromagnets have been an important subject in materials science. Semiconductors with Curie temperatures above room temperature could revolutionize the field of spintronics by allowing control of the magnetization via application of voltage as observed e.g. for the ferromagnetic material galfenol. Magnetic semiconductors, which are currently under investigation, still show a rather low Curie temperature making them inapplicable for application. However, GaMnAs seems to be a promising candidate for high Curie temperature material. GaMnAs is typically grown epitaxially on GaAs substrates with a limited manganese content of a few percent. This system was studied intensively in the past years. To understand the relation between ferromagnetic and structural properties, high resolution x-ray diffraction experiments were performed at beamline BL9 of DELTA using a photon energy of 20 keV and a helium flow cryostate setup. The small changes in the GaMnAs lattice were determined by measuring both, the GaAsMn (004) and the GaAs(004) reflection of the substrate which serves as an internal reference. Our investigation hints on an impact of the ferromagnetic order on the lattice of GaMnAs. However, the data analysis is still in progress.

HL 39.20 Tue 14:00 Poster F

Modeling Magnetism of Diluted Magnetic Semiconductors using the Gutzwiller Method — •Thorben Linneweber — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund

Diluted magnetic semiconductors are materials in which magnetic ions substitutionally or interstitially replace a fraction of the cations of the semiconductor host material. We aim to describe the magnetic properties of $Cd_{1-x}Mn_xTe$ by combining the theory of strongly correlated electrons to semiconductor band theory. We use a multiband hubbard model with s,p-orbitals for the host and s,p,d-orbitals for the manganese ions. The one-particle hamiltonian is obtained via downfolding from DFT calculations using the Wannier90 Code. The effect of the

strongly correlated Mn d-electrons is treated within the Gutzwiller method. To model the diluted nature of the magnetic substitutions a supercell approach is incorporated. As the manganese magnetic moment is known to be close to a $S = 5/2$ state the central question is how much this state is an atomic-like Hund's rule state. One of our further goals is to extract the coupling constants for a Heisenberg model.

HL 39.21 Tue 14:00 Poster F

Strain-controlled magnetically doped III-V semiconductors — •Stefan Stagraczyński[1], Czesław Jasiukiewicz[2], Vitalii Dugaev[2], and Jamal Berakdar[1] — [1]Institute für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle(Saale), Germany — [2]Department of Physics, University of Technology, 35-959 Rzeszów, Poland

We investigate the 6-band Kane model for the valence band structure of III-V magnetic semiconductors, motivated by finding a general way to effectively control magnetic properties which are strongly coupled with elastic properties. In particular, we map out how uni/bi-axial strain can be used to tune the system. We analyze the complex dependence of total energy on the applied magnetization and compressive/tensile strain under selected hole concentrations and explain the effects of magnetic anisotropy in semiconductors. As an example, we have chosen the GaMnAs semiconductors system. Applying strain the has a strong impact on the total energy and can increase the magnetic anisotropy substantially. Further, we find the dependency of the total energy on the hole concentration in the presence of strain, magnetization and its direction. The results show symmetry properties, the importance of strain and magnetization in the semiconductors system.

HL 39.22 Tue 14:00 Poster F

Hole spin g-factor anisotropy in coupled GaAs/AlAs quantum wells — •Michael Kempf[1], Christian Gradl[1], Dieter Schuh[1], Dominique Bougeard[1], Roland Winkler[2], Christian Schüller[1], and Tobias Korn[1] — [1]Universität Regensburg, D-93040 Regensburg, Germany — [2]Northern Illinois University, DeKalb, Illinois 60115, USA

Using time resolved Kerr rotation (TRKR) we measured the spin dynamics of hole ensembles at low temperatures in undoped coupled quantum well (QW) structures prepared on GaAs substrates with different growth directions. By gating the double QW system we were able to separate the optically generated electron-hole-pairs into the different QW's, leading to a dominance of holes in the broader QW. As a result, we achieved spin dephasing times of several hundreds of picoseconds for the hole ensembles.

Thus, we were able to measure a strong anisotropy of the in-plane hole g-factor. For this, we altered the direction of the magnetic field applied with respect to the QW [1-10] axis in the QW plane. The arising results were in good agreement with numerical expectations.

HL 39.23 Tue 14:00 Poster F

Persistent Spin States in Two-Dimensional Hole Gases in Strained Quantum Wells — •Paul Wenk[1], Michael Kammermeier[1], Klaus Richter[1], Roland Winkler[2], and John Schliemann[1] — [1]Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany — [2]Department of Physics, Northern Illinois University, IL 60115 DeKalb, US

In 2003 a particular relation between the spin-orbit coupling (SOC) due to bulk inversion asymmetry (Dresselhaus type SOC) and structure inversion asymmetry (Rashba type SOC) in two-dimensional (2D) electron systems has been found which gives rise to a spin-preserving symmetry.[1] Accordingly, we investigate in our present work the conditions for long-living spin-states in 2D hole gases in zincblende type semiconductor heterostructures. Extending our previous results on the persistent spin helix[5] by including, in addition to both Rashba and Dresselhaus SOC, a shear stress and a symmetric in-plane strain allows for the identification of new persistent spin states. The latter are in contrast to previous results[4,5] which require restrictions on the band model parameters (here the Luttinger parameters) which are difficult to realize in real materials.

* * *

[1] Schliemann *et al.*, PRL **90** 146801 (2003)
[2] Bernevig *et al.*, PRL **97** 236601 (2006)
[3] Kohda *et al.*, PRB **86** 081306 (2012)
[4] Sacksteder *et al.* PRB **89**, 161307(R) (2014)
[5] Dollinger *et al.* PRB **90**, 115306 (2014)

HL 39.24 Tue 14:00 Poster F

(Magneto-)Optical Characterization of Sputter Deposited $La_{0.75}Sr_{0.25}MnO_3$ Thin Films — •Patrick Thoma[1], Manuel Monecke[1], Oana T. Ciubotariu[1,2], Roxana Dudric[2], Dietrich R. T. Zahn[1], and Georgeta Salvan[1] — [1]Semiconductor Physics, Technische Universität Chemnitz, D-09107 Chemnitz, Germany — [2]Faculty of Physics, Babes-Bolyai University Cluj-Napoca, RO-400084 Cluj-Napoca, Romania

$La_{1-x}Sr_xMnO_3$ (LSMO) is considered as a promising material for spintronic devices. Furthermore, via changing preparation conditions and/or stoichiometry of LSMO, one can tune the magnetic and transport properties[1].

LSMO with x = 0.33 has been widely investigated in this context. Here, $La_{0.75}Sr_{0.25}MnO_3$ thin films of different thicknesses ranging from 10 to 300 nm were grown on (111) p-doped Silicon with native SiO_2 by pulsed radio frequency magnetron sputtering at room temperature. The oxygen flow rate during the deposition process as well as the post-annealing temperature were optimized in order to obtain smooth (roughness $<$ 1 nm) and crystalline films.

Access to the dielectric function was provided by measuring and modelling spectroscopic ellipsometry data and by recording magneto-optical Kerr effect (MOKE) spectra the off-diagonal elements of the dielectric tensor were evaluated.

[1]Majumdar, S., van Dijken, S.: Pulsed laser deposition of $La_{1-x}Sr_xMnO_3$: thin-film properties and spintronic applications. Journal of Physics D (2014)

HL 39.25 Tue 14:00 Poster F

Effect of Surface Acoustic Wave Induced Strain on Spin Dynamics — •Johannes Wanner[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

Surface acoustic waves (SAW) have proven to be useful for driving charge and spin in quantum wells. By effectively separating spatially electrons and holes, spin transport by a SAW eludes the Bir-Aronov-Pikus relaxation mechanism. The piezo-electric in-plane field of the SAW allows to concentrate carriers in narrow pockets [1]. The suppression of the Dyakonov-Perel' spin relaxation mechanism based on the dominating spin-orbit interactions (Dresselhaus and Rashba) can thus be explained [2]. In this work, we study additional relaxation mechanisms, namely spin-orbit interaction due to strain and an out-of-plane electric field.

[1] H. Sanada et al., Phys. Rev. Lett. **106**, 216602 (2011); O. Couto et al., Phys. Rev. B **78**, 153305 (2008)
[2] J. Wanner et al., Adv. Mater. Interfaces **1**, 1400181 (2014)

HL 39.26 Tue 14:00 Poster F

Spectroscopy of surface-induced noise using shallow spins in diamond — •Christoph Müller[1], Thomas Unden[1], Yoav Romach[2], Lachlan Rogers[1], Boris Naydenov[1], Liam McGuinness[1], Nir Bar-Gill[2], and Fedor Jelezko[1] — [1]Institute for Quantum Optics and Center for Integrated Quantum Science and Technology, University of Ulm, 89081 Ulm, Germany — [2]The Racah Institute of Physics, The Center for Nanoscience and Nanotechnology, The Hebrew University of Jerusalem, Jerusalem 91904, Israel

Nitrogen-vacancy centres (NV) in diamond located a few nanometers below the surface were exploit to gain insight into the dynamics of the surface noise spectrum they experience. A double-Lorentzian noise spectrum was resolved, consisting of a slow component arising from spin-spin interactions of an electronic spin bath and a faster component related to phononic coupling. Dynamical decoupling sequences were used to decouple the NV spin from this surface noise and enhance their coherence properties.

HL 39.27 Tue 14:00 Poster F

NMR spectroscopy with single spin sensitivity — •Himadri Chatterjee[1], Christoph Müller[1], Xi Kong[1,2], Jiangming Cai[3], Junichi Isoya[4], Jiangfeng Du[2], Martin Plenio[3], Boris Naydenov[1], Liam McGuinness[1], and Fedor Jelezko[1] — [1]Institute for Quantum Optics, Ulm University, Albert-Einstein-Allee 11, Ulm 89081, Germany — [2]Synergetic Innovation Center of Quantum Information and Quantum Physics, University of Science and Technology of China, Hefei 230026, China — [3]Institute for Theoretical Physics, Albert-Einstein Allee 11, University of Ulm, Ulm D-89081, Germany — [4]Research Center for Knowledge Communities, University of Tsukuba,

1-2 Kasuya, Tsukuba, Ibaraki 305-8550 Japan

Nitrogen-vacancy (NV) centres in diamond located as close as a few nanometers to the diamond surface were exploit as a NMR quantum sensor to detect signals from strongly coupled nuclear spins placed on the surface. We achieved depth calibration for the NV in the range of tenth of nanometers by using 1-H spins and detection of down to 4 individual spins by using 29-Si. Using advanced techniques from signal processing (compressed sensing) the location of these spins could be calculated with Angström resolution.

HL 39.28 Tue 14:00 Poster F

Creation and Stabilization of Shallow Nitrogen-Vacancy Centers by Surface Plasma Termination — •Christian Osterkamp[1], Johannes Lang[1], Jochen Scharpf[1], Christoph Müller[1], Liam Paul McGuiness[1], Thomas Diemant[2], Rolf Jürgen Behm[2], Boris Naydenov[1], and Fedor Jelezko[1] — [1]Institut für Quantenoptik, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany — [2]Institut für Oberflächenchemie und Katalyse, Ulm University, Albert-Einstein-Allee 47, 89081 Ulm, Germany

Nitrogen-vacancy centers (NV) in diamond a few nanometers below the crystal surface can be used as magnetic field sensors with very high sensitivity and spatial resolution. The fluorescence of single NVs can be detected and it's electron spin can be polarized, read-out and manipulated at ambient conditions. We created shallow NV centers by nitrogen delta doping during a plasma enhanced chemical vapor deposition (PECVD) growth process. After stabilizing the NV's negative charge state by a SF6 plasma treatment, the hydrogen nuclear magentic resonance signal from protons in the immersion oil were detected.

HL 39.29 Tue 14:00 Poster F

All-optically induced EPR in Mn-doped quantum wells — •Markus Kuhnert, Ilya Akimov, Dimitri Yakovlev, and Manfred Bayer — TU Dortmund

The field of spintronics, which in contrast to electronics, uses the spin instead of charge as information carrier, presents many interesting possibilities. For proper implementation of spintronic devices, research of adequate materials and methods is required. Here we present the results of our research into Manganese doped GaAs quantum wells, which might offer long lived spin coherence as well as spin manipulation mediated by the magnetic Manganese ions.

Following initial studies of electron lifetime in Manganese-doped GaAs quantum wells via time resolved Kerr effect and time resolved Photoluminescence measurements, further investigation into such samples is done by Electron paramagnetic resonance measurements. In this case, a method of all optical Electron paramagnetic resonance was developed. This is achieved by intensity modulation of the incident laser beam by a frequency of about 9.2 GHz and applying varying external magnetic fields.

HL 39.30 Tue 14:00 Poster F

Spin Noise Spectroscopy on single InAs Quantum Dots — •Julia Wiegand[1], Ramin Dahbashi[1], Jens Hübner[1], Klaus Pierz[2], Arne Ludwig[3], Andreas Wieck[3], and Michael Oestreich[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, Abteilung Nanostrukturen, Appelstraße 2, D-30167 Hannover, Germany — [2]Physikalisch Technische Bundesanstalt, Bundesallee 100, D-38116 Braunschweig, Germany — [3]Ruhr-Universität Bochum, Angewandte Festkörperphysik, Universitätsstraße 150, D-44801 Bochum, Germany

The spin dynamics of electrons and holes confined in InAs quantum dots (QDs) are of particular interest for future applications in solid state quantum information processing. We employ spin noise spectroscopy (SNS) to access the intrinsic spin dynamics of confined carriers in individual QDs [1]. Measurements of single heavy hole spin dynamics reveal very long spin lifetimes up to 180 μs and a strong dependence of the longitudinal heavy hole spin relexation time for low magnetic fields [2]. The observed parasitic influence of charge fluctuations in the QD vicinity can be reduced by embedding the QDs in a Schottky diode structure. This also yields the advantages of deterministic charge control and tuning of the QD resonance via the quantum confined Stark effect.

[1] J. Hübner, F. Berski, R. Dahbashi, and M. Oestreich, physica status solidi (b) **251**, 1824 (2014).

[2] R. Dahbashi, J. Hübner, F. Berski, K. Pierz, and M. Oestreich, Phys. Rev. Lett. **112**, 156601 (2014).

HL 39.31 Tue 14:00 Poster F

Spin noise spectroscopy of artificial atoms in isotopically enriched ^{28}Si:P — •Michael Beck[1], Helge Riemann[2], Jens Hübner[1], and Michael Oestreich[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr.2, D-30167 Hannover — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, D-12489 Berlin

Spins of donor atoms in a silicon host are promising candidates for the implementation of quantum information devices [1]. The decoupling of donor atoms from the nuclear spin bath of the host lattice by means of isotopical enrichement leads to very long coherence times of donor electron spins [2]. Here, we will employ semiconductor spin noise spectroscopy [3] to investigate the spin dynamics of donor bound electrons in ^{28}Si:P in the millikelvin temperature regime. The nonperturbative character of this method allows for the extraction of the intrinsic electron spin coherence time and is anticipated to reveal additional dephasing mechanisms at ultra low temperatures.

[1] B.E. Kane, Nature **393**, 133 (1998).

[2] A.M. Tyryshkin, S. Tojo, J.J.L Morton, H. Riemann, N.A. Abrosimov, P. Becker, HJ. Pohl, T. Schenkel, M.L.W Thewalt, K.M. Itoh, S.A. Lyon, Nature Matter. **11**, 143, (2012).

[3] J. Hübner, F. Berski, R. Dahbashi and M. Oestreich, physica status solidi (b) **251**, 1824 (2014).

HL 39.32 Tue 14:00 Poster F

Stokes Polarimetry of the Voigt Effect in Semiconductors — •Pavel Sterin, Fabian Berski, Agnes Beichert, Jens Hübner, and Michael Oestreich — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany

The recently observed intriguing connection between spin-polarization control of optically injected carriers by linearly polarized light and magnetically induced birefringence raises the need in a method of precise characterization of the light beam polarization [1]. This birefringence in non-centrosymmetric materials under the influence of magnetic fields is known as the macroscopic Voigt effect and can cause significant changes of the degree of linear polarization. The change in polarization scales with the second power of the applied transversal magnetic field strength and depends strongly on parameters like the angle of incidence, the sample temperature, and the laser energy.

Here, we employ a self-built Stokes polarimeter and develop a customized Mueller-matrix formalism, which allows us to recover all important magnetic field dependent polarization properties of the light. We accurately investigate this setup and determine its limitations and applicability for such highly sensitive measurements [2].

[1] K. Schmalbuch, S. Göbbels, P. Schäfers, C. Rodenbücher, P. Schlammes, T. Schäpers, M. Lepsa, G. Güntherodt, B. Beschoten, Phys. Rev. Lett., **105**, 246603 (2010) [2] C. Flueraru, S. Latoui, J. Besse, P. Legendre, IEEE T INSTRUM MEAS, **57**, 731 (2008)

HL 39.33 Tue 14:00 Poster F

Optical analysis of ultrapure GaAs:Si for spintronics — •Magnus Neumann[1], Fabian Berski[1], Andreas Wieck[2], Jens Hübner[1], and Michael Oestreich[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, 30167 Hannover — [2]Angewandte Festkörperphysik, Ruhr-Universität Bochum, Universitätsstr. 150, 44780 Bochum

Isolated donor electron spins in GaAs are suitable candidates for performing quantum information processing. Their intrinsic spin dynamics can be probed by spin noise spectroscopy [1] which requires detailed knowledge of the donor bound exciton resonances and other related optical transitions in the spectral window of interest. Therefore we perform optical absorption measurements in the (D^0X) regime on a free-standing layer of high quality MBE-grown GaAs with residual impurity density of $n \sim 10^{14}\,\mathrm{cm}^{-3}$. Besides the well-known bound exciton transitions we quantify the pronounced peak-splitting of the free exciton resonance which is consistently explained within the exciton-polariton framework [2]. A quantative lineshape analysis confirms the high purity of our sample [3] and helps to monitor the (D^0X) occupancy.

[1] J. Hübner, F. Berski, R. Dahbashi, and M. Oestreich, physica status solidi (b) **251**, 1824 (2014).

[2] E.S. Koteles, J. Lee, J.P. Salerno, and M.O. Vassell, Phys. Rev. Lett. **55**, 867 (1985).

[3] W.L. Bloss, E.S. Koteles, E.M. Brody, B.J. Sowell, J.P. Salerno, and J.V. Gormley, Solid State Communications **54**, 103 (1985).

HL 39.34 Tue 14:00 Poster F

Enhanced spin noise spectroscopy by interferometric detection — •Jennifer Haack, Ramin Dahbashi, Fabian Berski, Jens Hübner, and Michael Oestreich — Leibniz Universität Hannover, Institut für Festkörperphysik, Abteilung Nanostrukturen, Appelstraße 2, D-30167 Hannover, Germany

We present an enhanced method for minimally invasive measurements of the spin dynamic. In the past few years spin noise spectroscopy (SNS) has emerged into a versatile tool to study different semiconductor spin systems [1], e.g., bulk GaAs, quantum wells, and even individual quantum dots [2]. Especially the measurements on single hole spins in InAs quantum dots have pointed out very long spin lifetimes but despite very low laser intensities there was still a significant perturbation limiting the detectable intrinsic hole spin lifetime [2]. Therefore we introduce homodyne detection as an extension to the standard SN detection. Homodyne detection amplifies the signal by a local oscillator interfering with the conventional SN probe laser. We show a first experimental validation of this detection scheme yielding an increased signal to noise ratio in the well understood example system of Rb vapor [3].

[1] J. Hübner, F. Berski, R. Dahbashi, and M. Oestreich, physica status solidi (b) **251**, 1824 (2014).

[2] R. Dahbashi, J. Hübner, F. Berski, K. Pierz, and M. Oestreich, Phys. Rev. Lett **112**, 156601 (2014).

[3] H. Horn, G.M. Müller, E. Rasel, L. Santos, J. Hübner, and M. Oestreich, Phys. Rev. A **84**, 043851 (2011).

HL 39.35 Tue 14:00 Poster F

Controlling the frequency of ultra-fast polarization oscillations in Spin-VCSELs — •Markus Lindemann[1], Henning Höpfner[1], Nils C. Gerhardt[1], Martin R. Hofmann[1], Tobias Pusch[2], and Rainer Michalzik[2] — [1]Photonics and Terahertz Technology, Ruhr-University Bochum, 44780 Bochum, Germany — [2]Institute of Optoelectronics, Ulm University, 89081 Ulm, Germany

Spin-polarized optoelectronic devices offer several advantages in comparison to their conventional counterparts. One of these benefits is the possibility of polarization manipulation, as the optical polarization degree is connected with the carrier spin via the optical selection rules. The modulation speed of the spin is fast in comparison to the modulation frequency of the laser's intensity, which is limited by the dynamics of the carrier-photon system. Therefore the polarization modulation bandwidth generally exceeds the direct intensity modulation bandwidth. Due to cavity anisotropies the VCSEL bears two orthogonal linear polarized modes. In case of spin-injection, both modes evolve lasing operation simultaneously. This leads to an oscillation in the circular polarization degree. By switching this oscillation on and off with spin injection, short polarization bursts can be generated (H. Höpfner et al, Appl. Phys. Lett., 104, 022409 (2014)). The frequency of this oscillation and therefore the minimal width of the polarization bursts depend on the frequency distance of the two VCSEL modes exclusively. This is determined by the birefringence of the lasing material. We investigate optimization strategies to reach very high oscillation frequencies by manipulating the birefringence via mechanical strain.

HL 39.36 Tue 14:00 Poster F

Characterization of nitrogen-vacancy centers (NVs) in ^{13}C controlled diamond layers produced by CVD growth — •Alexander Geier, Christian Osterkamp, Boris Naydenov, and Fedor Jelezko — Institut für Quantenoptik, Ulm University, Albert Einstein Allee 11, Ulm 89081, Germany

Optical read-out and spin manipulation makes the negatively charged nitrogen-vacancy center's (NV) electron spin one of the leading solid-state quantum bits operating under ambient conditions. For quantum technology applications it is necessary to create NVs on demand. We produce NV centers by delta doping during a plasma enhanced chemical vapor deposition (PECVD) process. By changing the ratio of ^{12}C/ ^{13}C atoms in the growth chamber we are able to produce isotopically pure diamonds. A well controlled ^{13}C concentration is important for creating a quantum register where an NV is coupled to several nearby ^{13}C atoms[1], [2].

[1]: Childress et al., *Coherent Dynamics of Coupled Electron and Nuclear Spin Qubits in diamond*, in: Science Vol. 314 no.5797 pp. 281-285 DOI:10.1126/science.1131871(2006)

[2]: Waldherr et al., *Quantum Error Correction in a Solid-State Hybrid Spin Register*, in: Nautre 506(7487), S.204-207, DOI: 10.1038/nature12919 (2014)

HL 39.37 Tue 14:00 Poster F

Microstrip resonators for silicon-carbide quantum microwave emitters — •Johannes Fichtner[1], Andreas Sperlich[1], Hannes Kraus[1], Georgy Astakhov[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

Silicon vacancies in silicon carbide (SiC) were recently found to possess an unique excitation pathway. Optical pumping results in deactivation into a metastable state, which then selectively populates the higher energy $\pm 3/2$ manifold of the spin quartet ground state. This population inversion allows stimulated emission of radiation [1].

When placed in a resonator, microwave amplification in SiC vacancies is possible. The amplification (gain) is highly dependent on the filling factor of the resonator. Our approach to increase the gain is the use of microstrip resonators instead of usual box resonators. A microstrip is an electrical transmission line consisting of a conduction strip separated from a conducting ground plane by a dielectric.

Here we present the first results on our circuit board design and its performance. The most important properties of the microstrip waveguide are its characteristic impedance and resonance frequency. The influence of the resonator geometry were studied. Effects of different edge shapes (so called mitred bends) and feed line gaps were also examined.

[1] H. Kraus, V. Soltamov, D. Riedel, S. Väth, F. Fuchs, A. Sperlich, P. Baranov, V. Dyakonov and G. Astakhov, Nat. Phys. 10, 157 (2014)

HL 39.38 Tue 14:00 Poster F

Small nuclear spin environments in graphene quantum dots — •Daniel Hetterich, Moritz Fuchs, and Björn Trauzettel — Institute for Theoretical Physics IV , University of Würzburg

Graphene based quantum dots (QD) constitute interesting systems for both quantum computation and the physics of quantum information. An electron spin confined to such a QD is in contact with a bath of nuclear spins via an anisotropic hyperfine interaction (HI). If the HI is the most important interaction, the spins form a star-like system with the electron spin in its center. Most interestingly, isotopic purification allows to change the ratio of spin carrying ^{13}C with respect to spinless ^{12}C and, hence, to control the number K of nuclear spins. In order to complement previous studies of the anisotropic HI in graphene for large bath sizes, we investigate the spin dynamics for a small number of nuclear spins by means of exact diagonalization. Considering different types of initial states and various configurations of the nuclei within the dot, we analyze the time evolution of the electron spin with a focus on equilibration. The results of our simulations are in accordance with analytical estimations.

HL 40: Focus Session: Role of polarization fields in nitride devices I

Devices based on GaN and related compounds have conquered the fields of transistors, laser and illumination because of their unique materials properties. Polarization fields in particular have strong impact on device characteristics such as current transport in transistors and emission wavelengths in light emitters. This session is devoted to highlight the role of polarization fields in general and with regard to different device performances. Leading experts on theory, materials growth and characterization, and device fabrication will discuss phenomena arising from the physics of polarization fields in nitrides.

Organization: André Strittmatter (OvGU Magdeburg) and Michael Jetter (IHFG, U Stuttgart)

Time: Wednesday 9:30–11:15 Location: ER 164

Invited Talk HL 40.1 Wed 9:30 ER 164

Boon and bane of polarization induced effects in group III-nitride based heterostructures — •Oliver Ambacher — Fraunhofer Institute for Applied Solid State Physics, Freiburg, Germany

Gradients of spontaneous and piezoelectric polarization at surfaces and interfaces of group III-nitride based heterostructures having hexagonal crystal structure can cause huge sheet charges. These fixed sheet charges dominate the band edge as well as the concentration profiles of free carriers. Boon of polarization induced effects are high mobility two dimensional carrier gases with large sheet concentration appearing without intentional doping and opening up new concepts for high power as well as for high frequency transistors. Boon and bane is the sensitivity of polarization induced carrier profiles towards any change of surface potential which might be caused by charged defects, ions or polar molecules. This effect makes it very difficult to achieve suitable surface passivation and long term stable group III-nitride based electronics but opens up an interesting field of very charge sensitive devices suitable for pH-sensors or the detection dangerous polar molecules in gases and liquids. Based on an explanation of non-linear spontaneous and piezoelectric polarization in ternary group III-nitride hexagonal crystals ($c - Al_xM_{1-x}N$, M:= Ga, In, Sc) the state of the art as well as novel electronic and sensor devices will be presented

HL 40.2 Wed 10:00 ER 164

Composition of lattice-matched AlInN at the early stage of growth — •Philipp Horenburg[1], Uwe Rossow[1], Ernst Ronald Buss[1], Heiko Bremers[1], Daniel Henzler[2], Felix Schwarzhuber[2], Josef Zweck[2], and Andreas Hangleiter[1] — [1]Institute of Applied Physics, TU Braunschweig, Germany — [2]Institute of Experimental and Applied Physics, University of Regensburg, Germany

With a nominal indium content of about 18%, $Al_{1-x}In_xN$ is a-lattice matched to GaN. As compared to $Al_{1-x}Ga_xN$, lattice-matched $Al_{1-x}In_xN$ has a higher contrast in refractive index to GaN. These advantageous properties make AlInN a promising material for Bragg-reflectors and cladding layers in optical devices. However, the epitaxy of lattice matched AlInN is a complex task due to the very different ideal growth conditions of AlN and InN. In this contribution, we will show that the effective In content of thin AlInN layers depends on their thickness. A series of tenfold superlattice structures with varying thickness of the AlInN layers and GaN interlayers of approximately 1 nm was grown by low-pressure MOVPE. Assuming a ternary AlInN layer, our observations suggest the formation of an indium depleted phase at the initial stage of growth. On the other hand, TEM-EDX measurements on AlInN single layers hint at parasitic gallium incorporation in the first few nanometers in AlInN growth, which can be misinterpreted assuming ternary layers. Parasitic Ga in the AlInN would also lead to an overestimation of the Al content assuming ternary AlInN layers in simulation of XRD-profiles.

HL 40.3 Wed 10:15 ER 164

Structural and optical properties of MOVPE grown InGaN/AlInGaN MQWs — •Silvio Neugebauer, Jürgen Bläsing, Armin Dadgar, and André Strittmatter — Institute of Experimental Physics, Otto-von- Guericke-University Magdeburg, Germany

Conventional InGaN/GaN light emitting diodes designed for the green spectral range lack in efficiency due to spontaneous and piezoelectric polarization fields. These fields have negative impact on the LED performance by reducing the recombination probability and wavelength stability of the active medium which is known as the quantum-confined Stark effect. Better device performance could be possibly achieved by using AlInGaN barriers instead of conventional GaN barriers. For a particular InGaN composition it is possible to eliminate the difference in total polarization across the QW/barrier interface by choosing a proper AlInGaN composition. In this context InGaN/AlInGaN MQWs have been grown by MOVPE. Within a set of samples the composition of the barriers have been varied from pure GaN to fully polarization-matched AlInGaN with respect to the InGaN. For better compositional and structural control, these AlInGaN barriers have been grown using the pulsed flow regime. In PL experiments we observe a blueshift of the MQW emission with increasing nominal polarization matching of the barriers. This is consistent with reduced electric fields across the quantum well region. Unfortunately, the whole MQW stack gets additionally strained due to the high indium content of the AlInGaN barrier leading to lattice relaxation as revealed by XRD.

HL 40.4 Wed 10:30 ER 164

Optical polarization of AlGaN quantum well LEDs with emission wavelength near 245 nm — •Martin Guttmann[1], Christoph Reich[1], Frank Mehnke[1], Christian Kuhn[1], Tim Wernicke[1], Jens Rass[1,2], Mickael Lapeyrade[2], Sven Einfeldt[2], Arne Knauer[2], Viola Kueller[2], 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

For $Al_xGa_{1-x}N$ quantum wells (QWs) the order of the valence bands at the center of the Brillouin zone depends on the aluminum content and the strain state, and hence the optical polarization of the in-plane emission. We measured the optical polarization of AlGaN quantum well light emitting diodes (LEDs) with emission wavelength between 235 nm and 265 nm, corresponding to an aluminum content between 80% and 60% in the QWs. We observed a dominant TE emission for the compressively strained AlGaN multiple quantum wells in the entire wavelength range. The degree of polarization, i.e. $(I_{TE} - I_{TM})/(I_{TE} + I_{TM})$, decreases from 0.85 at 265 nm to 0.5 at 239 nm. From the TE/TM spectra and the temperature dependent polarization we were able to determine the energy difference between the two topmost valence bands to be e.g. 30 meV for 243 nm LEDs. The deviation from the expected splitting energy of -150 meV for unstrained $Al_{0.7}Ga_{0.3}N$ QWs can be explained by the large compressive strain in the QWs.

Invited Talk HL 40.5 Wed 10:45 ER 164

Overview of theoretical aspects of semi-polar and non-polar nitride surfaces — •John Northrup — Palo Alto Research Center (PARC), Palo Alto, California, USA

I will provide an overview of theoretical arguments employed to assess the effect of surface orientation on impurity incorporation in GaN. I will present an argument based on energetics explaining why indium incorporation on semipolar surfaces such as (11-22) is expected to be greater than on the m-plane surface. I will also discuss the structure of Mg-induced pyramidal inversion domains that form in heavily Mg-doped GaN. Unraveling the formation mechanism of these defects is a challenge for theory.

HL 41: Topological insulators: Theory (with DS/MA/O/TT)

Time: Wednesday 9:30–11:30 Location: ER 270

HL 41.1 Wed 9:30 ER 270

Weyl and Dirac semimetals: A platform for new interface phenomena — •Adolfo G. Grushin[1], Jorn W. F. Venderbos[2], and Jens H. Bardarson[3] — [1]Max Planck Institute for the physics of Complex Systems, Dresden, Germany — [2]Massachusetts Institute of Technology, Cambridge, MA, USA — [3]Max Planck Institute for the physics of Complex Systems, Dresden, Germany

The Weyl semimetal (WSM) state is sometimes loosely referred to as the three-dimensional cousin of graphene since its low energy theory is described by an even number of copies of the Weyl Hamiltonian. Closely related to WSM, the Dirac semimetals hosts the Weyl nodes at the same point in the Brillouin Zone and it is realised in Cd_3As_2 and Na_3Bi compounds. In this talk I will explore the rich surface state physics that these states can host and how can it be probed, including coexistence of Dirac and Fermi arc states at the topological insulator-weyl semimetal interfaces as well as signatures of the chiral anomaly.

HL 41.2 Wed 9:45 ER 270

Spin chirality tuning and Weyl semimetal in strained $HgS_{1-x}Te_x$ — •Tomáš Rauch[1], Steven Achilles[1], Jürgen Henk[1], and Ingrid Mertig[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle (Saale), Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle (Saale), Germany

We have theoretically investigated the phase diagram of $HgS_{1-x}Te_x$. The parameters which have been varied are the concentration x and the in-plane strain, which could be applied by an appropriate substrate in an experiment. In the topological phase diagram we found a normal metallic phase, two topological insulator phases with different spin chiralities of the surface states and a Weyl semi-metal phase. The phases have been probed by calculating topological invariants and the dispersion of the surface states for both crystal terminations of the (001) surface by an *ab-initio* based tight-binding model.

HL 41.3 Wed 10:00 ER 270

Topological phases in (interfacial) phase-change materials — •Peter Schmitz, Wei Zhang, and Riccardo Mazzarello — Institute for Theoretical Solid State Physics, RWTH Aachen University

We investigate the topological, spectral and structural properties of $[Sb_2Te_3]_x[GeTe]_y$ (GST) compounds, some of which are interfacial phase change materials (IPCMs), as a function of strain and stacking sequence by performing a DFT study of bulk and slab models and discuss the relevance of a 3D (topological) Dirac semimetal phase ((T)DSM), eg. to GST225.
IPCMs can perform fast reversible transitions, induced by electric fields or heat, between crystalline states of different stacking. Since they also possess strong spin-orbit coupling and a strong topological insulator (STI) + normal insulator(NI) layering, they are a promising platform to investigate nontrivial interface states and direct applications to data storage in terms of switching topological phases. Until now they were shown to exhibit STIs and *unstable* DSM-like critical states corresponding to STI/NI transitions [1]. Then recently [2] a *robust* TDSM phase was predicted for crystals having certain rotational symmetries: The STI/NI transition point can be extended to a line and 2 Dirac points appear in the bulk spectrum.
Analyzing whether such phases can be obtained in GST compounds is also interesting since the problem of a TDSM in a multilayer structure has not yet been discussed.
[1] J. Tominaga et al, Adv. Mat. Inter. 1 (2014);
[2] B. Yang and N. Nagaosa, Nature Commun. 5, 4898 (2014)

HL 41.4 Wed 10:15 ER 270

Effect of Bi bilayers on the topological states of Bi_2Se_3: A first-principles study — Kirsten Govaerts[1], Kyungwha Park[2], Christophe De Beule[1], Dirk Lamoen[1], and •Bart Partoens[1] — [1]CMT-group and EMAT, University of Antwerp, Belgium — [2]Virginia Tech, Department of Physics, USA

Bi_2Se_3 and vice versa, has not been explored much. Bi bilayers are often present between the quintuple layers of Bi_2Se_3, since $(Bi_2)_n(Bi_2Se_3)_m$ form stable ground-state structures. Moreover, Bi_2Se_3 is a good substrate for growing ultrathin Bi bilayers. By first-principles techniques, we first show that there is no preferable surface termination by either Bi or Se. Next, we investigate the electronic structure of Bi bilayers on top of, or inside a Bi_2Se_3 slab. If the Bi bilayers are on top, we observe a charge transfer to the quintuple layers that increases the binding energy of the surface Dirac cones. The extra states, originating from the Bi bilayers, were declared to form a topological Dirac cone, but here we show that these are ordinary Rashba-split states. This result, together with the appearance of a new Dirac cone that is localized slightly deeper, might necessitate the reinterpretation of several experimental results. When the Bi bilayers are located inside the Bi_2Se_3 slab, they tend to split the slab into two topological insulators with clear surface states. Interface states can also be observed, but an energy gap persists because of strong coupling between the neighboring quintuple layers and the Bi bilayers.

HL 41.5 Wed 10:30 ER 270

Topological states in α-Sn and HgTe quantum wells: a comparison of ab-initio results — •Sebastian Küfner and Friedhelm Bechstedt — Friedrich Schiller Universität Jena

Quantum well (QW) structures based on HgTe are theroretically predicted and experimentally verified to exhibit the quantum-spin Hall phase. Despite the similarities of the bulk band structures, studies of α-Sn QW structures are missing. We compare the properties of QW structures made by the different zero-gap semiconductors α-Sn and HgTe, but both sandwiched in nearly lattice-matched CdTe barriers by means of first-principles calculations including quasiparticle corrections and spin-orbit interaction. The two well materials possess different space groups O_h^7 (diamond structure) and T_d^2 (zinc-blende structure). The spin-orbit interaction, in particular that in the p-derived valence states, is different due to the contribution of both atoms in the unit cell (α-Sn) and mainly the anion (HgTe) to the states at the top of the valence bands, and the different local electrostatic properties due to the different bonding character in the QW layers and their interfaces with the CdTe barrier material. We investigate the similarities and differences of the two embedded zero-gap semiconductors on the formation of quantum-well, edge and interface states in detail.

HL 41.6 Wed 10:45 ER 270

Quasiparticle band structure of the topological insulator Bi_2Se_3 — •Tobias Förster, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

Bi_2Se_3 is a prototype topological insulator. Its simple surface band structure with only one Dirac point makes it an ideal system for exploring the properties of topological surface states. Up to now, the vast majority of theoretical investigations of the electronic structure of Bi_2Se_3 has utilized DFT calculations. In Bi_2Se_3 and related compounds, however, many body perturbation theory in the GW approximation yields both quantitative and qualitative quasiparticle corrections of the DFT bulk band structures [1].

Here we discuss results for bulk Bi_2Se_3 from GW calculations employing a localized basis as well as from a perturbative LDA+GdW approach [2]. The latter provides a numerically very efficient method for the calculation of quasiparticle corrections with only slightly reduced precision compared to GW. The applicability of the LDA+GdW formalism to the Bi_2Se_3 surface with the Dirac state will also be addressed.

[1] I. Aguilera *et al.*, Phys. Rev. B **88**, 045206 (2013)
[2] M. Rohlfing, Phys. Rev. B **82**, 205127 (2010)

HL 41.7 Wed 11:00 ER 270

Calculation of topological invariants from a maximally localized Wannier functions derived model Hamiltonian — •Patrick M. Buhl, Chengwang Niu, Yuriy Mokrousov, Daniel Wortmann, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Using density-functional methods it is possible to provide an accurate description of topological phases in complex materials. We demonstrate how topological characterization can be performed in a unified manner based on Wannier functions generated from the full-potential linearized augmented plane-wave method as implemented in the FLEUR

code [1]. Taking as examples bcc Fe, Na_3Bi and PbTe we compute various topological invariants and identify topologically non-trivial points in the electronic structure of these materials in bulk and their close relation to the surface electronic structure. In particular, we focus on the Weyl semimetallic phase as a transitional phase between various topological phases in the same material and on the role of the Weyl points in the electronic structure for topological properties. Financial support by the HGF-YIG Programme VH-NG-513 and SPP 1666 of the DFG is gratefully acknowledged.

[1] F. Freimuth *et al.*, Phys. Rev. B **78**, 035120 (2008)

HL 41.8 Wed 11:15 ER 270

Functionalized Bismuth Films: Giant Gap Quantum Spin Hall and Valley-Polarized Quantum Anomalous Hall States — •Chengwang Niu, Gustav Bihlmayer, Hongbin Zhang, Daniel Wortmann, Stefan Blügel, and Yuriy Mokrousov — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The search for new large band gap quantum spin Hall (QSH) and quantum anomalous Hall (QAH) insulators is critical for their realistic applications at room temperature [1,2]. Here we predict, based on first principles calculations, that the band gap of QSH and QAH states can be as large as 1.01 eV and 0.35 eV in an H-decorated Bi(111) film [3]. The origin of this giant band gap lies both in the large spin-orbit interaction of Bi and the H-mediated exceptional electronic and structural properties. Moreover, we find that the QAH state also possesses the properties of quantum valley Hall state, thus intrinsically realising the so-called valley-polarized QAH effect. We further investigate the realization of large gap QSH and QAH states in an H-decorated Bi($\bar{1}$10) film and X-decorated (X=F, Cl, Br, and I) Bi(111) films.

This work was supported by the Priority Program 1666 of the DFG and project VH-NG-513 of the HGF.

[1]M. Hasan and C. Kane, Rev. Mod. Phys. **82**, 3045 (2010).
[2]X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. **83**, 1057 (2011).
[3]Chengwang Niu, Gustav Bihlmayer, Hongbin Zhang, Daniel Wortmann, Stefan Blügel, and Yuriy Mokrousov, submitted.

HL 42: Devices

Time: Wednesday 9:30–12:00 Location: EW 015

HL 42.1 Wed 9:30 EW 015

Charging dynamics of a floating gate transistor with site-controlled quantum dots — •Patrick Maier[1], Fabian Hartmann[1], Monika Emmerling[1], Christian Schneider[1], Sven Höfling[1,2], Martin Kamp[1], and Lukas Worschech[1] — [1]Technische Physik, Physikalisches Institut, Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]present address: SUPA, School of Physics and Astronomy, University of St. Andrews, St. Andrews, KY16 9SS, UK

Quantum dots can serve as floating gates when positioned in close vicinity to a transistor channel. We have used templates in combination with regrowth techniques by means of molecular beam epitaxy to position single InAs quantum dots in a GaAs based quantum wire. The floating gate properties were studied in terms of transport measurements. By sampling of different gate voltage sweeps for the determination of charging and discharging thresholds, it was found that discharging takes place at short time scales of microseconds, whereas several seconds of waiting times within a distinct negative gate voltage range were needed to charge the quantum dots. Such quantum dot structures have the potential to implement logic functions comprising charge and time dependent ingredients such as counting of signals or learning rules.

HL 42.2 Wed 9:45 EW 015

Charge transition levels of oxygen, lanthanum and fluorine related defect structures in bulk hafniumdioxide (HfO2): an ab initio investigation. — •Roman Leitsmann[1], Florian Lazarevic[1], Rolf Öttking[2], Ebrahim Nadimi[3], and Philipp Plänitz[1] — [1]AQcomputare GmbH, 09125 Chemnitz, Germany — [2]Institute of Physics, Illmenau University of Technology, 98693 Illmenau, Germany — [3]K. N. Toosi University of Technology, Faculty of Computer and Electrical Engineering, 14317-14191 Tehran, Iran

Intrinsic defect structures and impurity atoms are one of the main source of leakage current in metal-oxide-semiconductor devices. Using state of the art density functional theory we have investigated oxygen, lanthanum, and fluorine related defect structures and possible combinations of them. In particular we have calculated their charge transition levels in bulk m-HfO2. The obtained results are able to explain the experimentally observed reduction of the trap density after NF3 treatment [1].

[1] M. Drescher et al., J. Vac. Sci. Technol. accepted (2014).

HL 42.3 Wed 10:00 EW 015

Resonant tunnelling structures to improve the erase time in memory devices based on quantum dots — •Ismail Firat Arikan[1,2], Tobias Nowozin[1], Dieter Bimberg[1], and Nurten Oncan[2] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany — [2]Department of Physics, Faculty of Science, Istanbul University, 34134 Vezneciler, Istanbul, Turkey

We develop a memory device based on self-assembled quantum dots (QDs) called QD-Flash in order to combine the advantage of both DRAM and Flash Memory, i.e. non-volatility, fast write time (ns) and good endurance. While the write performance is promising, there is a trade-off for erasing performance: When the localization energy of the holes in the QDs is increased to further increase the storage time, the erase time also increases due to the increased tunnelling barrier. Implementing a superlattice structure, which allows resonant tunnelling as erasing mechanism, eliminates the trade-off between storage and erase time. In such a structure, it is possible to switch the transparency between very high and very low values by varying a bias voltage.

In this work, the concept of designing such a superlattice structure is presented. The structures are simulated using a One-Dimensional Poisson Solver and a Non-Equilibrium Green's Function Formalism. Results are presented.

HL 42.4 Wed 10:15 EW 015

Growth of $In_{0.5}Ga_{0.5}As$/GaP quantum dots, manipulation of optical transitions by epitaxial means, and application in nano memory cells — •Gernot Stracke, Elisa Sala, Leo Bonato, Manuel Gschrey, Sven Rodt, Sören Selve, Tore Niermann, Christopher Prohl, Andrea Lenz, Holger Eisele, Andrei Schliwa, André Strittmatter, and Dieter Bimberg — Institut für Festkörperphysik, Institut für Optik und Atomare Physik und Zentraleinrichtung Elektronenmikroskopie, Technische Universität Berlin

InGaAs quantum dots (QDs) embedded in GaP have recently attracted attention for nano memory cells and monolithic integration of III/V-devices on silicon. A QD size- and strain- dependent transition from indirect to direct optical emission was predicted. Here we report on direct-gap $In_{0.5}Ga_{0.5}As$/GaP(001) QDs grown by metalorganic vapor phase epitaxy with strong optical emission. To initiate the three-dimensional growth mode of $In_{0.5}Ga_{0.5}As$ on GaP, the GaP surface is covered with 2 monolayers (ML) of GaAs prior to InGaAs deposition. A second GaAs layer of 1-2 ML thickness grown on top of the QDs allows for improved strain relief of the QDs and results in a red-shift of QD luminescence from 722 nm to 843 nm, and an increase in luminescence intensity by more than one order of magnitude. The storage time of holes in $In_{0.5}Ga_{0.5}As$/AlP QDs is determined by deep level transition spectroscopy to 230 s at room temperature, the highest value hitherto measured in QDs. Thus, QDs in a (Ga,Al)P matrix represent promising candidates for future nano memory devices.

Coffee break

HL 42.5 Wed 10:45 EW 015

High-resolution in-situ electron beam lithography for deterministic nanophotonic device processing — •Manuel Gschrey, Ronny Schmidt, Arsenty Kaganskiy, Sven Rodt, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, D-10623 Berlin

Advances in the field of quantum communication and computation using single semiconductor quantum dots (QDs) as emitters of single and indistinguishable photons rely crucially on the development of novel deterministic device technologies. As such, in-situ electron-beam lithography combines the benefits of high-resolution electron-beam lithography (EBL) and deterministic fabrication of nanostructures via convenient preceding luminescence mapping by cathodoluminescence [1]. For the application of this technique, a thorough understanding of the alignment accuracy, the writing resolution and the low temperature resist properties is inevitable. In this work we address these important points by a statistical analysis of our in-situ lithography technology platform. We find the the alignment accuracy is well below 50 nm and that circular mesas and wires with feature sizes down to 100 nm can be realized routinely. Moreover, studying the dose and temperature dependence of various common resists has revealed that polymethylmethacrylate (PMMA) is most suitable for 2D and 3D EBL at cryogenic temperatures.

[1] M. Gschrey et. al, APL 102, 251113 (2013)
[2] M. Gschrey et. al, J. Vac. Sci. Technol. B 32, 061601 (2014)

HL 42.6 Wed 11:00 EW 015

On the Photocurrent-Voltage Relations of Resonant Tunneling Photodetectors — •Andreas Pfenning[1], Fabian Hartmann[1], Fabian Langer[1], Sven Höfling[1,2], Martin Kamp[1], and Lukas Worschech[1] — [1]Technische Physik, Physikalisches Institut, Universität Würzburg and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Am Hubland, D-97074 Würzburg, Germany — [2]SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, KY16 9SS, United Kingdom

We present a study of the photocurrent-voltage relations and photogenerated charge accumulation dynamics of resonant tunneling diode (RTD) photodetectors. The RTDs are based on an AlGaAs/GaAs double barrier structure with a nearby and lattice matched GaInNAs absorption layer. The RTDs were studied for light sensing at the telecommunication wavelength λ=1.3 μm by means of electro-optical transport measurements. A strong nonlinear photocurrent-voltage relation was found and is attributed to three voltage dependent parameters: the quantum efficiency η(V), the mean lifetime of photogenerated and accumulated charge carriers τ(V) and the RTD's current-voltage characteristic in the dark I(V).

HL 42.7 Wed 11:15 EW 015

Ultraviolet photodiodes from visible-blind to solar-blind spectral range based on $(Ga_{1-x},In_x)_2O_3$ thin films — •Zhipeng Zhang, Holger von Wenckstern, Stefan Müller, Daniel Splith, Jörg Lenzner, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Fakultät für Physik und Geowissenschaften, Institut für Experimentelle Physik II, Linnéstraße 5, 04103, Leipzig

We report on the fabrication of ultraviolet photodiode arrays based on Si-doped $(Ga_{1-x},In_x)_2O_3$ thin films [1] having a monotonous lateral variation of the indium content x from 0 to 0.8 as determined by energy-dispersive X-ray diffraction spectroscopy. The wavelength-selectivity of the device from visible-blind to solar-blind spectral range is realized by using a continuous composition spread approach [2,3] for pulsed-laser deposition. We ablate a single but segmented target consisting of semicircular segments of In_2O_3 and Ga_2O_3 both containing 0.1 wt.% SiO_2 in addition.

The structural properties of the thin film are investigated by spatially resolved X-ray diffraction measurements revealing phase separation for $x > 0.2$. The photoresponse of the photodiodes is determined from a metal-semiconductor-metal structure at room temperature. The onset of the absorption was tuned from 4.8 to 3.2 eV with increasing indium content within a single 2 inch wafer sample.

[1] H. von Wenckstern et al., Semic. Sci. Technol., accepted (2014)
[2] H. von Wenckstern et al., CrystEngComm. **15**, 10020 (2013)
[3] Z. Zhang et al., IEEE J. Sel. Top. Quantum Electr. **20**, 3801606 (2014)

HL 42.8 Wed 11:30 EW 015

Stability of QD excited-state laser emission under simultaneous ground-state perturbation — •Yücel Kaptan[1], André Röhm[2], Bastian Herzog[1], Benjamin Lingnau[2], Holger Schmeckebier[3], Dejan Arsenijević[3], Vissarion Mikhelashvili[4], Oliver Schöps[1], Mirco Kolarczik[1], Gadi Eisenstein[4], Dieter Bimberg[3], Ulrike Woggon[1], Nina Owschimikow[1], and Kathy Lüdge[2] — [1]Institut für Optik und Atomare Physik, Technische Universität Berlin, Berlin, Germany — [2]Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany — [3]Institut für Festkörperphysik, Technische Universität Berlin, Berlin, Germany — [4]Technion Institute of Technology, Faculty of Electrical Engineering, Haifa, Israel

State of the art in optoelectronic devices based on In(Ga)As-quantum dots (QDs) is the primary use of the energetically lowest bound QD state, the ground state (GS). Using also excited states (ES) may provide additional functionalities. We investigate QD ES lasers and provide conclusions for the realization of multi-state QD devices. We study the impact of GS amplification on simultaneous ES lasing via time-resolved emission measurements and find that a depopulation of the QD GS is followed by a drop in ES lasing intensity, strongly depending on wavelength of the depletion pulse and injection current. Numerical simulations based on laser rate equations reproduce the experimental results by taking into account the different dynamics of lasing and non-lasing QD subensembles within the inhomogeneously broadened spectrum [1]. [1] Y. Kaptan et al., Appl. Phys. Lett. 105, 191105 (2014)

HL 42.9 Wed 11:45 EW 015

25 Gb/s phase modulation with 1.3 μm semiconductor optical amplifiers based on InAs quantum dots — •Anissa Zeghuzi[1], Holger Schmeckebier[1], Mirko Stubenrauch[1], Christian Meuer[2], Christian-Alexander Bunge[3], and Dieter Bimberg[1] — [1]Technische Universität Berlin — [2]Fraunhofer Heinrich-Hertz-Institut Berlin — [3]Hochschule für Telekommunikation Leipzig

The number of components and thus costs in optical networks, e.g. in PON, can be significantly reduced by merging modulators and amplifiers. Since the real and the complex part of the susceptibility are decoupled in QD devices, the phase can be changed individually. The phase modulation is realized by means of the direct modulation induced change of current density, resulting in a change of effective refractive index of the ridge waveguide. The SOAs are driven in the QD ground state saturation regime with a high suppression of amplitude modulation. Therefore no patterning occurs in contrast to on-off- keying modulation scheme. Thus amplitude modulation was limited to 6 Gb/s, but phase modulation up to 25 Gb/s is demonstrated without any additional electrical pre- or post-processing (BER $< 10^{-9}$). Furthermore modulation of 20 Gb/s bit rate is achieved at a small cw input power of only - 11 dBm.

HL 43: Ultra-fast phenomena

Time: Wednesday 9:30–10:45 Location: EW 202

HL 43.1 Wed 9:30 EW 202

Bandgap behaviour of ultrashort laser pulse excited silicon — •Bernd Bauerhenne, Eeuwe S. Zijlstra, and Martin E. Garcia — Theoretische Physik - Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

After an intensive ultrashort laser pulse excites silicon, it melts within the next 500 fs. Due to the drastic changes of the atomic positions, the band gap vanishes after ~120 fs and so molten silicon becomes metallic. We studied this effect ab inito with LDA DFT molecular dynamics simulations.

HL 43.2 Wed 9:45 EW 202

Ultrafast coherent phonon dynamics during the phase transition of the quasi one-dimensional Ta_2NiSe_5 — •Selene Mor[1], Marc Herzog[1], Claude Monney[1,2], Martin Wolf[1], and Julia Stähler[1] — [1]Fritz-Haber-Institut der MPG, Dep. of Phys. Chem., Berlin, Germany — [2]Institut für Physik, University of Zürich, Switzerland

Ta_2NiSe_5 is a layered compound in which atomic chains are aligned in layers, forming a quasi one-dimensional crystal structure. At 328 K, the system shows a structural change accompanied by an electronic phase transition (PT) from a low temperature (LT) (potentially excitonic) insulator to a semiconductor. Our aim is to unveil the microscopic mechanisms underlying this PT by investigating the non-equilibrium dynamics after optical excitation. The system is excited with a femtosecond laser pulse at 800 nm and the mid-infrared (MIR) transient optical response is monitored by ultrafast optical spectroscopy. We observe a fast rise of transient reflectivity, which decays exponentially within 2-3 ps. This incoherent response is superimposed by several coherent phonon oscillations. In particular, we observe a 4 THz phonon that is specific of the LT phase, which is confirmed by temperature dependent Raman spectroscopy. The time evolution of this LT phase phonon reveals a finite lifetime of few ps. Furthermore, a non linear behavior is observed for both the coherent and incoherent response as a function of excitation fluence. The fluence and sample temperature dependence suggest that the PT can be driven by photoexcitation on an ultrafast timescale.

HL 43.3 Wed 10:00 EW 202

Ultrafast exciton dissociation and coherent polaron formation in polymer fullerene blends observed by femtosecond spectroscopy — •Ephraim Sommer[1], Antonietta De Sio[1], Carlo A. Rozzi[2], Margherita Maiuri[3], Julien Rehault[3], Giulio Cerullo[3], and Christoph Lienau[1] — [1]Institut für Physik, Carl von Ossietzky Universität, 26129 Oldenburg, Germany — [2]Istituto Nanoscienze Consiglio Nazionale delle Ricerche (CNR), Centro S3, via Campi 213a, 41125 Modena, Italy — [3]Istituto di Fotonica e Nanotecnologie CNR, Dipartimento di Fisica, Politecnico di Milano, 20133 Milano, Italy

Blends of conjugated polymers (P3HT) and fullerene (PCBM) derivatives are prototype systems of organic photovoltaic devices. The primary charge-generation mechanism involves a light-induced electron transfer from the polymer to the fullerene acceptor.

Here we show ultrabroadband (500-1400nm) pump probe measurements with sub 15-fs time resolution of a pristine polymer thin-film and a blend of P3HT and PCBM, which reveal direct signatures of ultrafast charge dissociation. In particular we trace the dynamics of the interface excitons in the blended material. We find that they dissociate into charge transfer excitons within about 50fs [1]. In addition we find in both pristine and blended films evidence for an ultrafast buildup of polaron pair states. We analyze and discuss the ultrafast polaron pair dynamics on the basis of pump probe and coherent two-dimensional spectroscopy.

[1] S. M. Falke et al. Science 344, 1001-1005 (2014)

HL 43.4 Wed 10:15 EW 202

Asynchronous Optical Sampling of Rolled-up GaAs/InGaAs Superlattices — •Delia Brick[1], Martin Schubert[1], Chuan He[1], Martin Grossmann[1], Vivienne Meier[2], Guodong Li[2], Daniel Grimm[2], Oliver G. Schmidt[2], and Thomas Dekorsy[1] — [1]Universität Konstanz, Deutschland — [2]IFW Dresden, Deutschland

Strained bilayers of different materials can be rolled up to form radial superlattices by controlled release of the bilayers which were deposited on a sacrificial layer [1]. This new kind of rolled-up superlattices has not only a broad field of applications but is also interesting by itself [1,2]. It is important for these tubes to be uniform and defect free, therefore it is of great interest to characterize the superlattice tubes through a fast, non-invasive method like femtosecond pump-probe spectroscopy using asynchronous optical sampling (ASOPS) [3].

Rolled-up GaAs/InGaAs superlattices are optically excited and detected by ASOPS. The acoustic phonon modes are analyzed. The folding of the dispersion relation of the superlattice can be measured and it is possible to determine the quality of the layers by seeing large changes in the spectra. Scans over the length of the tubes can provide information on the homogeneity. Furthermore measurements at different temperatures are performed to measure phonon lifetimes.

References: [1] Deneke et al; Journal of Physics D: Applied Physics; 103, 233114 (2009) [2] Angelova et al; Applied Physics Letters; 100, 201904 (2012) [3] Ristow et al, Applied Physics Letters; 103, 233114 (2013)

HL 43.5 Wed 10:30 EW 202

Nonlinear Coupling of Phonons to Ferroelastic Domain Walls in $SrTiO_3$ Observed by Ultrafast Light Scattering from Phonons — •Lena Maerten, André Bojahr, Matthias Rössle, and Matias Bargheer — Insitut für Physik und Astronomie, Universität Potsdam, Germany

We excite high amplitude strain waves in $SrTiO_3$ (STO) using metal transducer films and monitor the strain propagation by ultrafast broadband transient reflectivity experiments. The phonon oscillations observed in temperature dependent measurements give access to the linear and nonlinear acoustic response of STO in the 100 GHz range across its ferroelastic transition. We interpret the linear response as a coupling to the ferroelastic soft mode and the nonlinear behaviour as a strain dependent coupling of phonons to ferroelastic domain walls [1]. We evaluate the wavevector dependent attenuation of the excited phonon modes and discuss, how the presence of domain walls affects the sound attenuation in STO in different temperature regimes.

[1] L. Maerten, A. Bojahr, M. Rössle, M. Gohlke and M. Bargheer, Coupling of GHz phonons to ferroelastic domain walls in $SrTiO_3$, Phys. Rev. Let., accepted

HL 44: Quantum dots: Preparation and characterization

Time: Wednesday 9:30–13:00 Location: EW 203

HL 44.1 Wed 9:30 EW 203

Recent advances in growth of high- density InP based InAs/InGaAlAs quantum dots with reduced size inhomogeneity — •Saddam Banyoudeh and Johann Peter Reithmaier — Technische Physik, Institute of Nanostructure Technologies and Analytics (INA), University of Kassel

High-density 1.55 μm emitting quantum dot (QD) layers with a narrow spectral gain are requested for high-performance optoelectronic devices, like high-speed directly modulated communication lasers. We report about the influence of different growth parameters on the formation of 1.5 μm emitting InAs/InGaAlAs quantum dots (QDs) based on InP substrate. The InAs/InGaAlAs QDs were grown in a solid source molecular beam epitaxy system. The photoluminescence spectroscopy (PL) and atomic force microscope (AFM) were used to investigate the impact of the growth parameters, like V/III ratio, growth temperature of the InGaAlAs nucleation layer and growth rate of QD layers, on optical and structural properties of the formed QDs. The improved QD materials with dot densities up to 6 x 10^{10} cm^{-2} show a new record-low linewidth of 17 meV for a single QD layer and of 26 meV for multi QD layers, respectively (measurments performed at 10 K).

HL 44.2 Wed 9:45 EW 203

Growth and structure of $In_{0.50}Ga_{0.50}Sb$ quantum dots on GaP — •Elisa Maddalena Sala, Gernot Stracke, Andre' Strittmatter, and Dieter Bimberg — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany

III-V self-assembled QDs on GaP have recently attracted great interest for application in nano memory cells. As demonstrated by Marent, Geller and Bimberg et al, such QDs can be employed as storage units in a novel type of non-volatile nano memory, the QD-Flash. In this context, a proper choice of QD material is of decisive importance: by embedding $In_{0.50}Ga_{0.50}Sb$ QDs in a GaP matrix, storage times of more than 10 years can be obtained. Here we demonstrate the Stranski-Krastanov (S-K) growth of $In_{0.50}Ga_{0.50}Sb$ QDs on GaP(001) in metalorganic vapor phase epitaxy (MOVPE) environment for the first time. As reported in our previous works on InGaAs/GaP, a thin GaAs interlayer prior to QD deposition plays a decisive role in the surface energetics. $In_{0.50}Ga_{0.50}Sb$ QD growth is partially suppressed for GaAs coverage of less than 5 ML. Utilizing a 5 ML- thick GaAs layer, the transition from 2D to 3D growth is determined to about 0.20 ML and the QD density shows a logarithmic dependence on initial layer thickness, revealing a typical S-K growth mode. Prior to QD material deposition, a short Sb-flush is used to initiate antimony incorporation. Experimental results show that Sb apparently modifies the growth kinetics by reducing the surface diffusion length of gallium and indium atoms.

HL 44.3 Wed 10:00 EW 203

Atomic structure of InAs(Sb)/GaAs submonolayer stacks — •Zeno Diemer, Andrea Lenz, Christopher Prohl, David Quandt, Udo W. Pohl, André Strittmatter, Dieter Bimberg, Mario Dähne, and Holger Eisele — Technische Universität Berlin, Institut für Festkörperphysik, 10623 Berlin, Germany

Submonolayer-grown semiconductor nanostructures are promising for high power and high speed laser devices. Recent cross-sectional scanning tunneling microscopy (XSTM) studies of InAs/GaAs submonolayer stacks have shown the formation of InAs agglomerations with lateral sizes of about 5 nm, heights of about 2 nm, and a high density above $10^{12}/cm^2$. In this work, the structural changes upon additional supply of Sb, shown by cathodoluminescence to result in a stronger localization of charge carriers, are studied on the atomic scale using XSTM. The InAs(Sb) agglomerations show slightly smaller sizes than equivalent submonolayer structures grown without Sb. From atomically resolved filled-state XSTM images the Sb incorporation could be determined simply by counting the Sb atoms. The Sb atoms are mostly incorporated in the submonolayer structures. From an analysis of the local lattice parameter the In content could be determined, being considerably smaller than the nominally deposited amount of In. Also the distance of the submonolayer stacks along growth direction is reduced by about 30% with additional Sb. These reductions from the nominal values are due to a reduced growth rate of InGaAs and GaAs on Sb-containing growth surfaces.

This work was supported by the DFG, Sfb 787, TP A2 and A4.

HL 44.4 Wed 10:15 EW 203

Localization of charge carriers in MOCVD-grown InAs(Sb)/GaAs sub-monolayer stacks — •D. Quandt, J.-H. Schulze, A. Schliwa, M. Gschrey, S. Rodt, Z. Diemer, C. Prohl, A. Lenz, H. Eisele, A. Strittmatter, U. W. Pohl, S. Reitzenstein, and D. Bimberg — Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstraße 36, D-10623 Berlin

Conventional growth of InAs/GaAs sub-monolayer stacks results in the formation of high density InAs islands with strong vertical electronic coupling. Additionally, lateral electronic coupling is possible for sufficiently large densities, resulting in weakened three-dimensional confinement of electrons and holes. The addition of Sb to the growth sequence results in a stronger localization of charge carriers, as shown by cathodoluminescence measurements, in which individual emission lines appear in the luminescence spectrum, and temperature-dependent photoluminescence measurements revealing an S-shape in the temperature-dependent peak energy position. 8-band k·p simulations have been utilized to investigate the influence of Sb on the wavefunctions of electrons and holes. The structural properties of the sub-monolayers have been investigated by cross-sectional scanning tunneling microscopy, showing a smaller size of the In agglomerations as compared to sub-monolayers grown without Sb as well as a slight clustering tendency of the Sb atoms.

HL 44.5 Wed 10:30 EW 203

Cross-sectional Scanning Tunneling Microscopy Analysis of InGaAs/GaP Quantum Dots — •Christopher Prohl[1], Andrea Lenz[1], Holger Eisele[1], Gernot Stracke[1], André Strittmatter[1], Udo W. Pohl[1], Dieter Bimberg[1], Mario Dähne[1], Yuncheng Song[2], and Minjoo Larry Lee[2] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Department of Electrical Engineering, Yale University, New Haven, Connecticut 06520-8284, USA

GaP with its particular low lattice mismatch to Si offers the possibility to monolithically integrate III-V nanotechnology into Si. Recently, the topic of self-assembled InGaAs/GaP quantum dots (QDs) came more into focus because of their possible applications in new nanomemory cells. Furthermore, the first light emitting diode based on epitaxially grown InGaAs QDs on a monolithic GaP/Si substrate has already been demonstrated. In this contribution, cross-sectional scanning tunneling microscopy (XSTM) was used to structurally analyze differently grown InGaAs/GaP QDs on the atomic scale, investigating both, samples grown by metalorganic vapor-phase epitaxy (MOVPE) and molecular beam epitaxy (MBE). High-resolution images and a quantitative analysis of the local stoichiometry demonstrate that for a nominal MOVPE material amount of e.g. 3.0 monolayers (ML) GaAs and 2.0 ML $In_{0.25}Ga_{0.75}As$, indium-rich QDs with a truncated pyramidal shape, a reversed cone stoichiometry and a QD density of 2.4×10^{11} cm^{-2} form. In comparison, MBE samples with the same deposited material amount show QDs with similar size, shape and density.

HL 44.6 Wed 10:45 EW 203

Stoichiometry determination of InGaAs/GaP quantum dots — Daehwan Jung[1], Christopher Prohl[2], Yuncheng Song[1], Minjoo Larry Lee[1], and •Andrea Lenz[1,2] — [1]Department of Electrical Engineering, Yale University, New Haven, CT, 06511, USA — [2]Technische Universität Berlin, Institut für Festkörperphysik, 10623 Berlin, Germany

InGaAs/GaP quantum dots are promising for the integration of III-V nanostructures in the well-established silicon-device technology. In order to understand and improve optoelectronic device characteristics of InGaAs quantum dots grown under various growth conditions, detailed investigations on their size, shape and stoichiometry are performed. In this presentation the stoichiometry of InGaAs quantum dots is revealed by energy dispersive X-ray spectra (EDX) in a scanning transmission electron microscope and also by cross-sectional scanning tunneling microscopy (XSTM). From XSTM images the local stoichiomety across a quantum-dot layer is determined by an evaluation of the local lattice parameter and a comparison with reference values

from strain relaxation calculations. EDX and XSTM were applied on the same sample and benefit strongly from each other: It is revealed that P atoms are absent in the quantum dots and InAs is incorporated within the quantum-dot center, especially for the case of a thin GaAs layer deposited on the GaP matrix material prior to the InGaAs growth.
This work was supported by the DFG, project LE 3317/1-1.

HL 44.7 Wed 11:00 EW 203

Deep-Level Transient Spectroscopy on In0.5Ga0.5As/GaP quantum dots with AlP barrier — •Leo Bonato[1], Elisa Sala[1], Gernot Stracke[1], Tobias Nowozin[1], André Strittmatter[1], and Dieter Bimberg[1,2] — [1]Institut für Festkörperphysik, TU Berlin, Hardenbergstr. 36, 10623 Berlin — [2]King Abdulaziz University, Jeddah, Saudi Arabia

Aiming to use self-assembled quantum dots (QDs) as storage units for novel memory devices [1], we studied the charge-carrier dynamics during the processes of charging and discharging QDs by using Deep-Level Transient Spectroscopy (DLTS). We investigated In0.5Ga0.5As QDs grown on a GaAs interlayer in GaP, with an additional AlP barrier, which yielded a localization energy of 1.14 eV and a storage time at room temperature of 230 s. This marks a definite improvement over the previous record values of 0.8 eV [2] and 1.6 s [1].

[1] A. Marent et al., The QD-Flash: a quantum dot-based memory device, Semicond. Sci. Technol. 26 (2011) 014026

[2] T. Nowozin et al., 800 meV localization energy in GaSb/GaAs/Al0.3Ga0.7As quantum dots, Appl. Phys. Lett. 102 (2013) 052115

Coffee break

HL 44.8 Wed 11:30 EW 203

Growth of GaN quantum dots on AlN by MOVPE — •Konrad Bellmann[1], Torsten Ernst[1], Tim Wernicke[1], Andre Strittmatter[1,2], and Michael Kneissl[1] — [1]Technische Universität Berlin, Institute of Solid State Physics, Secretariat EW6-1, Hardenbergstrasse 36, 10623 Berlin, Germany — [2]Otto-von-Guericke Universität Magdeburg, FNW/IEP/AHE, Universitätsplatz 2, 39106 Magdeburg

GaN quantum dots(QDs) embedded in an AlN matrix are very promising to achieve single photon sources at room temperature. This work will present a systematic study of GaN growth on an AlN layer by metal organic vapor phase epitaxy(MOVPE). Due to the 2.4 % lattice mismatch GaN growth on AlN is very sensitive to the surface energy during growth. A high V/III ratio >300 can shift the balance between surface energy and strain energy towards two dimensional growth. A low V/III ratio on the other hand shifts the balance towards Stranski Krastanow growth. We have investigated the GaN growth at 840 °C at different V/III ratios ranging between 70 and 1200 as well as different growth times from 0 s to 40 s. Independent of the V/III ratio GaN is first nucleating on the terrace until a uniform monolayer is formed. At high V/III ratio additional material gathers at the step edge leading to two dimensional growth with nonuniform edges. Growth at low V/III ratios results in three dimensional islands. The density increases during growth from $10^8\,cm^{-2}$ to $10^{10}\,cm^{-2}$. Typical QDs exhibit heights of 1 - 4 nm and diameter of 20 - 50 nm. The growth results are summarized in a phase diagram based on the model by Daruka and Barabasi.

HL 44.9 Wed 11:45 EW 203

Growth of Site-Controlled InAs Quantum Dots by MOVPE — •Marc Sartison, Matthias Paul, Jan Kettler, Michael Jetter, and Peter Michler — Universität Stuttgart, Institut für Halbleiteroptik und Funktionelle Grenzflächen and Research Center SCoPE, Allmandring 3, 70569 Stuttgart

In the last decade, it has been demonstrated, that semiconductor quantum dots (QDs) have the potential to be excellent light sources for the application in single-photon devices. Normally, QDs with a high optical quality and structrual purity are grown self-assembled with a low spatial density. Hence, it is a challenging task to integrate QDs into optical circuits on chip, a precise control of the QD position is essential. It also has been shown, that the surface potential can be locally modified to create sites of higher nucleation probability by prepatterning the substrates. In this contribution, we present approaches of the site-controlled growth of InAs QDs on prepatterned GaAs substrates. To create nucleation sites, the substrate is structured with a hexagonal hole pattern, which is etched either by wet, or a combination of wet and dry chemical etching. Afterwards, the templates are overgrown with different GaAs buffer structures in our MOVPE system. The evolution of the holes and the nucleation behavior of the InAs QDs is monitored by AFM and SEM measurements. To reveal the optical characteristics, the QDs were capped with a GaAs layer. The microphotoluminescence measurements show single QD emission lines and two wetting layer peaks resulting from variations in the wetting layer thickness inside the holes and in the planar region in between.

HL 44.10 Wed 12:00 EW 203

Towards site-controlled In(Ga)As quantum dots at telecom wavelengths — •Caterina Clausen, Matthias Paul, Marc Sartison, Jan Kettler, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen and Research Center SCoPE, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

Single photon sources and sources of entangled photon pairs play one main part in quantum cryptography and quantum information technologies. The emission wavelength of 1310 nm correspond to the telecom O-band. In this range the dispersion and absorption of optical fibers is minimal. This characteristic is needed for loss free transmission in present communications networks. Semiconductor quantum dots (QDs) are excellent candidates for such applications due to very good optical properties and low area densities. The advantage of site-controlled grown QDs is simple integration into devices . The studied structures are produced by metal-organic vapor-phase epitaxy on exactly oriented GaAs substrates. The strain surrounding the QDs is reduced by a $In_{10}Ga_{90}As$ layer directly over the InGaAs-QDs. This leads to actual larger QDs, reduces the effective band gap, and shifts the emission to higher wavelengths. For the growth of positioned QDs, GaAs substrates are pre-structured with a hexagonal hole pattern. A GaAs buffer layer ensures a (100) growth surface in the etched holes. Then the QD material is deposited. It is possible to influence the nucleation in the holes by choosing the right growth parameter.

HL 44.11 Wed 12:15 EW 203

Direct growth of high-density InAs/GaAs core-shell quantum dots on silicon towards a new light emitting silicon based material platform — •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, InAs/GaAs core/shell quantum dots are grown in a solid source molecular beam epitaxy system directly on the silicon substrate. For efficient light emitting devices (e.g. LED, Laser) we aim for high-density QD layers with light emission in the range of 1.3 μm. The influence of growth parameters, like growth temperature, V/III ratio, deposited material thickness, on structural and optical properties are investigated and characterized by low-temperature photoluminescence (PL) spectroscopy and atomic force microscopy. Dot densities of $> 10^{10}\ cm^{-2}$ were obtained and first ensemble PL spectra will be discussed.

HL 44.12 Wed 12:30 EW 203

Strain in colloidal CdSe/CdS core/shell nanocrystals — •Narine Ghazarian[1], Amelie Biermann[1], Tangi Aubert[2], Marco Cirillo[2], Andrei Schliwa[1], Zeger Hens[2], Janina Maultzsch[1], Axel Hoffmann[1], and Christian Thomsen[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Germany — [2]Physics and Chemistry of Nanostructures, Ghent University, Belgium

In the last decade colloidal quantum dots have attracted particular attention due to their unique size-tunable emission wavelength from UV to IR, their high photoluminescence quantum yield and long lifetime, thus they offer uses in the field of optoelectronics and biotechnology. Surface defects cause non-radiative recombination of charge carriers. One solution to this can be the coating with a shell material. However, overcoating the core with a shell leads to strain inside

the core/shell nanocrystals (NC) caused by the lattice mismatch between the different materials. Since strain has a significant bearing on optical properties, it is important to know what impact parameters such as temperature, reaction duration, crystal size and shell thickness have. In order to be able to assess the influences of these parameters on strain, we investigate different series in CdSe/CdS core/shell NCs with wurtzite and zinc blende structure by using Raman spectroscopy. We consistently find that core and shell show compressive and tensile strain, respectively. Increasing the shell thickness results an increased compressive strain in the core and relaxation of the tensile strain in the shell.

HL 44.13 Wed 12:45 EW 203

In situ Raman monitoring of silica shell formation on colloidal CdSe/CdSe quantum dots — •Philipp Baumeister[1], Amelie Biermann[1], Tangi Aubert[2], Zeger Hens[2], Janina Maultzsch[1], and Axel Hoffmann[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Germany — [2]Physics and Chemistry of Nanostructures, Ghent University, Ghent, Belgium

Colloidal CdSe/CdS quantum dots offer possibilities for a variety of applications, in particular for biological imaging. Due to their high luminescence yield, discrete spectrum and stability, quantum dots used as biological markers are in many cases superior to regular dyes. The toxicity of CdSe and CdS remains a problem for biological uses. Furthermore, for those applications the quantum dots need to be modified for water solubility and acid resistance. One approach to solve these problems is the coating the quantum dots with a silica shell.

In this talk we discuss the influence of the silica shell synthesis on the encapsulated CdSe/CdS quantum dots utilizing in situ Raman spectroscopy. This made it possible to monitor the formation of the silica shell in real time. We were able to measure an increasing strain in the CdS-shell during the first hours of the synthesis, despite the silica shell being an amorphous material.

HL 45: Organic electronics and photovoltaics: OPV II (CPP with HL/TT)

Time: Wednesday 9:30–13:00 Location: C 130

HL 45.1 Wed 9:30 C 130

Impact of Mesoscale Order on Energetics in Organic Semiconductors — •Carl Poelking[1], Max Tietze[2], Chris Elschner[2], Selina Olthof[3], Dirk Hertel[3], Björn Baumeier[1], Frank Würthner[4], Klaus Meerholz[3], Karl Leo[2], and Denis Andrienko[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Institut für Angewandte Photophysik, Dresden, Germany — [3]Physikalische Chemie, Universität zu Köln, Germany — [4]Institut für Organische Chemie, Universität Würzburg, Germany

The interaction of charged excitations with the molecular surrounding in organic semiconductors is strictly long-ranged, due to their quadrupolar building blocks and preferential or absolute structural order. We show how atomistic simulations access the resulting energetics of charges and charge pairs and derived quantities, notably the charge-density-dependent open-circuit voltage across organic heterojunctions, with excellent accuracy. We compute level diagrams for a variety of donor-fullerene interfaces, with direct experimental validation. The underlying simulation approach takes into account long-range electrostatic effects that persist up to the mesoscale. The resulting mesoscale fields not only produce flat level profiles, but provide orientation-dependent push-out forces across a donor-acceptor interphase that can drive the charge-separation process. Correct polarity of these push-out forces is a requirement for functional solar cells, with operation closely above an isopolar point as the optimum tradeoff between magnitude of these push-out forces and the photovoltaic gap.

HL 45.2 Wed 9:45 C 130

Signature of the Dirac cone in the excitation gaps of linear oligoacenes — •Richard Korytár — Institut für Nanotechnologie, Karlsruher Institut für Technologie, Herrmann-von-Helmholtzplatz 1, 76344 Eggenstein-Leopoldshafen

Linear oligoacenes (linearly fused benzene rings) are one of the prototypical examples of quantum wires and the simplest realization of the so called nano-graphene. We show that contrary to a widely held belief, the excitation gaps of oligoacenes can display oscillations of period 11 (rings) as a function of the molecule's length. By inspection of the polyacene electronic band-structure, we show that the incommensurate oscillations are caused by the presence of an accidental degeneracy at the Fermi level, reminiscent to the Dirac cone of graphene. Our predictions are supported by calculations based on density functional theory. We clarify the role of interactions by studying a parameterized Hubbard model with density matrix renormalization group. Our findings may have implications for organic electronics and research of materials for energy conversion.

HL 45.3 Wed 10:00 C 130

Probing Interfacial Properties in Polymer:Fullerene Bulk Heterojunctions — •Christian Kästner[1], Daniel A. M. Egbe[2], and Harald Hoppe[1] — [1]Institute of Physics, Technische Universität Ilmenau, Ilmenau, Germany — [2]Linz Institute for Organic Solar Cells, Johannes Kepler University, Linz, Austria

We investigated the properties of donor-acceptor interfaces occurring in fine-tuned ternary bulk heterojunctions and were able to quantitatively correlate spectroscopic information with domain phase order. Relaxation energies for AnE-PV donor polymers as well as of PCBM were found to range within 100-200 meV.

HL 45.4 Wed 10:15 C 130

The Effect of Solvent Additive on Generation, Recombination and Extraction in PTB7:PCBM Solar Cells: A conclusive Experimental and Numerical Simulation Study — •Juliane Kniepert[1], Ilja Lange[1], Thomas Brenner[1], Jan Anton Koster[2], and Dieter Neher[1] — [1]Universität Potsdam, Germany — [2]University of Groningen, The Netherlands

Time delayed collection field (TDCF), bias amplified charge extraction (BACE) and space charge limited current (SCLC) measurements are combined with complete numerical device simulations to unveil the effect of the solvent additive 1,8-diiodooctane (DIO) on the performance of PTB7:PCBM bulk heterojunction solar cells. DIO is shown to increase the charge generation rate, reduce geminate and bimolecular recombination and increase the electron mobility. In total, the reduction of loss currents by processing with the additive raises the power conversion efficiency of the PTB7:PCBM blend by a factor of almost three. Our device simulations show unambiguously that the effect of the additive on the shape of the current-voltage curve cannot be ascribed to the variation of only the mobility, the recombination or the field-dependence of generation. It is only when the changes of all three parameters are taken into account that the simulation matches the experimental J-V-characteristics under all illumination conditions and for a wide range of voltages.

HL 45.5 Wed 10:30 C 130

Quantification of loss channels in bulk heterojunction organic solar cells based on DPP-type donor-acceptor copolymers blended with PC71BM — •Julian Robert Ochsmann[1], Deepak Chandran[2,3], Kwang-Sup Lee[3], and Frédéric Laquai[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Dublin City University, Dublin, Ireland — [3]Hannam University, Daejeon, South Korea

A promising approach to improve the performance of bulk-heterojunction (BHJ) organic solar cells (OSC) is to use low-bandgap polymers as electron donor materials as they enhance the photon absorption of the photoactive layer in the near infrared wavelength range and thereby increase the photocurrent. In addition, low-bandgap polymers are suitable for use in tandem solar cells, since their absorption spectrum is complementary to that of mid-bandgap polymers such as P3HT or PCDTBT, which allows for photocurrent matching of front and back cells. A promising class of low-bandgap polymers for single- and multijunction solar cells are donor-acceptor type copolymers based on diketopyrrolopyrrole (DPP) units. In this study we investigate the photovoltaic performance and the photophysics of two DPP-based copolymers, namely PTDPP-TT and PFDPP-TT, blended with PC71BM and applied in single junction BHJ solar cells. The photophysics of the OSC devices were investigated with broadband tran-

sient absorption pump-probe spectroscopy (TA) and analyzed with a previously reported model of charge recombination that allows to quantify the loss channels in devices.

HL 45.6 Wed 10:45 C 130

Efficiency-Limiting Processes in Low-Bandgap Polymer:Perylene Diimide Photovoltaic Blends — •Dominik Gehrig[1], Steffen Roland[2], Ian Howard[1], Dieter Neher[2], and Frédéric Laquai[1] — [1]Max-Planck-Institut für Polymerforschung, Mainz — [2]Institut für Physik und Astronomie, Physik weicher Materie, Universität Potsdam

In this work, we present a photophysical study on blends of a low-bandgap polymer, namely PBDTTT-C, as donor in combination with a PDI-based electron acceptor.[1] Exciton and charge carrier dynamics as well as loss mechanisms are investigated by sub-picosecond to microsecond pump-probe transient absorption (TA) and time-resolved photoluminescence (TRPL) spectroscopy in combination with multivariate curve resolution (MCR) data analysis. A largely diffusion-limited exciton dissociation at the donor acceptor interface and consequently a slow charge generation is observed. Time-delayed collection field (TDCF) experiments reveal a strongly field-dependent charge generation process in turn leading to low fill factors in devices. However, once free charges are generated they recombine non-geminately on a ns-us timescale indicating that they can be potentially extracted as photocurrent. By comparison of the PBDTTT-C:PDI charge generation efficiency with that of a PBDTTT-C:fullerene blend, we identify inefficient charge generation and fast non-geminate recombination competing with charge extraction to be the main bottlenecks of photocurrent generation in the investigated polymer:PDI blends.

[1] Gehrig et al., J. Phys. Chem. C 2014, 118, 20077

HL 45.7 Wed 11:00 C 130

Effect of solvent vapor annealing on perylene-based solar cells — •Stefan Grob[1], Mark Gruber[1], Andrew Bartynski[2], Theresa Linderl[1], Mark Thompson[2], and Wolfgang Brütting[1] — [1]University of Augsburg, Augsburg, Germany — [2]University of Southern California, Los Angeles, USA

Diindenoperylene (DIP) and Tetraphenyldibenzoperiflanthene (DBP) are two common materials used in organic solar cell devices. While DIP is growing crystalline, showing good charge and exciton transport but only weak absorption, DBP exhibits an amorphous character, leading to lower carrier mobility and a short exciton diffusion length, however, DBP reveals a distinctly higher absorption. For both materials we investigate the influence of solvent vapor annealing (SVA) on solar cell performance. In general, SVA leads to a reorganization of the treated materials due to a partial re-solubilization of the layers, allowing the molecules to rearrange into structures characterized by a higher degree of order [1]. Though, for DBP, extended annealing times lead to a strong aggregation of the molecules, resulting in inhomogeneous layers unfavorable for solar cells. For DIP cells however, SVA leads to an increase in fill factor (FF) and also a slight increase in short-circuit current density (Jsc) due to interface roughening. Nevertheless, the best results are obtained by combining annealed DIP layers with strongly absorbing DBP and C70 on top. Thereby, we obtain the same increase in FF but a higher gain in Jsc, elevating the power conversion efficiency by almost 20 % up to more than 4 %.

[1] G. De Luca et al., J. Mater. Chem., 2010, 20, 2493-2498

15 min. break

HL 45.8 Wed 11:30 C 130

Morphology Tuning by Side-chain Variation in Bulk-Hetero-Junction Solar Cells Based on Merocyanines — •Dirk Hertel, Julian Nowak, Stephanie Rüth, Ruth Bruker, Jürgen Schelter, and Klaus Meerholz — Universität zu Köln, Department Chemie, Luxemburgerstrasse 116, 50939 Köln

Organic photovoltaics (OPV) offers the potential of mass-produced renewable energy. Within the last decade the efficiency of organic solar cells has increased from 3 % to 10 %, mainly based on better understanding and control of morphology. We investigate merocyanines (MC), a class of low-molecular-weight colorants, as donor material in organic solar cells. These molecules are processable via both deposition techniques showing remarkable power conversion efficiencies (PCE) beyond 4% for SOL- and 6% for VAC-processed devices. Despite these impressive numbers the understanding of the influence of morphology on charge generation, transport and recombination in MCs is in its infancy. To aim towards even higher PCEs we have systematically varied the side-chain of a prototypical donor-acceptor MC with a high ground state dipole moment. By applying atomic-force mircroscopy, transmission electron microscopy and x-ray diffraction we are able to elucidate the thin film structure and show how side-chain variation reduces domain size and improves device data. We are able to correlate crystal size to optical, morphological and device data. There is an optimum side chain length and contrary to previous observations the MC:PCBM blend layers processed from solution perform better in OPVs than layers processed by thermal deposition under vacuum.

HL 45.9 Wed 11:45 C 130

Exploring the performance enhancement potential of the tapering technology for block-copolymer solar cells using a novel particle-based multiscale solar-cell algorithm — Anton Pershin, Sergii Donets, and •Stephan Baeurle — Institut für Physikalische und Theoretische Chemie, Universität Regensburg, 93040 Regensburg, Deutschland

Tapered block copolymers offer an exciting opportunity to tailor the interfacial region between different components by conserving their phase-separated mesoscale structure, which enable the generation of polymer systems with the desired spatio-dynamic properties. In this presentation, we explore their usefulness for optimizing the photovoltaic performance of polymer bulk heterojunctions. To this end, we apply a recently developed particle-based multiscale solar-cell algorithm [1,2] and investigate the effect of random tapering at the chemical junctions between the electron-donor- (D) and electron-acceptor-(A) blocks on the photovoltaic properties of various lamellar-like polyfluorene-based block-copolymer systems. Our simulation results [2] reveal that introducing a tapered middle block with optimal length leads to a significant increase of the exciton dissociation efficiency, but deteriorates the charge transport efficiency only moderately. This results in a gain of the internal quantum efficiency from 25 up to 39 % by increasing the thickness of the active layer of the solar cell from 10 up to 50 nm in direction to the DA interface. Literature: [1] A. Pershin, S. Donets, S.A. Baeurle, Polymer 55, 3736 (2014); [2] A. Pershin, S. Donets, S.A. Baeurle, Polymer 55, 1507 (2014).

HL 45.10 Wed 12:00 C 130

Effect of alcohol treatment on the morphology and performance of PTB7:PC71BM bulk heterojunction solar cells — Shuai Guo[1], Biye Cao[1], Weijia Wang[1], Jean-Francois Moulin[2], and •Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]Helmholtz-Zentrum Geesthacht am MLZ, Lichtenbergstr. 1, 85747 Garching

The environmentally friendly alcohol treatment of bulk heterojunction (BHJ) polymer solar cells using the low bandgap copolymer based on thieno[3,4-b]thiophene-alt-benzodithiophene units (PTB7) and [6,6]-phenyl-C71-butyric acid methyl ester (PC71BM) is studied. Different alcohols are tested and besides the most commonly used methanol treatment, other alcohols such as ethanol, 2-propanol, and 1-butanol also improve the device performance as compared to untreated solar cells. Changes of the surface structure caused by the alcohol treatment are probed with AFM and the modification of inner film morphology is probed by time of flight-grazing incidence small angle neutron scattering (TOF-GISANS). UV/Vis measurements show that the thickness of all BHJ films remains unchanged by the different solvent treatments. Thus, the enhanced device performance induced by the alcohol treatments is correlated to the reconstruction of the inner film structures probed with TOF-GISANS and the modified energy levels at the interfaces between the BHJ layer and the aluminum electrodes, evident by the enhanced short-circuit current and open-circuit voltage of the I-V curves.

HL 45.11 Wed 12:15 C 130

Control of Structural Order and Phase Separation in Polymer-Fullerene Solar Cells — •Christian Kästner[1], Daniel A. M. Egbe[2], and Harald Hoppe[1] — [1]Institute of Physics, Technische Universität Ilmenau, Ilmenau, Germany — [2]Linz Institute for Organic Solar Cells, Johannes Kepler University, Linz, Austria

It is common knowledge that polymer aggregation and phase separation in blends with fullerene derivatives is a delicate issue and crucially impacts the photovoltaic parameters of polymer based solar cells. On the one side, strongly intermixed polymer:fullerene phases provide large interfacial area and consequently large exciton dissociation rates and thus charge carrier generation. On

the other side, pristine, and eligibly ordered, polymer or fullerene domains support exciton delocalization and efficient charge transport. Herein, we present versatile routes to control the morphology by applying side-chain modifications to the polymer and fullerene, tuning the polymer:fullerene blend ratio and controlling the order within the bulk heterojunction via ternary blends. On the basis of an anthracene-containing poly(p-phenylene-ethynylene)-alt-poly(p-phenylene-vinylene) (PPE-PPV) copolymer backbone we investigated a number of these structure-property-relations. As an imposing result it is demonstrated that via manipulation of molecular structure and processing parameters enables tuning bulk morphologies at will.

HL 45.12 Wed 12:30 C 130

Influence of post-production thermal stress on organic photovoltaic cells — •Arne Hendel, Marlis Ortel, and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

One of the mayor challenges of organic photovoltaic cells towards large scale industrial production is the lifetime of the organic solar cells. Accelerated lifetime tests can be performed by applying thermal stress to the devices. In this study, PTB7:PCBM bulk hetero-junction solar cells were exposed in a post-production thermal heat step to temperatures up to 140°C. The reaction to thermal stress was investigated by impedance analysis and light intensity dependent I-V characteristics. It was found that the overall conductivity improved by thermal stress. In addition, an asymmetric series resistance which depends strongly on the light intensity was found by the light intensity dependent measurements. Furthermore, an investigation of the diode characteristic in dark revealed a deterioration of the blocking behaviour for reverse voltages. The results of the impedance analysis and light intensity dependent measurements were compared to AM1.5G I-V characterization, which was used to monitor the degradation of the device performance. A physical device model including the contact properties of the solar cells is presented to explain the findings.

HL 45.13 Wed 12:45 C 130

How intrinsic photo-degradation impacts photovoltaic device performance in organic solar cells — •Thomas Heumueller[1], Timothy Burke[2], William Mateker[2], Michael McGehee[2], and Christoph Brabec[1,3] — [1]Universität Erlangen-Nürnberg — [2]Stanford University — [3]ZAE Bayern

As organic PV efficiencies exceed 10%, the science of stabilization and lifetime gains importance. Several degradation phenomena in organic solar cells are related to an increase in trap density, but the mechanisms of how different types of traps affect open-circuit voltage, short-circuit current and fill factor need considerably more investigation. To separate effects from several different degradation mechanisms that usually occur at the same time, we perform tests under controlled environmental conditions and distinguish between bulk and interface effects by de-laminating and replacing electrodes. Interfacial degradation is observed to predominantly affect the fill factor, most likely due to the formation of energetic barriers and can be reversed by reapplying new electrodes. Bulk degradation in amorphous systems, like PCDTBT, results in a loss of open circuit voltage. Using charge extraction and transient photovoltage we show that the Voc losses are not caused by increased recombination, but rather by a broadening in the density of states. Crystalline materials demonstrate an increased stability against Voc losses, most likely due to a high charge carrier density at Voc. Sometimes a characteristic loss of short circuit current is observed in crystalline materials. We show that those losses can be prevented by choosing a different acceptor material.

HL 46: Graphene: Dynamics (O with HL/TT)

Time: Wednesday 10:30–13:00 Location: MA 041

HL 46.1 Wed 10:30 MA 041

Electron-phonon interactions and carrier transport in graphene — •tae yun kim[1], nicola marzari[2], and cheol-hwan park[1] — [1]Department of Physics, Seoul National University, Seoul 151-747, Korea — [2]Theory and Simulations of Materials (THEOS) and National Center for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

The transport properties of graphene have received much attention partly for its possible applications in electronic devices. In particular, as recently reported, electron-phonon interactions are important in determining the intrinsic carrier transport properties [1,2]. Based on previous studies, we investigate further the carrier transport properties of graphene in terms of carrier density and other physical variables and find connection with experimental results on this matter.

This work was supported by Korean NRF funded by MSIP (Grant No. NRF-2013R1A1A1076141). Computational resources have been provided by Aspiring Researcher Program through Seoul National University (SNU) in 2014.

[1] C.-H. Park, N. Bonini, T. Sohier, G. Samsonidze, B. Kozinsky, M. Calandra, F. Mauri, and N. Marzari, Nano Lett. 14, 1113 (2014).

[2] T. Sohier, M. Calandra, C.-H. Park, N. Bonini, N. Marzari, and F. Mauri, Phys. Rev. B 90, 125414 (2014).

HL 46.2 Wed 10:45 MA 041

Non-linear luminescence and four-wave mixing from graphene, probed by femtosecond pulse shaping — •Richard Ciesielski[1], Alberto Comin[1], Matthias Handloser[1], Torben Winzer[2], Ermin Malic[2], and Achim Hartschuh[1] — [1]Ludwig-Maximilians-Universität, AK Hartschuh, Butenandtstr. 5-11, 81377 München — [2]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany

Ultrafast optical excitation of graphene leads to two main nonlinear emission signals in the visible. The first was described as incoherent non-linear photoluminescence (NLPL). The second results from near-degenerate four-wave mixing which is extraordinarily strong in graphene as compared to other materials. We investigated the two types of emission for different layer thickness using confocal microscopy and a 15 fs pulsed laser at 1.55 eV with a pulse shaper. Spectrally resolved autocorrelation scans revealed a continuously decreasing decay time of the NLPL from 1.2 eV towards 2.8 eV. Comparing the dynamics observed for different layers allows us to identify the influence of substrate induced doping. Finally, we were able to separate a weaker third contribution induced by the microscopic polarization of graphene [1].

Financial support by the DFG through the Nanosystems Initiative Munich (NIM) and the ERC (NEWNANOSPEC) is gratefully acknowledged.

[1] T. Winzer, R. Ciesielski, M. Handloser et al., arXiv:1411.0531v1 (2014).

HL 46.3 Wed 11:00 MA 041

Microscopic description of intraband absorption in graphene — •Faris Kadi[1], Ermin Malic[1], Torben Winzer[1], Manfred Helm[2], Fabian Göttfert[2], Martin Mittendorff[2], Stephan Winnerl[2], and Andreas Knorr[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany — [2]Helmholtz- Zentrum Dresden-Rossendorf, Dresden, Germany

We present a microscopic explanation for the occurrence of the controversially discussed transient negative differential transmission observed in optical pump-probe measurements in graphene [1]. Within the density matrix formalism we investigate the transient transmission with respect to optical interband as well as phonon-assisted intraband transitions. While interband processes yield a positive contribution due to absorption bleaching, we find intraband transitions to decrease differential transmission. Interestingly, in the low excitation regime, the phonon-assisted absorption prevails over the absorption bleaching resulting in the experimentally observed negative differential transmission [2]. The zero-crossing occurs within the first hundreds of femtoseconds and is followed by a recovery of the transmission spectrum on a picosecond timescale in a good agreement with experimental observations. [1] S.Winnerl, F. Göttfert, M. Mittendorff, et al., Journal of Physics: Condensed Matter 25, 054202 (2013) [2] F. Kadi, T. Winzer, E. Malić, et al., Phys. Rev. Lett. 113, 035502, (2014)

HL 46.4 Wed 11:15 MA 041

Anisotropic Intravalley Scattering in Strongly Doped Graphene — •Daniela Dombrowski[1], Wouter Jolie[1], Sven Runte[1], Marin Petrović[2], Fabian Craes[1], Jürgen Klinkhammer[1], Marko Kralj[2], Predrag Lazić[3], Eran Sela[4], and Carsten Busse[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Institut za fiziku, Croatia — [3]Institut Ruđer Bošković, Croatia — [4]Raymond and Beverly Sackler School of Physics and Astronomy, Tel-Aviv University, Israel

We perform Fourier-transform scanning tunneling spectroscopy (FT-STS) studies on Cs intercalated graphene on Ir(111). Angle-resolved photoemission spectroscopy (ARPES) measurements show, that the Cs strongly n-dopes graphene and shifts the Fermi level into the region of strong trigonal warping. We observe intervalley scattering and additionally a clear feature of intravalley scattering, which exhibits an anisotropic intensity distribution with dominant scattering in Γ-M direction.

In the linear region of the Dirac cone, conservation of pseudospin leads to the suppression of intravalley scattering since the direction of the pseudospin is either parallel or antiparallel to the momentum, thus the system has well defined chirality. This is no longer valid in the trigonal warping region near the Van-Hove singularity.

The FT-STS results are supplemented by density functional calculations of the electronic band structure and simulations of the scattering pattern based on the T-matrix theory.

HL 46.5 Wed 11:30 MA 041

Theory of coherent light emission in graphene — •Roland Jago, Torben Winzer, Andreas Knorr, and Ermin Malic — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany

Within the density matrix formalism we present a microscopic and full quantized theoretical description of the coupled carrier, phonon and photon dynamics in graphene implemented in a photonic crystal nanocavity. We demonstrate that under strong optical excitation a spectrally broad and long-lived population inversion can be achieved. In the case of free-standing graphene non-radiative Coulomb-induced carrier-recombination on a femtosecond time scale prevents an efficient emission of coherent photons. To partially suppress this ultrafast recombination, we propose to support graphene on a substrate having high-dielectric screening. In this case, our calculations reveal a temporarily extended population inversion, that remains stable up to some tens of picoseconds under realistic conditions. In particular we observe the emission of coherent laser light suggesting graphene as gain medium for lasers [2].

[1] T. Winzer, E. Malic and A. Knorr, Phys. Rev. B 87, 165413 (2013) [2] R. Jago, T. Winzer, A. Knorr and E. Malic, arXiv:1409.8182 (2014)

HL 46.6 Wed 11:45 MA 041

Phonon dynamics of graphene on copper substrate — •Naira S. Grigoryan, Eeuwe S. Zijlstra, and Martin E. Garcia — Theoretical Physics, University of Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

In the framework of density functional theoretical calculations, the lattice dynamical properties of graphene with and without a Cu(111) substrate have been investigated and analyzed using our in-house code for highly excited valence electron systems (CHIVES). We find that the lattice dynamics exhibits large sensitivity to the presence of copper. In particular, the appearance of a nearly dispersionless phonon branch at ~1.5THz makes this system a potential mirror for light molecules. We further show that there is a lifting of the degeneracy of the ZO and ZA modes at the M- point.

HL 46.7 Wed 12:00 MA 041

Non-equilibrium Carrier Relaxation in Graphene investigated with tr-ARPES — •Mariana Chavez Cervantes[1], Raghu Tomar[1], Hubertus Bromberger[1], Haiyun Liu[1], Stefan Link[2], Ulrich Starke[2], Andrea Cavalleri[1,3], and Isabella Gierz[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany — [3]Department of Physics, Clarendon Laboratory, University of Oxford, Oxford, United Kingdom

We used time- and angle-resolved photoemission spectroscopy (tr-ARPES) based on high order harmonics generation for the extreme ultra-violet (XUV) probe to investigate the relaxation of photo-excited carriers in quasi-freestanding epitaxial graphene samples. From the data we determined the energy dependence of the scattering rate that, according to Ref. [1,2], is predicted to follow the imaginary part of the *equilibrium* self-energy. In order to test this hypothesis we compare the scattering rate measured at different sample temperatures and for different pump fluences with the equilibrium self-energy determined from high-resolution static ARPES experiments as described in Ref. [3,4].

[1] M. Sentef et al., Phys. Rev. X 3, 041033 (2013)
[2] A. F. Kemper et al., Phys. Rev. B 90, 075126 (2014)
[3] A. Bostwick et al., Nat. Phys. 3, 36 (2007)
[4] I. Gierz et al., Faraday Disc. 171 (1), 311 (2014)

Invited Talk HL 46.8 Wed 12:15 MA 041

Electronic structure and electron dynamics in two-dimensional materials — •Philip Hofmann — Department of Physics and Astronomy, Aarhus University

Two-dimensional materials can be grown epitaxially and in high quality on different substrates, and this can be exploited to study their electronic structure and different many-body effects. In this talk I will review the growth and electronic properties of epitaxial graphene, bilayer graphene and single-layer MoS_2. Specifically, I will focus on the electronic structure of these materials as studied by angle-resolved photoemission spectroscopy. This technique does not only give access to the materials' band structure but also to many-body effects such as the electron-electron and electron-phonon interaction. This is particularly so for the time-resolved variety of the technique in which the carrier dynamics can be followed in real time.

HL 46.9 Wed 12:45 MA 041

Dirac carrier thermalization on the sub 10fs timescale observed by tr-ARPES — •Sven Aeschlimann[1,2], Mariana Chavez Cervantes[1], Francesca Calegari[1,3], Cephise Cacho[4], Emma Springate[4], Stefan Link[2], Ulrich Starke[2], Klaus Kern[2,5], Andrea Cavalleri[1,6], Christian R. Ast[2], and Isabella Gierz[1] — [1]MPI for the Structure and Dynamics of Matter, Hamburg, Germany — [2]MPI for Solid State Research, Stuttgart, Germany — [3]IFN, Consiglio Nazionale delle Ricerche, Milano, Italy — [4]Central Laser Facility, STFC Rutherford Appleton Laboratory, Harwell, United Kingdom — [5]EPFL, Lausanne, Switzerland — [6]University of Oxford, United Kingdom

We used time- and angle-resolved photoemission spectroscopy (tr-ARPES) with extreme ultra-violet (XUV) probe pulses from high order harmonics generation (HHG) to observe the ultrafast electron dynamics in photo-excited quasi-freestanding epitaxial graphene monolayers. By the use of the hollow core fiber compression technique, we produced 8 fs pulses, which are utilized both for driving HHG and for photo-excitation. These ultrashort pulses allowed us to observe the initial thermalization of photo-excited carriers via electron-electron scattering with unprecedented temporal resolution. We find that, at early times, the carrier distribution neither follows a Fermi-Dirac distribution nor the non-equilibrium distribution expected for a population-inverted state [1]. We attribute this to the short duration of the pump pulse on the order of the electron-electron scattering time.

[1] I. Gierz et al., Nature Materials 12, 1119 (2013)

HL 47: Frontiers of electronic structure theory: Organics and materials

Time: Wednesday 10:30–13:30 Location: MA 004

Invited Talk HL 47.1 Wed 10:30 MA 004

Transport and excitations in biased nano-junctions: DFT-based simulations — •Mads Brandbyge — Dept. of Micro and Nanotechnology, DTU-Nanotech, and Center for Nanostructured Graphene (CNG) Technical University of Denmark, Build. 345 east, 2800 Kongens Lyngby, DENMARK

In nano-junctions the electronic current is forced through a bottleneck down to the single molecular or atomic level. The highly non-equilibrium electronic system in such junctions results in various excitations such as phonons or plasmons. The phonon interaction directly yield signals in the current which can be probed in current-voltage spectroscopy, while the plasmon interaction can result in light emission which seems to be related to the current fluctuations/noise at finite frequency. The low frequency shot noise can provide information about the elastic transport channels and underlying spin-dependent electronic structure of the junctions. We will discuss how theory based on non-equilibrium Greens functions in combination with density functional theory or beyond, can be compared to experimental results, and provide important insights into excitations, the underlying transport channels, and electronic structure of the junctions. The electronic current will not only excite phonons. Energy non-conserving current-induced forces may control the resulting heat flow and heat distribution in the junctions, and in some cases lead to a break-down of the harmonic approximation.

HL 47.2 Wed 11:00 MA 004

Role of atomic multiplets in intermediate valence SmB_6 and PuB_6 systems — •Alexander B. Shick[1], Alexander I. Lichtenstein[2], and Mikhail I. Katsnelson[3] — [1]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic — [2]Institute of Theoretical Physics, University of Hamburg, Hamburg, Germany — [3]Radboud University Nijmegen, The Netherlands

The materials with strong electron correlations are important because of the fundamental properties, and the technological applications. Recently, SmB_6 (as well as PuB_6) was proposed as 3D topological insulator [1]. The electronic structure calculations are performed combining the LDA with an exact diagonalization of the Anderson impurity model [2] for [Sm,Pu]B_6. For the Sm atom in SmB_6, intermediate valence ground state (GS) is found with the f-shell occupation $\langle n_{4f}\rangle = 5.6$. The GS is a singlet, and the first excited triplet state ~ 3 meV higher in the energy. The f-orbital density of states is in agreement with experimental PE spectra. SmB_6 is a narrow band insulator already in LDA, with the direct band gap of ~ 10 meV. The electron correlations increase the band gap which now becomes indirect. For the Pu atom in PuB_6, we also find intermediate valence ($\langle n_{5f}\rangle = 5.5$) singlet GS. The calculations illustrate that many-body effects are relevant to form the indirect band gap, and support the idea of "topological Kondo insulator" in SmB_6. [1] M. Dzero *et al.*, Phys. Rev. Lett. **104**, 106408 (2010); [2] A. B. Shick *et al.*, Phys. Rev. B **87**, 020505(R) (2013).

HL 47.3 Wed 11:15 MA 004

Transition paths and cohesive energies in alpha-sexithiophene polymorphs — •Bernhard Klett, Caterina Cocchi, and Claudia Draxl — Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

Like many organic crystals, oligothiophenes display polymorphism. Different molecular orientations and stacking arrangements are known to influence electronic and transport properties. An in-depth theoretical understanding of the energetics in these systems is crucial to control their growth and fully exploit their potential. In fact, their outstanding opto-electronic features make oligothiophenes excellent candidates for a number of technological applications, ranging from thin-film transistors to photovoltaic cells. We investigate alpha-sexithiophene in view of the transition between the high-temperature (HT) and low-temperature (LT) phase. With the full-potential all-electron density-functional theory code exciting [1], we analyse the cohesive properties of the two polymorphs. Our results indicate HT as the most stable phase, in agreement with previous molecular-dynamics simulations [2]. We also explore a transition path between the two polymorphs, suggesting different reaction coordinates. Our findings allow for estimating the energy barrier between the two phases, hence gaining insight into the microscopic mechanisms ruling polymorphism in organic crystals. [1] A. Gulans, et al., J. Phys.: Condens. Matter 26, 363202 (2014). [2] R. G. Della Valle, et al., J. Phys. Chem. A, 112, 6715 (2008).

HL 47.4 Wed 11:30 MA 004

Importance of the reorganization energy barrier in computational design of porphyrin-based solar cells with cobalt-based redox mediators — •Kristian Baruël Ørnsø, Elvar Örn Jónsson, Juan Maria Garcia-Lastra, Karsten Wedel Jacobsen, and Kristian Sommer Thygesen — Center for Atomic-scale Materials Design, Department of Physics, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark

The shift from iodide based redox mediators in dye sensitized solar cells towards octahedral cobalt complexes has lead to a significant increase in the efficiency. However, due to the nature of this type of complexes the driving force required for the regeneration of the dye is very high and this limits the achievable efficiency. Here we show that the large driving force is a direct consequence of the large reorganization energy of the dye regeneration reaction. The reorganization energies for charge transfer between a simple zinc porphyrin dye and two popular cobalt based redox mediators is calculated using ab-initio molecular dynamics with explicit solvent. These results are then combined with a Marcus based extrapolation scheme to obtain the reorganization energies of more than five thousand porphyrin based dyes.We propose a scheme for scoring the performance of the porphyrin dyes which is able to identify already known high-performance dyes in addition to a number of even better candidates. Our analysis shows that large internal reorganization energy of the Co-based redox mediators is a main bottleneck for achieving higher efficiencies.

HL 47.5 Wed 11:45 MA 004

Ab initio Simulation of Optical Limiting: The Case of Metal-Free Phthalocyanine — •Caterina Cocchi[1,2], Deborah Prezzi[2], Alice Ruini[2,3], Elisa Molinari[2,3], and Carlo Andrea Rozzi[2] — [1]Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany — [2]Centro S3, CNR Istituto-Nanoscienze, Modena, Italy — [3]Dipartimento di Scienze Fisiche, Informatiche, Matematiche, University of Modena and Reggio Emilia, Italy

Optical limiting (OL) is a nonlinear process that is relevant for an entire class of devices related to the protection of light-sensitive elements, including the human eye, from intense light sources. While extensively studied experimentally, an accurate theoretical investigation of this phenomenon is still missing. In the framework of time-dependent density-functional theory, we present a fully ab initio, non-perturbative description of OL properties of a metal-free phthalocyanine, a prototypical macrocyclic organic compound. By applying a broadband electric field of increasing intensity, we confirm that reverse saturable absorption is the leading mechanism for OL phenomena in this class of systems, and reveal that a number of dipole-forbidden excitations are populated by excited-state absorption at more intense external fields. The excellent agreement with the available experimental data supports our approach as an effective and powerful tool to describe and predict OL [1]. [1] C. Cocchi et al., Phys. Rev. Lett. 112, 198303 (2014).

HL 47.6 Wed 12:00 MA 004

High-throughput Screening of Perovskite Oxides and Related Compounds for Light Harvesting Applications — •Ivano E. Castelli[1], Nicola Marzari[1], Kristian S. Thygesen[2], and Karsten W. Jacobsen[2] — [1]Theory and Simulation of Materials, and EPFL National Center for Computational Design and Discovery of Novel Materials (MARVEL), EPFL, Lausanne, Switzerland — [2]Center for Atomic-scale Materials Design, Technical University of Denmark, Kgs. Lyngby, Denmark

Solar energy harvesting in a photoelectrochemical (PEC) cell, where water is split into hydrogen and oxygen, is an attractive and renewable contribution to our global needs of increasing energy demand and storage. We explore the possibility of identifying novel photocatalysts for PECs with the use of high-throughput quantum mechanical simulations. We devise inexpensive approaches to calculate systematically the structural and electronic properties of 19000 cubic ABX3 perovskites, obtained by combining 52 possible metals as A- or B-

cations, together with oxygen, nitrogen, sulfur and fluorine as anions. Using the screening criteria of stability and bandgap, 20 promising materials have been identified for visible-light harvesting [1]. The problem of corrosion has been addressed, determining the Pourbaix diagrams of the candidates through a combination of experimental and computational data [2]. We also suggest a handful of lower symmetry layered and rare-earth perovskites for further theoretical and experimental investigation. References: [1] I. E. Castelli et al., Energy Environ. Sci. 5, 9034 (2012). [2] I. E. Castelli et al., Topics in Catalysis 57, 265 (2014).

HL 47.7 Wed 12:15 MA 004

Understanding and designing novel materials for energy — •Silvana Botti — Friedrich-Schiller-Universität Jena, Germany

I will present an overview of our most recent theoretical/computational developments and some examples of their application to calculate from first-principles the structural and electronic properties of materials for energy production, storage, and saving.

The systems we are interested in are varied, ranging from thin-films absorbers and transparent conductive oxides for solar cells, to thermoelectrics, light-weight materials for constructions, complex hydrides for on-board hydrogen storage.

Nowadays, ab initio approaches based on density functional theory ally accuracy and efficiency, which make them suitable for understanding the physics not only of simple bulk crystals, but also of nanostructures, crystals with defects, doped crystals, interfaces, alloys, etc. As a consequence, ab initio calculations are finally able to analyze the "real" samples measured in experiments, allowing accurate comparisons of both ground-state and excited-state properties.

Moreover, ab initio methods can be used together with structural prediction algorithms and evolutionary algorithms to solve the inverse problem, i.e. find the best material for a specific application, providing a precious guide for experimental search of novel materials.

HL 47.8 Wed 12:30 MA 004

Accurate density-functional theory calculation of bulk properties of 65 elemental solids — •Sven Lubeck[1], Andris Gulans[1,2], and Claudia Draxl[1] — [1]Humboldt-Universität zu Berlin, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Density-functional theory (DFT) is a common method for calculating various properties of molecules and solids. While a large part of errors in DFT calculations stems from approximations to the exchange-correlation functional, there are additional not well controlled errors introduced by numerical implementation of electronic structure codes. In this work, we present accurate benchmark calculations of equation of state for 65 non-magnetic elemental solids. The data have been obtained using the full-potential augmented-plane-waves (APW) code `exciting` [1]. High accuracy has been achieved by constructing a converged APW+lo basis set, which yields consistent bulk properties of considered solids for a range of augmentation sphere sizes. Using methodology suggested in Ref. [2], we compare our results to those obtained with WIEN2k [2] and find the average and maximum Δ-values of 0.3 meV/atom and 2.1 meV/atom, respectively.

[1] A. Gulans, S. Kontur, C. Meisenbichler, D. Nabok, P. Pavone, S. Rigamonti, S. Sagmeister, U. Werner, and C. Draxl, J. Phys.: Condens. Matter 26, 363202 (2014).

[2] K. Lejaeghere, V. Van Speybroeck, G. Van Oost and S. Cottenier, Critical Reviews in Solid State and Materials Sciences 39, 1-24 (2014).

HL 47.9 Wed 12:45 MA 004

Electronic phase transitions of bismuth under strain from relativistic self-consistent *GW* calculations — Irene Aguilera, •Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We present quasiparticle self-consistent *GW* (QS*GW*) calculations of semimetallic bulk Bi. We go beyond the conventional QS*GW* method by including the spin-orbit coupling throughout the self-consistency cycle. This approach improves the description of the electron and the hole pockets considerably with respect to standard density functional theory (DFT), leading to excellent agreement with experiment. We employ this relativistic QS*GW* approach to conduct a study of the semimetal-to-semiconductor and the trivial-to-topological transitions that Bi experiences under strain. While DFT predicts that an unphysically large strain is needed for such transitions, we show that the relativistic QS*GW* description of the electronic structure moves the required strain into a regime that is likely to be realizable in experiment. We acknowledge financial support from the Alexander von Humboldt Foundation and from the Helmholtz Association through the Virtual Institute for Topological Insulators (VITI).

HL 47.10 Wed 13:00 MA 004

A GW algorithm of reduced complexity for organic crystals — •Saber Gueddida[1], Dietrich Foerster[1], Peter Koval[2], and Daniel Sanchez-Portal[2] — [1]Laboratoire Ondes et Matière d'Aquitaine, University of Bordeaux, France — [2]Donostia International Physics Center, San Sebastian, Spain

Density functional theory (DFT) provides a variational estimate of the electronic structure and geometry of many materials in their ground state. By its construction, DFT is unsuited for a description of the excited states, and particularly so for semi conductors. For these, one resorts to Hedin's GW approximation that gives rather good bands and gaps. A practical limitation of this approach is its computational cost that increases with the fourth power (N**4) of the number of atoms N per unit cell. Starting in 2007 [1], we have developed methods of "reduced complexity" that lower the growth of CPU time in calculations of electronic structure from N**4 to N**3, both for optical absorption [2] and in the GW approximation for finite systems [3]. Here we report on the extension of our methods to crystals, where we reduce the growth of CPU time again from N**4 to N**3, with N now the number of atoms in the unit cell of the crystal. Our work is motivated by organic semiconductors that have too many atoms in their unit cell for O(N**4) algorithms to be practical. Our results should help to improve and optimize organic solar cells. [1] D. Foerster, J. Chem. Phys. 128 (34108) 2008. [2] P. Koval, D. Foerster and O. Coulaud, J. Chem. Theory Comp. 6 (2654) 2010 . [3] D. Foerster, P. Koval, and D. Sánchez-Portal, J. Chem. Phys. 135, 74105 (2011) .

HL 47.11 Wed 13:15 MA 004

Modeling anisotropic organic molecules at patterned semiconductor surfaces — •Nicola Kleppmann and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Hybrid systems consisting of organic molecules at inorganic semiconductor surfaces are gaining increasing importance as thin film devices for optoelectronics. Their large charge carrier densities and tuneable resonance energies make them ideal candidates for semiconductor devices. However, the efficiency of such devices strongly depends on the self-organized structure formed by the adsorbed molecules, which depends, in turn, on the complex interplay of growth conditions and molecular properties. Recent ab initio calculations and experiments inspire us to examine the growth of sexiphenyl (6P) on ZnO(10-10) as a model system to understand self-organization of highly anisotropic molecules [1]. We develop a coarse-grained interaction hamiltonian of 6P molecules using a Gay-Berne potential and a linear quadrupole interaction term with additional substrate influence. We perform both equilibrium and non-equilibrium (growth) Monte Carlo simulations on a 2D lattice, where the rotational degrees of freedom of the molecules are continuous. We use these simulations to investigate orientational ordering in the condensed state, which is characterized by local descriptors such as order parameters and angular distributions.

[1] N. Kleppmann, and S. H. L. Klapp, submitted to JCP

[2] S. Bommel, N. Kleppmann et al., Nat Comm 5, 5388 (2014)

HL 48: Focus Session (with O): Nanophotonic concepts and materials for energy harvesting - Plasmonics, transformation optics, upconversion, and beyond I

Nanostructured and novel photonic materials can control the spectral composition of light, its propagation characteristics, and its interaction with matter. The use of these abilities is particularly rewarding in the context of energy harvesting in semi-conductor materials. This focused session appreciates and presents the most recent advancement in this field of research, where progress has been made from a conceptual but also from a materials perspective.

Organization: Carsten Rockstuhl (KIT, Karlsruhe), Jan Christoph Goldschmidt (FhG ISE, Freiburg), Ralf Wehrspohn (MLU Halle), Uli Lemmer (KIT, Karlsruhe)

Time: Wednesday 11:00–13:00 Location: EW 201

Invited Talk HL 48.1 Wed 11:00 EW 201

Transformation Optics: From Fundamentals to Applications for Energy Harvesting — •Martin Wegener and Martin Schumann — Institute of Applied Physics and Institute of Nanotechnology, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany

Transformation optics can be seen as a versatile tool for designing devices in optics and other areas of physics. In this talk, we start by giving a broad introduction into this concept. A striking paradigm is invisibility cloaking. We briefly review experimental demonstrations in optics, thermodynamics, and mechanics. Next, we discuss a possible application: In order to extract the electrical power from solar cells, metal contacts at the sun-facing surface are required. Unfortunately, these contacts create optically dead areas, reducing the overall current per area by a few percent. We present a solution to this problem by using microstructures that are designed by transformation optics and that cloak the contacts. An experimental proof-of-principle demonstration based on three-dimensional direct-laser-writing optical laser lithography is given.

Invited Talk HL 48.2 Wed 11:30 EW 201

Nanostructures and materials for intermediate band solar cells — •Antonio Martí — Instituto de Energía Solar, ETSI Telecomunicación, Universidad Politécnica de Madrid

Intermediate band solar cells (IBSCs) seek for materials that can harvest photons with energy lower than the semiconductor bandgap without degrading the output voltage of the cell. One of these material systems relies on the use of quantum dots (QDs). Under this approach, photons are harvested thanks to the energy states of the electrons confined in the quantum dots. In this contribution we review the theory that sustains the use of QDs for IBSC applications, the design constrains of these kind of solar cells, its limitations and challenges as well as the most recent experimental results. These experimental results refer to the empirical demonstration of the use of two below bandgap energy photons to generate an electron-hole pair and the preservation of the output voltage of the cell.

HL 48.3 Wed 12:00 EW 201

Emission quenching of magnetic dipole transitions near an absorbing optical nanoantenna — •Dmitry Chigrin, Deepu Kumar, and Gero von Plessen — RWTH Aachen University, 52074 Aachen, Germany

The optical emission of an ionic emitter near an absorbing optical nanoantenna (such as a metal nanoparticle) can be enhanced or quenched due to near-field effects induced by the nanoantenna. A comparison of emission quenching of electric dipole (ED) and magnetic dipole (MD) transitions in the close vicinity of a metal nanoparticle has been carried out in this work. It is demonstrated that the emission quenching of the MD transitions becomes dominant at substantially shorter distances to the surface of the absorbing nanoantenna as compared to the ED transitions. This difference in quenching behaviour is due to different asymptotic dependencies of the quasi-static radiative and non-radiative decay rates of ED and MD transitions near a metal nanoparticle. It is shown that in the extreme near-field regime the non-locality of the dielectric response of the metal cannot be neglected, which leads to a reduction in the emission quenching for both ED and MD transitions near the absorbing optical nanoantenna.

HL 48.4 Wed 12:15 EW 201

Light trapping with combined photonic elements — •Aimi Abass[1] and Bjorn Maes[2,3] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [2]Photonics Research Group (INTEC), Ghent University-imec, Sint-Pietersnieuwstraat 41, B-9000 Ghent, Belgium — [3]Micro- and Nanophotonic Materials Group, Faculty of Science, University of Mons, 20 place du Parc, B-7000 Mons, Belgium

Nanophotonics offers many avenues for enhancing solar cells. For example, one can tailor the incoming light flow to boost absorption via nanostructures. To ensure strong absorption over the whole spectral range of interest, one has to utilize many photonic phenomena. Oftentimes however, the nanoscale geometrical requirements for optimum excitation of one phenomenon can be at the expense of another. To address this challenge, we examine light trapping strategies with combined photonic elements and study conditions under which different elements complement each other. Here, we discuss the usage of dual interface gratings (DIGs) and diffuser-grating structures. The former enhances absorption by relying on guided mode excitation while the latter focuses on antireflection and scattering management. In such structures the responsibility of different optical components is split, enabling more flexibility in optimization. One main point of discussion is multiperiodic DIG systems, which provide a rich Fourier spectrum, while maintaining a straightforward geometry. In studying combined diffuser-grating structures, we developed a memory efficient calculation method, which evades dealing with rough diffuser geometries directly.

HL 48.5 Wed 12:30 EW 201

Tailoring Disorder of Nanophotonic Light-Trapping Concepts for Thin-Film Silicon Solar Cells — •Ulrich W. Paetzold[1], Karsten Bittkau[1], Y. J. Donie[2], Guillaume Goumard[2], Radwanul H. Siddique[2], Michael Smeets[1], Hendrik Hölscher[2], Reinhard Carius[1], Uwe Rau[1], and Uli Lemmer[2] — [1]IEK5 * Photovoltaik, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Light Technology Institute and Institute for Microstructure Technology, Karlsruhe Institute of Technology, Engesserstr. 13, 76131 Karlsruhe, Germany

Light-trapping is essential for high performance thin-film solar cells applying optically thin photoactive absorber layer such as a-Si:H with thicknesses below 500 nm. Conventional devices apply randomly textured transparent conductive oxide substrates serving as light-scattering front contacts as well as reflective light-scattering metal back contacts. In recent years, a substantial progress in the development of nanophotonic light-trapping schemes has been reported. In order, to further advance the nanophotonic concepts, the role of tailored disorder in these nanophotonic light trapping concepts is investigated. We present a systematic experimental as well as simulation study on the impact of disorder in nanophotonic light-trapping employing periodic grating couplers in thin-film solar cells. Our results demonstrate a spectrally broad enhanced light trapping effect, i.e., a significant improvement of photocurrent generation, after introducing disorder in advanced nanophotonic light trapping concepts which already beat state-of-the-art light trapping concepts.

HL 48.6 Wed 12:45 EW 201

Opaline Photonic Crystals as Back Side Reflector for Thin-Film Silicon Solar Cells — •Daniela Schneevoigt[1], Frederik Bub[1], Alexander N. Sprafke[1], Ralf B. Wehrspohn[1,2], André Hoffmann[3], Karsten Bittkau[3], Reinhard Carius[3], Samuel Wiesendanger[4], and Carsten Rockstuhl[5] — [1]Martin-Luther-Universität Halle-Wittenberg, Germany — [2]Fraunhofer IWM, Halle, Germany — [3]Forschungszentrum Jülich GmbH, Germany — [4]Friedrich-Schiller-Universität Jena, Germany — [5]Karlsruher Institut für Technologie, Germany

3D photonic crystals, such as opaline structures, have a tremendous

potential to increase the efficiency of solar cells by enabling advanced light management concepts. Especially opaline structures applied to the back side of a solar cell provide various functions that can enhance the light path in the cell. Light in a specific spectral interval that is not absorbed during its first passage through the solar cell is strongly back reflected if the opal satisfies a Bragg condition. Light at other wavelengths might be diffracted back into the cell by the opal. By both means the probability of light absorption and thus the efficiency of the solar cell is increased. Here, we present the successful fabrication of large-area opaline structures at the back side of 1μm thick hydrogenated microcrystalline silicon (μc-Si:H) single junction solar cells via an automated spray coating process. The optical, structural, and electrical characteristics of these structures on different μc-Si:H textures were analyzed and the photovoltaic characteristics of the completely integrated system were evaluated and compared to simulations.

HL 49: Quantum information systems: mostly concepts (with TT)

Time: Wednesday 11:00–13:00 Location: EW 202

HL 49.1 Wed 11:00 EW 202

Cold atom - semiconductor hybrid quantum system — •Jan-Philipp Jahn[1], Mathieu Munsch[1], Lucas Beguin[1], Andreas Kuhlmann[1], Aline Faber[1], Tobias Kampschulte[1], Andreas Jöckel[1], Armando Rastelli[2], Fei Ding[3], Oliver G. Schmidt[3], Nicolas Sangouard[1], Philipp Treutlein[1], and Richard J. Warburton[1] — [1]University of Basel, Switzerland — [2]Johannes-Kepler University Linz, Austria — [3]IFW Dresden, Germany

Semiconductor quantum dots are excellent single-photon sources, providing triggered single-photon emission at a high rate and with high spectral purity [1]. Independently, atomic ensembles have emerged as one of the best quantum memories for single photons, providing high efficiency storage and long memory lifetimes [2]. In this project, we combine these two physical systems to exploit the best features from both worlds. On the one hand, we have characterized a new type of self-assembled GaAs/AlGaAs quantum dots that emit narrowband ($\Delta\nu$ = 500 MHz) single-photons at a wavelength compatible with Rb atoms. Fine tuning of the photon frequency is achieved via strain. This allows us to perform spectroscopy of the Rb D2-line at the single-photon level, proving that we can address the different hyperfine transitions. On the other hand, we have developed a detailed theory of an EIT-based memory scheme in a dense ultracold ensemble of 87Rb atoms (OD>150) that achieves storage-and-retrieval efficiency exceeding 28% [3].

[1] R. J. Warburton, Nature Mater. 121, 483-493 (2013) [2] F. Bussières et al., J. Mod. Opt. 60, 1519 (2013) [3] M. T. Rakher et al., Phys. Rev. A 88, 053834 (2013)

HL 49.2 Wed 11:15 EW 202

Surface Acoustic Waves as a versatile tool for quantum information processing with solid-state spin qubits — •Martin J. A. Schuetz[1], Eric M. Kessler[2,3], J. Ignacio Cirac[1], Mikhail D. Lukin[2,3], Lieven M. K. Vandersypen[4], and Géza Giedke[1,5] — [1]Max-Planck-Institut für Quantenoptik, H.-Kopfermann-Str 1, D-85748 Garching — [2]ITAMP, Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts 02138, USA — [3]Physics Department, Harvard University, Cambridge, Massachusetts 02318, USA — [4]Kavli Institute of NanoScience, TU Delft, P.O. Box 5046, 2600 GA Delft, The Netherlands — [5]Donostia International Physics Center, Paseo Manuel de Lardizabal 4, E-20018 San Sebastian

Surface acoustic waves (SAW) offer a great variety of applications in the context of solid-state quantum information processing (QIP). The use of SAWs as transport shuttles for single electrons has been demonstrated, high-quality cavities for SAW can be fabricated, and their quantum nature has been explored coupling them to superconducting qubits.

We investigate theoretically the use of SAWs for QIP with spin qubits in GaAs quantum dots. We show that strong coupling between the qubit and SAW cavities is feasible with current cavity designs. We investigate the viability of "quantum acoustics" in this setting, where phononic cavities are used to couple spin qubits and phonons serve as propagating carriers of quantum information. Possibilities to extend these results to other spin qubits such as NV centers in diamond are discussed.

HL 49.3 Wed 11:30 EW 202

Creating and controlling entanglement using coherent time-delayed feedback — •Sven Moritz Hein, Franz Schulze, Alexander Carmele, and Andreas Knorr — Technische Universität Berlin, Institut für theoretische Physik, Nichtlineare Optik und Quantenelektronik, Hardenbergstraße 36, 10623 Berlin, Germany

Entanglement is a quantum-mechanical property interesting from a fundamental point of view as well as for future applications in quantum information science. We propose to use time-delayed quantum-coherent feedback to create and control entanglement between quantum-mechanical objects.

In classical physics, feedback schemes with a distinct feedback delay[1] are successfully applied to control unstable states and periodic orbits. We demonstrate by numerical simulations that this concept can be transferred to the quantum regime. Here, it can be used to enhance the entanglement of photons from a biexciton cascade[2] and also entangle cavities and other quantum nodes in a quantum network. To preserve quantum coherence, the feedback will be modeled in a fully quantum-mechanical way without the use of measurements.

[1] K. Pyragas, Phys. Lett. A 170, 421–428 (1992)
[2] S. M. Hein, et al., Phys. Rev. Lett. 113, 027401 (2014)

HL 49.4 Wed 11:45 EW 202

Temporal shaping of Gaussian single photon pulses — •Emanuel Peinke[1], Gaston Hornecker[2], Julien Claudon[1], Alexia Auffèves[2], and Jean-Michel Gérard[1] — [1]CEA/CNRS joint team "Nanophysics and Semiconductors", INAC, CEA and Université Grenoble Alpes, Grenoble, France — [2]CEA/CNRS joint team "Nanophysics and Semiconductors", Institut Néel, CNRS and Université Grenoble Alpes, Grenoble, France

Single photon pulses with a Gaussian temporal envelope constitute an important resource for optical quantum information processing [1]. We propose here a scheme to shape single photon pulses with high fidelity using a two-level emitter (e.g. a quantum dot (QD)) coupled to a frequency-tunable microcavity. By controlling the cavity resonance frequency on a time-scale shorter than the typical emitter spontaneous emission time, one controls the instantaneous emission rate and thus the temporal envelope of the emitted photon. For realistic experimental parameters, we show that nearly ideal Gaussian pulses can be generated with QD-semiconductor systems and superconducting Josephson circuits.

[1] P. P. Rohde, T. C. Ralph, and M. A. Nielsen. Optimal photons for quantum- information processing. Phys. Rev. A, 72:052332, Nov 2005.

HL 49.5 Wed 12:00 EW 202

Electric dipole spin resonance in the presence of valley degeneracy — •Marko Rancic and Guido Burkard — University of Konstanz

We theoretically investigate the electric dipole spin resonance (EDSR) in a single Si/SiGe quantum dot in the presence of a magnetic field gradient, e.g., produced by a micomagnet. The control of electron spin states can be achieved by applying an oscillatory electric field, which induces periodic back and forth motion of the electron spin inside the quantum dot. This motion inside a magnetic field gradient, produces an effective periodic in-plane magnetic field, and allows for driven spin rotations near resonance. By solving a Lindblad master equation, we discuss possible electron spin relaxation and decoherence mechanisms relevant to EDSR. In Si there is 5% of naturally occurring nuclear spin 1/2 isotope, which causes the electron spin to decohere. Nuclear spins are included in our model through the additional random Overhauser magnetic field. Furthermore, a valley dependent g-factor, combined with intervalley scattering gives rise to another electron spin decoherence mechanism. The goal of our study is to describe the efficiency of a spin echo sequence in the presence of all mentioned relaxation and decoherence mechanisms.

HL 49.6 Wed 12:15 EW 202

Resonant exchange qubit under influence of electrical noise — •Maximilian Russ and Guido Burkard — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

In this work we investigate the influence of electrical charge noise on a resonant exchange (RX) qubit in a triple quantum dot. This RX qubit is a variation of the exchange-only qubit [1] which responds only to a narrow-band resonant frequency [2,3]. Our noise model includes uncorrelated charge noise in each quantum dot giving rise to two independent (noisy) bias parameters. We calculate the energy splitting of the two qubit states as a function of these two bias detuning parameters to find "sweet spots", where the noise suppression is maximized. Our investigation shows that such sweet spots exist within the low bias regime, in which the bias detuning parameters have the same magnitude as the hopping parameters. The location of the sweet spots depends on the bias detuning and the hopping asymmetry between the quantum dots.

[1] D. P. DiVincenzo et al., Nature **408**, 339 (2000).
[2] J. Medford et al., Phys. Rev. Lett. **111**, 050501 (2013).
[3] J. M. Taylor, V. Srinivasa, and J. Medford, Phys. Rev. Lett. **111**, 050502 (2013).

HL 49.7 Wed 12:30 EW 202

Electrically controlled echo sequences for the exchange-only qubit — •Niklas Rohling and Guido Burkard — Department of Physics, University of Konstanz, Germany

We consider a model of an exchange-only qubit [1] in a triple quantum dot under the influence of the surrounding nuclear spin bath, which we describe by an inhomogeneous Overhauser field. This field can lead to decoherence and leakage out of the logical qubit space. When a strong external magnetic field is applied, the spin in each of the quantum dots precess effectively about the same axis. In this case, only one leakage state has to be taken into account [2]. For this situation, we present a purely exchange-based pulse sequence that corrects decoherence as well as leakage as long as the Overhauser field varies slowly compared to the pulse times. As the pulses rely on the exchange interaction, they can be electrically tuned similarly to the quantum gates of the qubit [1]. For the case of a well-known initial state, we further refine the sequence to allow for first-order correction of errors in the applied pulses in analogy to the Carr-Purcell-Meiboom-Gill sequence known from spin resonance techniques.

[1] D. P. DiVincenzo, D. Bacon, J. Kempe, G. Burkard, and K. B. Whaley, Nature **408**, 339 (2000)
[2] J.-T. Hung, J. Fei, M. Friesen, and X. Hu, Phys. Rev. B **90**, 045308 (2014)

HL 49.8 Wed 12:45 EW 202

Influence of Hyperfine Interaction on the Entanglement of Photons Generated by Biexciton Recombination — •Erik Welander, Julia Hildmann, and Guido Burkard — Department of Physics, University of Konstanz, Germany

The quantum state of the emitted light from the cascade recombination of a biexciton in a quantum dot is theoretically investigated including exciton fine structure splitting (FSS) and electron-nuclear spin hyperfine interactions. In an ideal situation, the emitted photons are entangled in polarization making the biexciton recombination process a candidate source of entangled photons necessary for the growing field of quantum communication and computation. The coherence of the exciton states in real quantum dots is affected by a finite FSS and the hyperfine interactions via the effective magnetic field known as the Overhauser field. We investigate the influence of both sources of decoherence and find that the FSS combined with a stochastic exciton lifetime is responsible for the main loss of entanglement. Furthermore, we examine the possibility of reducing the decoherence from the Overhauser field by partially polarizing the nuclear spins and applying an external magnetic field. We find that an increase in entanglement depends on the degree as well as the direction of nuclear spin polarization.

HL 50: Topological insulators: Transport (with MA/O/TT)

Time: Wednesday 11:45–13:00 Location: ER 270

HL 50.1 Wed 11:45 ER 270

Surface Transport on a Bulk Topological Insulator — •Frederik Edler[1], Lisa Kühnemund[1], Marco Bianchi[2], Ellen M.J. Hedegaard[3], Martin Bremholm[3], Bo B. Iversen[3], Philip Hofmann[2], and Christoph Tegenkamp[1] — [1]Inst. f. Festkörperphysik, Uni. Hannover — [2]Dep. of Physics and Astronomy, Uni. Aarhus — [3]CMC, Dep. of Chemistry and iNANO, Uni. Aarhus

Topological insulators are guaranteed to support metallic surface states on an insulating bulk, and one should thus expect that the electronic transport in these materials is dominated by the surfaces states. Alas, due to the high remaining bulk conductivity, surface contributions to transport have mainly only been singled out indirectly via quantum oscillations, or for devices based on gated and doped topological insulator thin films, a situation in which the surface carrier mobility could be limited by defect and interface scattering. This issue was first overcome for Bi_2Te_2Se where compensation of defects leads to low bulk conductivity and surface-dominated transport could directly be observed [1]. Here we present a direct measurement of surface-dominated conduction on atomically clean surfaces of Bi_2Te_3. Using a four tip STM for nano-scale four point transport measurements with variable contact distance we show that the transport at 30 K is again two-dimensional rather than three-dimensional. The sheet conductivity is $7.9(3)\times10^{-4}\Omega^{-1}$ corresponding to a mobility of 505 cm^2/Vs. Besides, results regarding the temperature dependence of the conductivity and the influence of structural defects, e.g steps, present after cleavage will be discussed. [1] Barreto et al., Nano Lett. **14**, 3755 (2014)

HL 50.2 Wed 12:00 ER 270

Aharonov-Bohm oscillations in quantum wire of topological insulator — •Louis Veyrat[1], Joseph Dufouleur[1], Romain Giraud[1], Emmanouil Xypakis[2], Jens Bardarson[2], Christian Nowka[1], Silke Hampel[1], and Bernd Büchner[1] — [1]IFW-Dresden — [2]MPIPKS

Studying Aharonov-Bohm (AB) effect in a nanowire of topological insulator is a convenient way to reveal the specific properties of the topological surface states (SS), which are spin-chiral Dirac fermions. In the short perimeter limit, we evidenced in a previous work the ballistic transport of the SS in the perimeter of the nanowire, revealed by the temperature dependance of the phase coherence length [1] and showing the weak scattering effect of disorder on Dirac fermions. The quantum transverse confinement of SS is further revealed by the observation of non-universal conductance fluctuations. In the longer perimeter limit, we surprisingly find that the transport remains ballistic in the perimeter, despite the presence of disorder. The interaction with disorder is revealed by specific phase-jump of the AB oscillations under transverse magnetic field.

[1] Dufouleur et al., Phys. Rev. Lett. 110, 186806 (2013)

HL 50.3 Wed 12:15 ER 270

The effect of strain on the two-dimensional topological insulator HgTe — •Philipp Leubner, Andreas Budewitz, Christoph Brüne, Hartmut Buhmann, and Laurens Molenkamp — Experimentelle Physik III, Fakultät für Physik, Universität Würzburg, Germany

In the past years, HgTe quantum wells have been used extensively to study the magnetotransport signature of two-dimensional topological insulators, namely the quantum spin Hall effect. It has been shown that the band structure of those systems strongly depends on the thickness of the quantum well, and that, in particular, the topology changes from trivial to nontrivial at a critical thickness of 6.3 nm.

As an additional degree of freedom, the influence of strain on the band structure is investigated in this work. By using different CdTe-ZnTe superlattices grown on GaAs as virtual substrates, we are able to tune the strain of the HgTe quantum well layer from tensile to compressive, and thus modify the shape of the valence band.

Depending on strain, temperature dependent transport measurements on nominally identical wells reveal either features of topological insulators or semimetals, with the obtained fitting parameters nicely agreeing with band structure calculations. Further experiments focus on the correlation between the magnitude of the inverted bandgap and stability of the quantum spin Hall edge states.

HL 50.4 Wed 12:30 ER 270

Transport measurements on Mn-doped HgTe quantum wells — •Andreas Budewitz, Kalle Bendias, Philipp Leubner, Christoph Brüne, Hartmut Buhmann, and Laurens W. Molenkamp — Universität Würzburg, Lehrstuhl für experimentelle Physik III

In 2007 HgTe quantum wells have been experimental identified as a quantum spin Hall system [1]. One open question is how quantum spin Hall states interplay with magnetic impurities. Especially the formation of the anomalous quantum Hall effect raises a lot of interest [2, 3]. Since Mn-doped HgTe is a paramagnetic topological insulator it is important to investigate the onset of the ν = -1 plateau at low fields. Here we present transport measurements on Mn-doped HgTe quantum wells. Therefore we show results on different temperatures, magnetic fields, Mn concentration and quantum well width. We discuss our results in comparison to undoped HgTe quantum wells.

[1] M. König, S. Wiedmann, C. Brüne, A. Roth, H. Buhmann, L. W. Molenkamp, X.-L. Qi and S.-C. Zhang, Science 318, 766 (2007)

[2] Chao-Xing Liu, Xiao-Lang Qi, Xi Dang, Zhong Fang and Shou-Cheng Zhang, PRL 101, 14682 (2008)

[3] Hsiu-Chang Hsu, Xin Liu and Chao-Xing Liu, Phys. Rev. B 88, 085315 (2013)

HL 50.5 Wed 12:45 ER 270

Quantum hall states equilibration in lateral heterojunctions on inverted HgTe quantum wells — •M. Reyes Calvo[1,2], Christoph Brüne[3], Christopher Ames[3], Philipp Leubner[3], Hartmut Buhmann[3], Laurens W. Molenkamp[3], and David Goldhaber-Gordon[1] — [1]Department of Physics, Stanford Universtiy, Stanford, U.S.A. — [2]C.I.C. Nanogune, San Sebastián, Spain — [3]Physikalisches Institut (EP3), Universität Würzburg, Würzburg, Germany

We study lateral heterojunctions on HgTe quantum wells with inverted band structure. At high densities and fields, we can explore the equilibration between Quantum Hall (QH) states with different filling factor. The resulting resistance plateaus are particularly clear in the n-n'-n quadrant and fit the expected values for a 2D electron gas heterojunction. The low density and moderate magnetic field regime is of more interest, since due to the inverted band structure of HgTe, Quantum Spin Hall (QSH) edge states could be present. In this regime, we observe unexpected features in the Hall resistance, which could be associated with the interplay between chiral QH edge modes and helical QSH edge modes.

HL 51: Focus Session: Role of polarization fields in nitride devices II

Continuation of the morning session "Role of polarization fields in nitride devices I"

Organization: André Strittmatter (OvGU Magdeburg) and Michael Jetter (IHFG, U Stuttgart)

Time: Wednesday 15:00–16:45 Location: ER 164

HL 51.1 Wed 15:00 ER 164

Nitrogen vacancies in III-V nitrides as non-radiative recombination centers: a first-principles investigation — •Ying Cui, Christoph Freysoldt, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40627 Düsseldorf

For LED technology, one of the unresolved problems is the nature of the non-radiative recombination processes. Theoretical calculations could be an ideal subsidiary to experiment to identify possible non-radiative recombination centers in LEDs where point defects are usually hard to detect. Here, we show an efficient and reliable strategy to study non-radiative recombination centers in III-V nitrides based on density functional theory with the HSE hybrid functional. Our calculations locate the transition state in the capture process by using defect level occupation as a natural reaction coordinate. We compare the results for nitrogen vacancies in the AlN-GaN-InN series and find that they are always efficient non-radiative recombination centers. Systematic trends along the series and implications for alloys are discussed.

HL 51.2 Wed 15:15 ER 164

Analysis of the anisotropic dielectric function of strained semipolar AlGaN — •Michael Winkler[1], Juliane Klamser[1], Martin Feneberg[1], Rüdiger Goldhahn[1], Joachim Stellmach[2], Martin Frentrup[2], Simon Ploch[2], Frank Mehnke[2], Tim Wernicke[2], and Michael Kneissl[2] — [1]Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg — [2]Institut für Festkörperphysik, Technische Universität Berlin

The linear optical responses of thick semipolar ($11\bar{2}2$) AlGaN films are analyzed quantitatively. The samples were grown by metal-organic vapor phase epitaxy on m-plane sapphire substrates spanning the whole composition range between GaN and AlN.

Due to the anisotropic nature of strain and non-vanishing shear-strain elements, the crystal symmetry is no longer wurtzite but monoclinic. This case is covered by **kp**-theoretical calculations yielding energy distances of transitions from different valence sub-bands and corresponding relative oscillator strengths for electric field vectors in different orientations, i.e. different optical polarization directions. These data are translated to model dielectric functions which are compared and fitted to experimental results obtained by spectroscopic ellipsometry.

The quantitative analysis allows a conversion back to wurtzite material yielding direct experimental evidence of the dependence of the crystal field energy on the aluminum concentration.

Invited Talk HL 51.3 Wed 15:30 ER 164

Impact of reduced polarization fields on the optical properties of semipolar nitride quantum wells — •Mitsuru Funato and Yoichi Kawakami — Department of Electronic Science and Engineering, Kyoto University, Kyoto, Japan

Semipolar InGaN and AlGaN quantum wells (QWs) are promising material systems for efficient light emitters and detectors because of the reduced polarization fields. We have been investigating their crystal growth and optical properties, and have demonstrated that the radiative recombination lifetimes are drastically shortened in both the QWs. The shorted lifetimes have consequences; for example, (1) the carrier diffusion is limited, which leads to spatially uniform emission in the microscope level, (2) the AlGaN emission line width is reduced to below 100 meV, and (3) the emission intensity at room temperature is enhanced. In the presentation, we will describe the recent progress in the understanding of the optical properties of the semipolar QWs, with a particular focus on the effect of reduced electric fields.

HL 51.4 Wed 16:00 ER 164

Nonradiative recombination mechanisms in non- and semipolar GaInN/GaN quantum wells — •Manuela Klisch, Torsten Langer, Holger Jönen, Fedor Alexej Ketzer, Heiko Bremers, Uwe Rossow, and Andreas Hangleiter — Institut für Angewandte Physik, TU Braunschweig

Via temperature-dependent time-resolved photoluminescence spectroscopy, we investigate the nonradiative recombination of excess charge carriers in non- and semipolar quantum well structures of varying indium composition grown via metalorganic vapor phase epitaxy on low defect density GaN. We demonstrate that for InN mole fractions of about 30% within the quantum well, the nonradiative carrier lifetimes in m-plane quantum wells match the corresponding values for polar quantum wells of about 100 ps. The shortening of nonradiative lifetimes with increasing indium content is weak compared to polar quantum wells indicating that the mechanisms of defect generation differ among different growth planes. Possibly, this is related to different influences of slip planes on the plastic relaxation of the compressively strained quantum wells. However, comparable nonradiative lifetimes for ($11\bar{2}2$)-, ($20\bar{2}1$)-, m- and a-plane quantum wells have been observed. Due to the small piezoelectric field component perpendicular to the quantum well plane, which reduces the radiative recombination probability in polar quantum wells, this observation is very promising to outperform the internal quantum efficiency of polar quantum wells towards green emission using non- or semipolar quantum wells.

HL 51.5 Wed 16:15 ER 164

Temperature-dependent Electro- and Photoluminescence on InGaN/GaN MQW LEDs — •Pascal Farin[1], Felix Nippert[1], Anna Nirschl[2], Alexander Wilm[2], Ines Pietzonka[2], Martin Strassburg[2], and Axel Hoffmann[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Germany — [2]OSRAM Opto Semiconductors GmbH, Regensburg, Germany

Current state-of-the-art multi quantum well light-emitting diodes (MQW LEDs) suffer from the droop phenomenon, a reduction in IQE at high operating currents. Several mechanisms including the Auger effect as well as saturation of the active region have been proposed to account for it. These have generally been investigated by means of electroluminescence (EL) and photoluminescence (PL). In order to distinguish between the different non-radiative recombination processes the influence of temperature and external electrical fields on the measurements is frequently utilized.

In this work temperature dependent results of EL and PL on InGaN/GaN MQW-LEDs are presented which allows a general comparison between the two measurements and offers insight into the loss mechanisms in these devices.

HL 51.6 Wed 16:30 ER 164

Investigation of the optical characteristics of semipolar InGaN/GaN quantum wells on pyramidal facets — •Martina Dombrowski, Jan Wagner, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen and Research Center SCoPE, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

The InGaN/GaN material system offers the possibility to reach the green spectral regime for semiconductor light emitters. However the development of such devices in an efficient way is still challenging. Strain introduced due to mismatching lattice constants in heterostructures creates a band tilt in the active region, leading to reduced recombination efficiency. One way to overcome this quantum confined Stark effect (QCSE) is to grow the quantum well on semipolar GaN facets. Since up to now semipolar and nonpolar GaN substrates are not widely available we grow pyramidal GaN structures by selected area growth (SAG). The semipolar facets of the pyramids are used as growth plane for InGaN quantum wells and show a reduced QCSE. To separate the influence of the electrical field and the influence of the three dimensional growth both semipolar and c-plane quantum wells were grown at the same spectral position. The optical and time-resolved photoluminescence measurements were performed and we compare the results for both type of samples.

HL 52: Topological insulators: Structure and electronic structure (with DS/MA/O/TT)

Time: Wednesday 15:00–16:30 Location: ER 270

HL 52.1 Wed 15:00 ER 270

New electron states at the Bi/InAs(111) interface — K Hricovini[1,2], J-M Mariot[3], •L Nicolaï[1,2,7], U Djukic[1], M C Richter[1,2], O Heckmann[1,2], T Balasubramanian[4], M Leandersson[4], J Sadowski[4], J Denlinger[5], I Vobornik[6], J Braun[7], H Ebert[7], and J Minár[7,8] — [1]LPMS, UCP,Cergy, France — [2]DSM-IRAMIS, SPEC, CEA-Saclay, France — [3]LCP-MR, UPMC Univ. Paris 06/CNRS, France — [4]MAX-lab, Lund Univ., Sweden — [5]ALS, Berkeley, USA — [6]EST, Trieste, Italy — [7]LMU Münich, Germany — [8]Univ. of West Bohemia, Plzeň, Czech Republic

The Bi(111) surface is a prototype system to study Rashba-split surface states. Theoretical studies [1] predicted non-trivial topological surface states appearing on a single bi-layer of Bi(111) and a more complex behaviour was suggested for a variable film thickness as a function of layer thickness [2]. This clearly indicates that the electronic properties of thin films of this material are far from being understood. Here we present combined theoretical and ARPES studies of the electronic structure of Bi(111) films grown on InAs(111). Bi growth is epitaxial and a monocrystal of very high quality is obtained after depositing several monolayers. The ARPES experiments on these samples show several new types of electronic states. It is shown that a part of these new states corresponds to novel bulk-like features. These features are well reproduced by the one-step model of photoemission as implemented in the SPR-KKR package [3].[1] M. Wada et al., Phys. Rev. B 83, 121310 (2011). [2] Z. Liu et al., Phys. Rev. Lett. 107, 136805 (2011). [3] H. Ebert, D. Ködderitzsch, J. Minár, Rep. Prog. Phys. 74, 096501 (2011).

HL 52.2 Wed 15:15 ER 270

Ultrafast currents at the surface of the topological insulator Bi_2Se_3 — •Lukas Braun[1], Luca Perfetti[2], Gregor Mussler[3], Markus Münzenberg[4], Martin Wolf[1], and Tobias Kampfrath[1] — [1]Fritz-Haber-Institut Berlin (MPG) — [2]Ecole Polytechnique Palaiseau — [3]Forschungszentrum Jülich — [4]Universität Greifswald

Optical excitation of topological insulators (TIs) can launch electron currents along the TI surface whose direction can be controlled by varying the polarization of the driving light [J. W. McIver *et al.*, Nat. Nanotech. **7**, 96]. So far, photocurrents have been detected with a time resolution from DC to picoseconds [C. W. Luo *et al.*, Adv. Opt. Mat. **1**, 804]. Since electrons moving through a solid typically undergo scattering on a 100fs time scale, it is highly desirable to generate and detect TI photocurrents with femtosecond time resolution in a contact-free manner. For this purpose, we excite n-doped Bi_2Se_3 (Fermi energy at 300meV) crystals with a femtosecond laser pulse (10fs, 1.55eV). The resulting photocurrent gives rise to the emission of a broadband terahertz (THz) electromagnetic pulse (1 to 20THz) whose transient electric field is detected by means of electro-optic sampling. We present a method that allows us to extract the transient current $j(t)$ from the measured field $E(t)$. The AC photocurrents are found to be dominated by shift currents along the surface and photo-Dember injection currents into the bulk. We finally discuss the origin of $j(t)$ and implications for the dynamics of photoexcited TI electrons.

HL 52.3 Wed 15:30 ER 270

Observation of the photon drag effect in epitaxially grown $(Bi_{1-x}Sb_x)_2Te_3$ based topological insulators — •H. Plank[1], L. E. Golub[2], P. Olbrich[1], T. Herrmann[1], S. Bauer[1], V. V. Bel'kov[2], G. Mussler[3], J. Kampmeier[3], D. Grützmacher[3], and S. D. Ganichev[1] — [1]University of Regensburg, Regensburg, Germany — [2]Ioffe Institute, St. Petersburg, Russia — [3]Jülich Aachen Research Alliance (JARA-FIT), Jülich, Germany

We report on the observation of a terahertz (THz) radiation induced photon drag effect in epitaxially grown $(Bi_{1-x}Sb_x)_2Te_3$ three-dimensional topological insulators. We demonstrate that the excitation with polarized radiation results in a dc electric photocurrent. While at normal incidence a current arises due to the photogalvanic effect in the surface states, caused by asymmetrical scattering of Dirac fermions [1], at oblique incidence it is overweighted by the trigonal photon drag effect. The currents are generated in n- and p-type $(Bi_{1-x}Sb_x)_2Te_3$ samples with various composition applying linearly and circularly polarized THz radiation. Results are analysed in terms of phenomenological theory and microscopic model based on transfer of photon momentum to free carriers resulting in an asymmetric distribution of electrons (holes) in k-space. Our analysis describes well all experimental findings including e.g. variation of the angle of incidence, radiation polarization and frequency. The observed trigonal photon drag and photogalvanic effect provide an opto-electronic method to study high frequency transport of Dirac fermions even at room temperature.

[1] P. Olbrich *et al.*, Phys. Rev. Lett. **113**, 096601(2014)

HL 52.4 Wed 15:45 ER 270

Cyclotron Resonance Induced Spin Polarized Photocurrents in Surface States of a 3D Topological Insulator — •K.-M. Dantscher[1], D.A. Kozlov[2], Z.D. Kvon[2], P. Faltermeier[1], M. Lindner[1], P. Olbrich[1], C. Zoth[1], G.V. Budkin[3], S.A. Tarasenko[3], V.V. Bel'kov[3], N.N. Mikhailov[2], S.A. Dvoretskii[2], D. Weiss[1], and S.D. Ganichev[1] — [1]University of Regensburg, Regensburg, Germany — [2]Institute of Semiconductor Physics, Novosibirsk, Russia — [3]Ioffe Institute, St. Petersburg, Russia

We report on the observation of cyclotron resonance (CR) induced photocurrents excited by cw radiation, with frequencies of 2.54, 1.62 and 0.69 THz in a 3D topological insulator based on 80 nm strained HgTe films. To support the complex study, including optical, opto-

electronic and electron transport experiments, various sample designs have been used. The measurements were done in a wide range of temperatures (1.6 to 120 K). We demonstrate that the photocurrent is generated in the topologically protected surface states. Studying the resonance response in the gated samples we examined the behaviour of the photocurrent and Dirac fermions cyclotron mass upon variation of Fermi energy. For large gate voltages we also detected CR in the bulk HgTe with the mass about two times larger than that obtained for the surface states. Based on this data we develop a microscopic theory of the effects and show that the asymmetry of light-matter coupling in the system of Dirac fermions subjected to an external magnetic field causes the electric current to flow. We show that the current is spin polarized.

HL 52.5 Wed 16:00 ER 270

Response of the topological surface state to surface disorder in $TlBiSe_2$ — Florian Pielmeier[1], •Andreas Eich[2], Gabriel Landolt[3,4], Bartosz Slomski[3,4], Julian Berwanger[1], Alexander A. Khajetoorians[5], Jens Wiebe[2], Roland Wiesendanger[2], Jürg Osterwalder[3], Franz J. Giessibl[1], and J. Hugo Dil[3,4,6] — [1]Institute of Experimental and Applied Physics, Universität Regensburg, D-93040 Regensburg, Germany — [2]Department of Physics, University of Hamburg, Jungiusstrasse 11, D-20355 Hamburg, Germany — [3]Physik-Institut, Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland — [4]Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen, Switzerland — [5]Institute of Molecules and Materials, Radboud University, 6500 GL Nijmegen, Netherlands — [6]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

By a combination of experimental techniques we show that the topmost layer of the topological insulator $TlBiSe_2$ as prepared by cleavage is formed by irregularly shaped Tl islands. No trivial surface states are observed in photoemission, which suggests that these islands can not be regarded as a clear surface termination. The topological surface state is, however, clearly resolved in photoemission experiments. This is interpreted as a direct evidence of its topological self-protection and shows the robust nature of the Dirac cone like surface state.

HL 52.6 Wed 16:15 ER 270

Wet etch process for HgTe nanostructure fabrication — •Kalle Bendias[1], Erwann Bocquillon[1], Alex Hughes[2], Christoph Brüne[1], Hartmut Buhmann[1], and Laurens W. Molenkamp[1] — [1]EP3, Physikalisches Institut, Universität Würzburg — [2]Department of Physics, Stanford University

Topological insulators (TI) are a new class of material with outstanding spin properties. Grown in 2d quantum wells HgTe does not only host Quantum Spin Hall edge channels [1][2], but also a giant Rashba splitting [3]. Both could lead to numerous applications in spintronic devices. In order to perform experiments such as spininjection, -probing [3] or quantum point contact collimation [4] a high carrier mobility and i.e. a long ballistic mean free path is essential.

The conventional processing method using ion milling to define the structure strongly affects these surface properties on small microstructures. In this talk the development and results of an alternative lithography etch method using KI:I:HBr as wet etchant are presented. Measurements on microstructures will be shown, indicating comparable mobilities on big and small structures.

[1] Markus König et al., Journal of the Physical Society of Japan 77.3 (2008), S. 031007.

[2] C. Brüne et al., Nature Physics 6.6 (2010), S. 448-454.

[3] J. Hinz et al., Semiconductor science and Technology 21.4 (2006), S 501-506.

[4] L.W. Molenkamp et al., Phys. Rev. B 41, 1274 (1990)

HL 53: Photonic crystals

Time: Wednesday 15:00–16:00 Location: EW 015

HL 53.1 Wed 15:00 EW 015

Transport in three-dimensional aperiodic structures: Experiments and calculations — •Michael Renner[1] und Georg von Freymann[1,2] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schrödinger-Str. 56, 67663 Kaiserslautern — [2]Fraunhofer-Institute for Physical Measurement Techniques (IPM), Erwin-Schrödinger-Str. 56, 67663 Kaiserslautern, Germany

To explore the mechanism of light transport in three-dimensional aperiodic structures we perform finite-difference time-domain (FDTD) simulations closely resembling our experimental geometry [1]. By incoherently adding individual mode profiles after excitation with Cassegrain-type point spread functions and taking into account the given collection optics we are able to reproduce experimental results obtained by an focal plane array (FPA) connected to a Fourier transform infrared spectrometer (FTIR). We confirm the experimentally observed sub-diffusive transport behavior in direct laser written polymer samples with different aperiodic spatial correlations. Structures based on the Rudin-Shapiro sequence show the strongest mode localization, in good agreement with the experiment. Comparisons with two-dimensional representations reveal less pronounced localization highlighting the importance of the aperiodic structuring in three dimensions.

[1] Renner, M. & von Freymann, G. Transverse Mode Localization in Three-Dimensional Deterministic Aperiodic Structures. Adv. Opt. Mater. 2, 226-230 (2014).

HL 53.2 Wed 15:15 EW 015

Fabrication of photonic crystal circuits based on GaN ultrathin membranes by maskless lithography — •Olesea Volciuc[1], Tudor Braniste[2], Veaceslav Sergentu[3], and Jürgen Gutowski[1] — [1]Institute of Solid State Physics, University of Bremen, Bremen 28334, Germany — [2]National Center for Materials Study and Testing, Technical University of Moldova, Chisinau 2004, Moldova — [3]Institute of Applied Physics, Academy of Sciences of Moldova, Chisinau 2028, Moldova

We report on maskless fabrication of photonic crystal (PhC) circuits based on ultrathin (d ~ 15 nm) nanoperforated GaN membranes exhibiting a triangular lattice arrangement of holes with diameters of 150 nm. In recent years, we have proposed and developed a cost-effective technology for GaN micro- and nano-structuring, the so-called surface charge lithography (SCL), which opened wide possibilities for a controlled fabrication of GaN ultrathin membranes. SCL is a maskless approach based on direct writing of negative charges on the surface of a semiconductor by a focused ion beam (FIB). These charges shield the material against photo-electrochemical (PEC) etching. Ultrathin GaN membranes suspended on specially designed GaN microstructures have been fabricated using a technological route based on SCL with two selected doses of ion beam treatment.

HL 53.3 Wed 15:30 EW 015

Fabrication of two dimensional photonic crystal membranes in cubic AlN/GaN — •Sarah Blumenthal[1], Matthias Buerger[1], Donat J. As[1], Andre Hildebrandt[2], and Jens Förstner[2] — [1]University of Paderborn, Faculty of Physics, Department of Optoelectronic Semiconductors — [2]University of Paderborn, Faculty of Physics, Department of Theoretical Electrical Engineering

Group III-Nitrides attracted much attention in the development of optical and quantum optical devices, operating in the UV spectral range. Microresonators enable to control the spontaneous emission of light and to realize an efficient single photon emitter (SPE). Promising candidates for such devices are 2D photonic crystal (PhC) nanocavities. Recently, SPE of hexagonal GaN quantum dots (QD) were already reported. However, h-GaN QDs exhibit strong internal electrical fields causing long radiative lifetimes. This can be overcome by the growth of cubic GaN QDs where no polarisation fields are present. We implemented a process to fabricate freestanding c-AlN/GaN membrane with a 2D hexagonal array of holes. This configuration leads to a large photonic band gap. The free standing membrane ensures an inplane light propagation. This PhC cavity processing is realized by electron beam lithography and different steps of reactive ion etching. Simulations were carried out to optimize the size of the holes, the distance between the holes and the thickness of the membrane. Furthermore, various cavities were fabricated by omitting three holes in a row (L3-cavity) and five holes in a row (L5-cavity).

HL 53.4 Wed 15:45 EW 015

GaAs-based photonic crystal microcavities with metallic contacts — Wadim Quiring[1], •Björn Jonas[1], 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

An elegant method to perform coherent control on a quantum dot two level system is to make use of an optical clock signal together with a synchronous electric HF-signal [1]. The application of this concept requires electrically contacted microcavities. To achieve this, we use MBE-grown membrans, which are designed as n-i-Schottky structures with an InGaAs quantum well as active layer in the intrinsic region. From this we have fabricated GaAs-based photonic crystal cavities with narrow electrodes, which provide an electric connection to the defect. Metalic contacts offer low sheet resistance and enable the transmission of high frequency signals, which are required for coherent optoelectronic manipulation. They also allow for electric tuning via the quantum confined Stark effect and for photocurrent (PC) readout. On those electrically contacted cavities we have performed PC spectroscopy under resonant excitation within a temperature range of 4 K - 310 K. We find strong cavity resonances in the PC spectrum and surprisingly high Q-factors up to 6000. Temperature increase results in an exponential enhancement of the PC and in an external quantum efficiency of 0.26 at room temperature. [1] S. Michaelis de Vasconcellos et. al, Nat. Photon., 4, 548 (2010)

HL 54: Focus Session: Nanophotonic concepts and materials for energy harvesting - Plasmonics, transformation optics, upconversion, and beyond II

Continuation of the morning session 'Nanophotonic concepts and materials for energy harvesting - Plasmonics, transformation optics, upconversion, and beyond I'

Organization: Carsten Rockstuhl (KIT, Karlsruhe), Jan Christoph Goldschmidt (FhG ISE, Freiburg), Ralf Wehrspohn (MLU Halle), Uli Lemmer (KIT, Karlsruhe)

Time: Wednesday 15:00–16:30 Location: EW 201

Invited Talk HL 54.1 Wed 15:00 EW 201

Nanophotonic light harvesting concepts from the visible to the mid-infrared — •Stefan A Maier — Imperial College London, London, UK

Surface polariton modes facilitate the controlled focusing of electromagnetic energy from the far to the near field, overcoming the diffraction limit of optics. This talk will discuss new developments in this field, focusing firstly on surface plasmon polaritons based on metallic nanostructures. Here, transformation optics serves as a useful design tool and also as a powerful formalism to reveal the underlying physics of the light harvesting process. At mid-infrared frequencies, surface phonon polariton modes in polar dielectrics are preferable due to longer phonon lifetimes and hence less absorption-induced damping. Examples of light harvesting with silicon carbide and hexagonal boron nitride nanostructures will be presented in the second part of the talk, including the characterization of hyperbolicity in polar van der Waals crystals.

Invited Talk HL 54.2 Wed 15:30 EW 201

Material Design of Luminescent Glasses and Glass Ceramics for White-LED Applications — •Stefan Schweizer[1,2], Franziska Steudel[2], Sebastian Loos[1], Bernd Ahrens[1,2], Peter Nolte[2], and Florian Wagner[1] — [1]South Westphalia University of Applied Sciences, Lübecker Ring 2, 59494 Soest — [2]Fraunhofer Application Center for Inorganic Phosphors, Branch Lab of Fraunhofer Institute for Mechanics of Materials IWM, Lübecker Ring 2, 59494 Soest

The majority of white light emitting diodes (LED) is based on a blue light emitting diode with a yellow phosphor on top. The phosphor powder, which converts a part of the blue light from the LED into yellow light, is usually embedded in an organic polymer and directly coated onto the LED chip. Heat-induced degradation of the encapsulate, however, results in an efficiency decrease and colour temperature change. Luminescent glasses or glass ceramics might represent an interesting alternative due to their higher thermal and chemical stability. Here, rare-earth single- and double-doped glasses and glass ceramics are investigated for their potential as photon converters. Interestingly, the colour coordinate of the double-doped glass can be varied over a broad spectral range by changing the rare-earth doping ratio accordingly. In addition, double-doping allows for a change in the colour coordinate by using different excitation wavelengths.

HL 54.3 Wed 16:00 EW 201

Enhancing Upconversion with a Bragg Structure — •Clarissa Hofmann, Barbara Herter, Stefan Fischer, and Jan Christoph Goldschmidt — Fraunhofer Institute for Solar Energy Systems, Heidenhofstraße 2, 79110 Freiburg, Germany, Phone: +49 (0) 761 4588-5922 Fax: + 49 (0) 761 4588-9250

Abstract intented for focused session on Nanophotonic Concepts and Materials for Energy Harvesting - Plasmonics, Transformation Optics, Upconversion, and Beyond

Upconversion describes the generation of one higher energy photon out of at least two lower energy photons. This upconversion process can be influenced by the environment of a photonic crystal, by a modulated local density of photon states (LDOS) and an enhanced local irradiance. We present the theoretical analysis of the photonic effects of a Bragg structure on the upconversion process of the embedded upconverter β-NaYF_4:25%Er^{3+}. Considering the modulated LDOS in a rate equation model of the upconversion dynamics, we show that this effect increases the maximum possible upconversion quantum yield (UCQY) from 14% to 16% for an optimised Bragg stack design. Furthermore, due to a high irradiance enhancement, it is possible to find a Bragg stack design for each investigated incident irradiance (100 W/m^2 - 5000 W/m^2) that yields the maximum possible UCQY of 16%. At 200 W/m^2 this corresponds to a UCQY enhancement factor of 6, making the Bragg stack a very effective photonic structure for increasing the UCQY, especially in the low irradiance range.

HL 54.4 Wed 16:15 EW 201

Metamaterial concepts for energy harvesting applications — •Carsten Rockstuhl[1,2], Aimi Abass[2], Stephan Fahr[3] und Samuel Wiesendanger[3] — [1]Institute of Theoretical Solid State Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), 76021 Karlsruhe, Germany — [3]Institute of Condensed Matter Theory and Solid State Optics, Abbe Center of Photonics, Friedrich-Schiller-Universität Jena, 07743 Jena, Germany

Metamaterials provide us unprecedented means to control the propagation of light and to tailor its interaction with matter. The latter aspect is specifically rewarding in the context of energy harvesting applications such as solar cells. There, a referential example that would particularly benefit from a better optical performance is a thin-film solar cell, where the light absorption in a thin layer across an extended spectral domain is poor and enhancing it is a well defined problem. In such situation, metamaterials may provide opportunities for new concepts that can contribute to the solution of this problem. Here, we present our latest results along these lines and show how metamaterial concepts can be used to enhance absorption in solar cells. This concerns the absorption enhancement in solar cells employing Fabry-Perot resonances that are made to be spectrally broad using complementary materials and the use of metamaterial devices perceived in the context of transformation optics for a similar purpose.

HL 55: Quantum dots: Interaction with environment

Time: Wednesday 15:00–16:45 Location: EW 203

HL 55.1 Wed 15:00 EW 203

Influence of crossed excitons on the carrier dynamics in dot-in-well structures — •Mirco Kolarczik, Nina Owschimikow, Yücel Kaptan, Nicolai Grosse, and Ulrike Woggon — Institut für Optik und Atomare Physik, Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany

Quantum dots (QDs) embedded in a quantum well (QW), the so-called DWELL system, are an important class of active media in optoelectronic devices. In addition to strain relaxation, the well provides an efficient way of injecting carriers into the QDs. We investigate the energy level structure formed by the combination of zero-, two- and three-dimensional confinement in an In(Ga)As-based DWELL system embedded in a GaAs matrix by ultrafast two-color pump-probe spectroscopy. We find that "crossed excitons", a Coulomb-correlated electron-hole pair with one carrier localized in the QD, and the complementary carrier in either the QW or the bulk, are formed in these systems [1]. The crossed excitons play an important role in the response of the system to an optical excitation as well as in the lateral coupling between QDs mediated by the well. They create an additional localized density of states around the QDs, that significantly modifies capture and escape processes between QDs and surrounding QW and bulk material.

[1] N. Owschimikow, M. Kolarczik, Y. Kaptan, N. Grosse, and U. Woggon, Appl. Phys. Lett. 105, 101108 (2014)

HL 55.2 Wed 15:15 EW 203

Geometrical Control of the Interatomic Coulombic Decay Process in Quantum Dots — Praphasiri Dolbundalchok[1] and •Annika Bande[1,2] — [1]Theoretische Chemie, Physikalisch-Chemisches Institut, Universität Heidelberg, Im Neuenheimer Feld 229, 69120 Heidelberg, Germany — [2]Institute of Methods for Material Development, Helmholtz-Zentrum Berlin and Joint Lab JuLiq with Department of Physics, FU Berlin, Albert-Einstein-Str. 15, 12489 Berlin, Germany

The elementary physical process of interatomic Coulombic decay (ICD) is recognized as an ultrafast energy transfer process between atoms and molecules induced by long range electron correlation. It was shown to be also possible in arrays of semiconductor quantum dots (QDs). An electron bound to an excited state of one of the QDs decays by transferring its energy to the neighboring QD from which a second electron is emitted.

Different from atomic ICD, ICD in QDs is postulated to find technological application either in infrared photo detectors or solar cells. Most appealing for this technological use is that by geometry variation of the QDs the ICD rate can be controlled.

In this work we present the control of the two-electron ICD process by geometry variation of QDs represented by electron binding potentials in electron dynamics calculations with the highly accurate multiconfiguration time-dependent Hartree (MCTDH) method for antisymmetric electronic wave functions.

HL 55.3 Wed 15:30 EW 203

Effects of inter-nanocrystal distance on luminescence quantum yield in ensembles of Si nanocrystals — •Sebastian Gutsch[1], Daniel Hiller[1], Margit Zacharias[1], Michael Greben[2], and Jan Valenta[2] — [1]Laboratory for Nanotechnology, University of Freiburg, Freiburg, Germany — [2]Laboratory of Optical Spectroscopy, Charles University, Prague, Czech Republic

The absolute photoluminescence (PL) quantum yield (QY) of multilayers of Si nanocrystals (NCs) separated by SiO2 barriers were thoroughly studied as function of the barrier thickness, excitation wavelength, and temperature. By mastering the plasma-enhanced chemical vapor deposition growth we produce a series of samples with the same size-distribution of SiNCs but variable interlayer barrier distance. These samples enable us to clearly demonstrate that the increase of barrier thickness from 1 nm to larger than 2 nm induces doubling of the PL QY value which corresponds to the change of number of close neighbors in the hcp structure. The temperature dependence of PL QY suggests that the PL QY changes are due to a thermally activated transport of excitation into non-radiative centers in dark NCs or in the matrix. We estimate that dark NCs represent about 68 % of the ensemble of NCs. The PL QY excitation spectra show no significant changes upon changing the barrier thickness and no clear carrier multiplication effects. The dominant effect is the gradual decrease of the PL QY with increasing excitation photon energy.

HL 55.4 Wed 15:45 EW 203

Signatures of Förster and Dexter transfer processes in two coupled quantum dots for linear and two-dimensional coherent optical spectroscopy — •Judith Specht, Andreas Knorr, and Marten Richter — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany

An in-depth investigation of the spin-dependent exciton dynamics in coupled nanostructures driven by coherent, ultrafast laser pulses is crucial for future applications e.g. in the field of quantum information processing. Two-dimensional coherent optical spectroscopy techniques serve as a powerful tool to study the microscopic coupling processes and the underlying excitation pathways. We show theoretically that it is possible to distinguish the signatures of the two different Coulomb induced resonance energy transfer mechanisms: Förster and Dexter coupling, using double quantum coherence spectroscopy.

Förster transfer denotes a purely dipole-dipole mediated interaction which can either transfer or flip the spin state of the excited electron, whereas Dexter coupling describes a direct exchange of electrons between the nanostructures. The possible excitation transfer pathways are selected by the polarizations of the exciting laser pulses and the mutual orientations of the two quantum dots.

We show that spectroscopic signatures reveal the type of excitation transfer process and the limitations imposed on the optical selection rules in the non-linear response.

HL 55.5 Wed 16:00 EW 203

Near unity fidelity single hole spin preparation on picosecond timescales — •Tobias Simmet[1], Per-Lennart Ardelt[1], Kai Müller[2], Alexander Kleinkauf[1], Alexander Bechtold[1], Gerhard Abstreiter[1], and Jonathan J. Finley[1] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany — [2]E. L. Ginzton Laboratory, Stanford University, Stanford, California 94305, USA

An isolated heavy-hole spin in optically active self-assembled InGaAs-GaAs quantum dots has emerged as a viable spin qubit, whereby the timescales for spin initialization, manipulation and read-out are crucial parameters. Here, we present a scheme for all optical, near fidelity heavy-hole spin initialization within ∼3ps by tunneling ionization from the optically prepared exciton state. By optimizing the thickness and Al-content of an AlGaAs tunneling barrier immediately adjacent to the quantum dot, we tailor the comparative tunneling escape rates of electron and heavy holes such that hole spins can be initialized with a fidelity >99% - even at zero magnetic fields - where optical spin initialization may be limited by electron-hole exchange interaction for the neutral exciton. Finally, we present how single heavy-hole spin storage and optical read-out via photocurrent can be optimized by time-gating the electric field using a spin storage device.

HL 55.6 Wed 16:15 EW 203

Excitation of complex spin dynamics patterns in a quantum-dot electron spin ensemble — •Henning Moldenhauer[1], Steffen Varwig[1], Irina A. Yugova[2], Alexandre René[1], Tomasz Kazimierczuk[1], Alex Greilich[1], Dmitri R. Yakovlev[1,3], Dirk Reuter[4], Andreas D. Wieck[4], and Manfred Bayer[1,3] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Spin Optics Laboratory, Saint-Petersburg State University, 198504 St. Petersburg, Russia — [3]Ioffe Physical-Technical Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia — [4]Angewandte Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany

We investigate on special periodic pulsed laser excitation protocols in (In,Ga)As/GaAs quantum dot spin ensembles to access more complex nontrivial dynamic patterns. Using a pump-probe setup we apply an additional rectification pulse to generate higher harmonics in the observed spin precession reflecting the orientation patterns of mode-locked spins in a dephased spin ensemble.

HL 55.7 Wed 16:30 EW 203

Formation of bound continuum excitons due to excitonic effects in intraband quantum dot spectroscopy. — •Sandra Kuhn and Marten Richter — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany

Coulomb induced effects on intraband transitions between bound quantum dot and unbound continuum states of the host material can play a role in a variety of experiments, due to their relevance to the dephasing properties of the quantum dot states as well as for bound to continuum intraband spectroscopy.

We present a theory based on the density matrix formalism to calculate bound to continuum intraband absorption spectra including Coulomb interaction. We study several bound to continuum quasi particles such as trions, biexciton or exciton, resulting in characteristic spectral signatures. In particular, our results show signatures of a bound exciton consisting of a localized carrier inside the quantum dot and a delocalized carrier of the continuum. To get information about the localization of this exciton we discuss the bound to continuum exciton wave function, which shows that the exciton is spatially delocalized in the vicinity of the quantum dot. Especially for the energetically higher states, the spatial extension of the exciton is much larger than the quantum dot extension of 10 nm, often up to 100 nm. This large wave function extension opens a way to study a new possibility of electronic coupling between different quantum dots.

HL 56: Frontiers of electronic structure theory: Optical excitations

Time: Wednesday 15:00–18:30 Location: MA 004

Invited Talk HL 56.1 Wed 15:00 MA 004

Ultrafast coherent dynamics in photovoltaics — •Carlo Andrea Rozzi[1], Sarah Maria Falke[2], Daniele Brida[3,4], Margherita Maiuri[4], Michele Amato[5], Ephraim Sommer[2], Antonietta De Sio[2], Angel Rubio[6,7], Giulio Cerullo[4], Elisa Molinari[1,8], and Christoph Lienau[2] — [1]CNR-NANO, Modena, Italy — [2]Carl von Ossietzky Universität, Oldenburg, Germany — [3]University of Konstanz, Germany — [4]CNR-IFN, Politecnico di Milano, Italy — [5]Universitè Paris-Sud, Orsay, France — [6]Universidad del País Vasco San Sebastián, Spain — [7]Fritz-Haber-Institut, Berlin, Germany — [8]Università di Modena e Reggio Emilia, Modena, Italy

The photoinduced charge-separation events occurring in photovoltaic systems have traditionally been interpreted in terms of the incoherent kinetics of optical excitations and of charge hopping, but recently signatures of quantum coherence were observed in energy transfer in photosynthetic bacteria and algae. We have studied charge separation in reference systems for artificial photosynthesis and photovoltaics by combining TDDFT simulations of the quantum dynamics and high time resolution femtosecond spectroscopy. We provide evidence that the coherent coupling between electronic and nuclear degrees of freedom is of key importance in triggering charge delocalization and transfer both in covalently bonded molecules and in bulk heterojunctions[1]. We have exploited the results of our research to design, syntesize and characterize a novel molecular scaffold for photovoltaic applications.[2] [1] Falke S., et al., Science, 344, 1001 (2014) [2] Pittalis S., et al., Adv. Func. Mat. (2014)

HL 56.2 Wed 15:30 MA 004

Real-time propagation of coupled Maxwell-Kohn-Sham systems — •Rene Jestädt[1], Heiko Appel[1,3], and Angel Rubio[1,2,3] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain — [3]Max-Planck-Institut für Struktur und Materie, Hamburg

Based on a recent extension of time-dependent density-functional theory to quantum electrodynamics [1], we show first steps of an implementation of Maxwell's equations coupled to time-dependent Kohn-Sham equations. Our implementation utilizes the Riemann-Silberstein vector of the electromagnetic field which allows to write Maxwell's equations in a symplectic spinor representation similar to the Dirac equation. This spinor representation allows us to use standard unitary propagation techniques [2] developed for the Schrödinger equation also for the coupled solution of Maxwell's equations and Kohn-Sham equations. We illustrate our implementation of such coupled Maxwell-Kohn-Sham systems in the real-space real-time code octopus [3] for small molecules coupled to optical cavities [4].

[1] M. Ruggenthaler et al., Phys. Rev. A **90**, 012508 (2014).
[2] A. Castro et al., J. Chem. Phys. **121** (2004).
[3] X. Andrade et al., J. Phys. Cond. Mat. **24** (2012).
[4] M.S. Tame et al., Nature Physics 9, 329-340 (2013).

HL 56.3 Wed 15:45 MA 004

Correlated Light-Matter Interactions in Cavity QED — •Johannes Flick[1], Camilla Pellegrini[2], Michael Ruggenthaler[3], Heiko Appel[1,4], Ilya V. Tokatly[1,5], and Angel Rubio[1,2,4] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Nano-bio Spectroscopy Group/ETSF Scientific Development Centre, Universidad del Pais Vasco UPV/EHU, San Sebastian — [3]Universität Innsbruck — [4]MPI for the Structure and Dynamics of Matter, Hamburg — [5]IKERBASQUE, Basque Foundation for Science, Bilbao

In the last decade, time-dependent density functional theory (TDDFT) has been successfully applied to a large variety of problems, such as calculations of absorption spectra, excitation energies, or dynamics in strong laser fields. Recently, we have generalized TDDFT to also describe electron-photon systems (QED-TDDFT) [1, 2]. Here, matter and light are treated on an equal quantized footing.
In this work, we present the first numerical calculations in the framework of QED-TDDFT. We show exact solutions for fully quantized prototype systems consisting of atoms or molecules placed in optical high-Q cavities and coupled to quantized electromagnetic modes. We focus on the electron-photon xc-contribution by calculating exact Kohn-Sham potentials using fixed-point inversions and present the performance of the first approximated xc-potential based on an optimized effective potential (OEP) approach.

[1] I. Tokatly, Phys. Rev. Lett. **110**, 233001 (2013).
[2] M. Ruggenthaler et.al., Phys. Rev. A **90**, 012508 (2014).

HL 56.4 Wed 16:00 MA 004

A hybrid QM/EMT approach to charge state corrections — •Osman Baris Malcioglu[1] and Michel Bockstedte[2] — [1]Lst.f.Theor.Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — [2]FB Materialwissenschaften & Physik Universität Salzburg, 5020 Salzburg, Austria

Localized charge at surfaces, interfaces, or in volume materials naturally occur due to the ionization of adsorbates or defects. A robust quantitative description of charged systems is a prerequisite to explore the physics of adsorbates, surface and bulk defects of materials such as metal oxides. The popular supercell approach requires charge neutrality per supercell. For charged systems this is enforced by compensation charges. The resulting spurious interaction can be corrected a-posteriori [1,2]. Recently, a scheme based on model fitting the localized charge and dielectric screening was proposed [1]. Here, we present a fully automated and efficient hybrid QM/EMT approach for handling long-reach fields. The response of the medium and the localized charge density of the ab-initio calculations are represented by a finite element function space. The relevant physical observables are obtained using an auto-adaptive mesh solver. We demonstrate applications of our approach to charge state corrections of surface and bulk defects slabs in comparison with the earlier approaches [1,2].

[1] H.-P. Komsa and A. Pasquarello, Phys. Rev. Lett. **110**, 095505 (2013).
[2] C. Freysoldt, J. Neugebauer, and C. G. Van de Walle, Phys. Rev. Lett. **102**, 016402 (2009).

HL 56.5 Wed 16:15 MA 004

Plasmon assisted double photoemission — •Michael Schüler, Yaroslav Pavlyukh, and Jamal Berakdar — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany

Coincidence measurements of double photoemission (DPE) represent a direct way of tracing the various facets of electronic correlations in molecular as well as extended systems, such as e. g. dynamical screening and collective excitations. One prominent example in this respect is the C_{60} molecule, for its plasmon resonances dominate the electronic

excitation spectrum. Motivated by recent experiments on this molecule we demonstrate how the phenomenon of plasmon-mediated DPE can be described by an effective four-level system coupled to the bosonic plasmon excitations. The model generalizes the classical *s*-model and is treated within the *GW* approximation with the parameter estimates from *ab initio* calculations. We solve the coupled fermionic-bosonic time-dependent Kadanoff-Baym equations governing the dynamics of the model triggered by the interaction with the laser field. The use of the generalized Kadanoff-Baym Ansatz allows to significantly reduce the computation cost of our method.

HL 56.6 Wed 16:30 MA 004

Calculating photoemission spectra with real-time density-functional theory — •Matthias Dauth and Stephan Kümmel — University of Bayreuth, Germany

Photoemission spectroscopy is one of the primary tools for characterizing molecules and solids. A traditional approach of predicting photoemission signals relies on the interpretation of single-particle eigenvalues, e.g., from Hartree-Fock or Density Functional Theory (DFT). Here we demonstrate that real-time DFT allows for going beyond this static picture. We calculate photoemission signals dynamically and estimate ionization cross sections. We first investigate gas phase spectra, in which an ensemble of molecules with random orientation is probed. However, our approach in particular also allows for calculating angular resolved signals, i.e., we can track the ejected electron distribution with respect to a fixed light polarization. Furthermore, no a priori assumptions about the final state of the outgoing electrons need to be made, but the final state emerges naturally from the calculation. Thus, real-time DFT emerges as a powerful tool for the dynamical first-principles prediction of photoemission processes.

HL 56.7 Wed 16:45 MA 004

***Ab initio* local field effects for surface second harmonic generation** — •Nicolas Tancogne-Dejean[1,2] and Valérie Véniard[1,2] — [1]Laboratoire des Solides Irradiés, Ecole Polytechnique, CNRS-CEA/DSM, F. 91128, Palaiseau, France — [2]European Theoritical Spectroscopy Facility (ETSF), France

A comprehensive understanding of the nonlinear optical properties of solids is crucial to improve the design and the analysis of new optical devices. Among these processes, Second-Harmonic Generation (SHG) is probably one of the most studied and has become, through the years a very powerful-non-invasive technique to characterize materials, because of its particular sensitivity to the symmetry of a system. In materials where inversion symmetry is present, optical Second Harmonic Generation is forbidden within the dipole approximation. But at a surface or an interface between two such materials, the inversion symmetry is broken and SHG is allowed.

Crystal local fields are generated by the induced microscopic response of the system to an external perturbation. As a consequence their effects will be particularly important close to discontinuities as interfaces or surfaces. Local fields are important for a good description of optical properties of materials, but their effects on surface SHG have never been studied.

We present here a new ab initio formalism that allows us to calculate the frequency-dependent surface second-order susceptibility $\chi^{(2)S}$ within TDDFT, where the local field effects are fully included and we have applied this formalism to Silicon surfaces.

HL 56.8 Wed 17:00 MA 004

Mapping atomic orbitals in the transmission electron microscope: seeing defects in graphene — •Lorenzo Pardini[1], Stefan Löffler[2,3], Giulio Biddau[1], Ralf Hambach[4], Ute Kaiser[4], Claudia Draxl[1,5], and Peter Schattschneider[2,3] — [1]Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany — [2]Institute of Solid State Physics, Vienna University of Technology, Austria — [3]University Service Centre for Transmission Electron Microscopy, Vienna University of Technology, Austria — [4]Central Facility for Electron Microscopy, University of Ulm, Germany — [5]European Theoretical Spectroscopy Facility (ETSF)

The possibility of mapping atomic orbitals by using energy-filtered transmission electron microscopy (EFTEM) has been considered for a long time and was recently demonstrated from a theoretical point of view. With the example of graphene, we predict how this approach can be used to map orbitals of a particular character. To this purpose, we have investigated graphene in its pristine structure and with two different kinds of defects, namely an isolated vacancy and a substitutional nitrogen atom. We show that basically three different kinds of images are to be expected, depending on the orbital character as determined from the corresponding projected density of states. To judge the feasibility of mapping such orbitals in a real microscope, we investigate the effect of the optics' aberrations, by simulating the lens system of two microscopes that are commonly used for electron energy loss spectrometry. We find that it should indeed be feasible to see atomic orbitals in a state-of-the-art EFTEM.

HL 56.9 Wed 17:15 MA 004

Inelastic X-Ray Scattering: Insights from and Benefits for Many-Body Theory — •Claudia Rödl, Igor Reshetnyak, Francesco Sottile, and Lucia Reining — Laboratoire des Solides Irradiés, Ecole Polytechnique, CNRS, CEA-DSM, 91128 Palaiseau cedex, France

Non-resonant inelastic x-ray scattering (IXS) probes the momentum- and frequency-dependent dynamic structure factor $S(\mathbf{q},\omega)$. It captures the neutral excitations of a many-body system, such as excitons, plasmons, and interband transitions. In particular, localized excitations that are forbidden in the optical limit of vanishing momentum transfer are accessible. $S(\mathbf{q},\omega)$ is proportional to the diagonal element of the electric susceptibility $\chi(\mathbf{q},\mathbf{q}',\omega)$. Thus, IXS directly probes the dielectric screening and, hence, the screened Coulomb interaction which governs, for instance, the formation of quasiparticles in photoemission spectroscopy and excitons in optical spectroscopy. Therefore, IXS provides a unique tool to disentangle the many-body physics of renormalized quasiparticles and neutral excitations. It may serve as a solid experimental reference for the development of new approaches in many-body theory. Moreover, the off-diagonal elements of $\chi(\mathbf{q},\mathbf{q}',\omega)$ can be probed by coherent inelastic x-ray scattering (CIXS). This technique, which is still at a pioneering stage, allows one to visualize plasmon-like and localized neutral excitations in real space. We calculate diagonal and off-diagonal elements of $\chi(\mathbf{q},\mathbf{q}',\omega)$ for semiconductors and transition-metal oxides in good agreement with experiment and discuss the rich physics that is contained in $\chi(\mathbf{q},\mathbf{q}',\omega)$.

HL 56.10 Wed 17:30 MA 004

Real-Space Multiple-Scattering X-ray Absorption Spectroscopy Calculations of *d*- and *f*-state Materials using a Hubbard Model — •Christian Vorwerk[1], Kevin Jorissen[1], John Rehr[1], and Towfiq Ahmed[2] — [1]Department of Physics, University of Washington, Seattle, Washington 98195 USA — [2]Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545 USA

We present calculations of the electronic structure and x-ray spectra of materials with correlated *d*- and *f*-electron states treated with the Hubbard model in a real-space multiple scattering (RSMS) formalism, and using a rotationally invariant local density approximation (LDA+U). Values of the Hubbard parameter U are calculated ab initio using the constrained random-phase approximation (cRPA). The real-space Green's function approach with Hubbard model corrections is an efficient way to describe localized electron states in strongly correlated systems, and their effect on core-level x-ray spectra. The method is shown to give the correct density of states and x-ray absorption spectra for Transition Metal- and Lanthanide-oxides such as Ce2O3 and NiO, where the traditional RSMS calculations fail.

Supported by DOE BES DE-FG02-97ER45623

HL 56.11 Wed 17:45 MA 004

Variants of Second Order Screened Exchange for spin polarized and non-polarized Uniform Electron Gas — •Felix Hummel and Georg Kresse — University of Vienna, Austria

The commonly used Random Phase Approximation (RPA) only contains exchange processes of first order. The Second Order Screened Exchange (SOSEX) correction includes one exchange process beyond first order, which is considered the leading order correction to the RPA, and it has proven to be very accurate for the Uniform Electron Gas (UEG) as well as for solids.

The memory requirement of SOSEX is however of $O(N^4)$. We present an approach with a memory requirement of $O(N^2)$ and its differences to other approaches with comparable complexity, such as AC-SOSEX, for the spin polarized and non-polarized UEG.

HL 56.12 Wed 18:00 MA 004

Ferromagnetism from strongly correlated electrons at the $LaAlO_3/SrTiO_3$ interface — •Frank Lechermann, Lewin Boehnke, Malte Behrmann, Daniel Grieger, and Christoph Piefke — I. Institut für Theoretische Physik, Universität Hamburg

We shed light on the interplay between structure and many-body effects relevant for itinerant ferromagnetism in $LaAlO_3/SrTiO_3$ heterostructures. The realistic correlated electronic structure is studied by means of the (spin-polarized) charge self-consistent combination of density functional theory (DFT) with dynamical mean-field theory (DMFT) beyond the realm of static correlation effects [1]. A ferromagnetic instability occurs only with oxygen vacancies and it is possible to account for the basic mechanism by an derived minimal Ti two-orbital e_g-t_{2g} description for the correlated subspace. Magnetic order affected by quantum fluctuations with a Ti moment of $0.2\mu_B$ builds up from effective double exchange, which can be traced to the dilute defect regime. [1] F. Lechermann, L. Boehnke, D. Grieger and C. Piefke, Phys. Rev. B 90, 085125 (2014)

HL 56.13 Wed 18:15 MA 004

NanoDMFT: Full ab initio description of strong correlations in nanoscale devices — •David Jacob — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle

In order to obtain a full first-principles description of the correlated electronic structure and transport properties of nanoscale devices we combine the Coulomb-Hole-Screened-Exchange (COHSEX) approximation with Dynamical Mean-Field Theory (DMFT). While the former yields an effective mean-field description of the weakly correlated conduction electrons, the DMFT part accounts for the dynamic correlations originating e.g. from the strongly interacting $3d$- or $4f$-shells of transition metal atoms or from the molecular orbitals of weakly coupled molecular devices. The combination with COHSEX instead of Density Functional Theory (DFT) improves upon our NanoDMFT approach [1] in two important aspects: First, from the screened interaction W we can calculate the effective Coulomb interaction U for the strongly interacting electrons. Second, unlike in DFT+DMFT calculations the double-counting correction for COHSEX+DMFT is exactly known and straight-forward to calculate. Hence the two quantities which are essentially parameters in the DFT based approach can now be calculated ab initio so that it is now possible to actually predict e.g. the occurance of the Kondo effect in magnetic atoms and molecules on metal surfaces and attached to metallic leads.

[1] D. Jacob *et al.*, PRL **103**, 016803 (2009); D. Jacob *et al.*, PRB **82**, 195115 (2010); M. Karolak *et al.*, PRL **107**, 146604 (2011); D. Jacob *et al.*, PRB **88**, 134417 (2013)

HL 57: Optical properties of bulk semiconductors

Time: Wednesday 16:15–18:00 Location: EW 015

HL 57.1 Wed 16:15 EW 015

Quantum defect of the Rydberg series for cuprous oxide — •Florian Schöne, Heinrich Stolz, and Stefan Scheel — Universität Rostock MNF/IfPH, 18055 Rostock, Germany

The bound-state energies of semiconductor excitons are commonly described by the hydrogenic Rydberg formula $E_n = -\mathrm{Ry}/n^2$. However, recent experiments in cuprous oxide[1] have shown that the energy levels for highly excited p-excitons of the yellow series deviate significantly from the established Rydberg formula. Amongst the possible origins of this deviation, such as frequency-dependent background permittivity and coupling to LO-phonons, the largest contributing factor is the nonparabolic shape of the Γ^{7+} valence band. Based on the Suzuki-Hensel-Hamiltonian[2] which covers spin-orbit and magnetic interactions on symmetry grounds, we are able to analytically describe the nonparabolicity of the valence bands. Applying the concept of quantum defects known from atomic physics, the deviations of the resulting bound-state energies from the hydrogenic Rydberg series can be effectively incorporated in a single parameter $\delta_{n,l}$ according to $E_{n,l} = -\mathrm{Ry}/(n-\delta_{n,l})^2$. We will show the results for the calculation of the first Rydberg-Ritz parameters for the lowest angular-momentum exciton states of the yellow series of Cu_2O.

[1] Kazimierczuk, T. *et al.*, Nature **514**, 343-347 (2014)
[2] Suzuki K., Hensel J. C., Phys. Rev. B **9**,4184 (1974)

HL 57.2 Wed 16:30 EW 015

Pulsed magnetic field spectroscopy up to 70 T on the dilute nitride GaAsN — •Faina Esser[1,2], Harald Schneider[1], Stephan Winnerl[1], Oleksiy Drachenko[3], Amalia Patanè[4], Mark Hopkinson[5], and Manfred Helm[1,2] — [1]Institute of Ion Beam Physics and Material Research, Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Technische Universität Dresden, Germany — [3]The Laboratoire National des Champs Magnétiques Intenses of Toulouse, France — [4]The University of Nottingham, United Kingdom — [5]The University of Sheffield, United Kingdom

Magnetic fields above 45 T offer great opportunities as a tool for materials research but can only be realized in the pulsed regime. We use pulsed magnetic fields up to 70 T for spectroscopic investigations of the dilute nitride GaAsN. This material is a promising candidate for optical applications because of the possibility for tuning its band gap by the nitrogen content. Our studies focus on the exploration of the band structure and in particular on the determination of the effective mass. Cyclotron-resonance spectroscopy indicates that the effective mass is not strongly affected by nitrogen in comparison to previous publications. Our magneto-photoluminescence investigations reveal the formation of localized and delocalized states as a result of the nitrogen incorporation. Delocalized states undergo transitions to localized ones in very high magnetic fields. This result is in good agreement with a pressure dependent study [1].

[1] J. Endicott, A. Patanè, D. Maude, L. Eaves, M. Hopkinson, and G. Hill, Phys. Rev. B 72, 041306(R) (2005)

HL 57.3 Wed 16:45 EW 015

Giant Magnetic-Field-Induced Third-Harmonic Generation in Semiconductor GaAs — David Brunne[1], •Walter Warkentin[1], Victor Pavlov[2], Roman Pisarev[2], Anna Rodina[2], and Dmitri Yakovlev[2] — [1]Experimentelle Physik 2, Technische Universität Dortmund, Dortmund, Germany — [2]Ioffe Physical-Technical Institute, Russian Academy of Sciences, St. Petersburg, Russia

GaAs has the noncentrosymmetric crystallographic structure of zinc blend type (P.G. $\bar{4}3m$) in which nonlinear optical process of third-harmonic generation (THG) is allowed in the electric dipole approximation. However, an external magnetic field on the order of 10 T gives rise to an enormous enhancement of the THG intensity by a factor of hundred. We observed a resonance in the THG spectra of GaAs in the vicinity of the 1s-excitonic state, which is related to the four-photon THG processes. The observed resonance is attributed to the intricate modification of polariton-excitonic structure in magnetic field mixing dark and bright 1s-excitonic states. Magnetic-field, rotational anisotropy and temperature studies allowed us to unambiguously confirm the magnetic-field-induced THG mechanism in GaAs. It is important that suggested mechanism of the THG enhancement can be valid for other semiconductors as well.

HL 57.4 Wed 17:00 EW 015

Determination of absolute Raman scattering cross sections in wz-GaN — •Christian Röder, Gert Irmer, Cameliu Himcinschi, and Jens Kortus — TU Bergakademie Freiberg, Institute of Theoretical Physics, Leipziger Str. 23, D-09599 Freiberg, Germany

Reports on relative or absolute Raman scattering cross sections of phonons in wurtzite-type GaN are scarce in literature. Loa *et al.* [1] report on measurements of absolute and relative Raman scattering efficiencies of phonons which are accessible in backscattering geometry. In this work relative Raman scattering efficiencies of all Raman active phonon modes in wz-GaN were obtained using various scattering geometries [2]. Taking the dependence of the scattering cross sections on the phonon frequencies into acount the complete Raman tensors of wz-GaN were ascertained. For the determination of the absolute scattering cross sections comparative measurements with standard substances such as cyclohexane (C_6H_{12}) and carbon tetrachloride (CCl_4) were performed.

The authors would like to thank the European Union (EFRE) as well as the Free State of Saxony for financial support within the ADDE project.

[1] Loa, I. *et al.*: J. Raman Spectrosc. **29**, 291 (1998)
[2] Irmer, G. *et al.*: J. Appl. Phys. accepted

HL 57.5 Wed 17:15 EW 015

First-Principles calculations of the single-particle properties

for novel Bismide and Nitride containing III-V semiconductors — •Phil Rosenow[1], Phillip Springer[1], Stephan W. Koch[2], and Ralf Tonner[3] — [1]Research Training Group GRK 1782, Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Department of Physics, Philipps-Universität Marburg, 35032 Marburg, Germany — [3]Department of Chemistry, Philipps-Universität Marburg, 35032 Marburg, Germany

Novel, Bi and/or N containing GaAs based semiconductor systems have great potential for optoelectronic applications ranging from lasers, LEDs, solar cells, all the way to detectors.(1) For the systematic microscopic modelling of such devices, it is a prerequisite to have reliable information on the electronic bandstructure and the single-particle wavefunctions of the respective materials. Here, we use DFT with the MBJLDA functional. Using the resulting bandstructure, we used a least-squares fitting procedure to extract $\mathbf{k}\cdot\mathbf{p}$ parameters.(2) Since the extracted $\mathbf{k}\cdot\mathbf{p}$ parameters incorporate the effects of other bands, they are effective parameters allowing to treat systems that have not been experimentally characterized in any way since all parameters can be obtained computationally. Effects of disorder in mixed systems can be treated as well by averaging over various congigurations.
(1) N. Koukourakis *et al.*, *Appl. Phys. Lett.* **2012**, 100, 092107-092103. (2) R. Oszwaldowski, M. Reichelt, T. Meier, S. W. Koch, M. Rohlfing, *Phys. Rev. B* **2005**, 71.

HL 57.6 Wed 17:30 EW 015

Microscopic Calculations of the Optical Properties of Novel Bismide and Nitride Containing III-V Semiconductors — •Phillip Springer[1], Phil Rosenow[1], Ralf Tonner[2], Jörg Hader[3], Jerome Moloney[3], Tineke Stroucken[4], and Stephan W. Koch[4] — [1]Research Training Group GRK 1782, Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Department of Chemistry, Philipps-Universität Marburg, 35032 Marburg, Germany — [3]NLCSTR Inc., Tucson, Arizona 85705, USA — [4]Department of Physics, Philipps-Universität Marburg, 35032 Marburg, Germany

Using first-principles calculations to determine the single-particle properties of novel dilute Bismide or Nitride systems, we compute the absorption, gain and luminescence properties of such systems. We extract effective $\mathbf{k}\cdot\mathbf{p}$ parameters from DFT calculations which are then utilized to obtain the band structure as well as the optical and Coulomb matrix elements between the relevant valence and conduction bands using a Luttinger anti-crossing model. On this basis, we calculate the optical properties within the framework of the semiconductor Bloch and luminescence equations.

HL 57.7 Wed 17:45 EW 015

Erbium-doped slot waveguides containing Silicon nanocrystals — Romy Hoffmann[1], •Jan Beyer[1], Volker Klemm[2], David Rafaja[2], Brett Johnson[3], Jeffrey C. McCallum[3], and Johannes Heitmann[1] — [1]Institute of Applied Physics, TU Bergakademie Freiberg, D-09596 Freiberg, Germany — [2]TU Bergakademie Freiberg, Institute of Materials Science, D-09596 Freiberg, Germany — [3]Centre for Quantum Computation and Communication Technology, School of Physics, University of Melbourne, Melbourne, Victoria 3010, Australia

Silicon-based waveguides are intensely investigated with regard to their potential applications in e.g. inter-chip optical data transmission and data manipulation, e.g. as waveguide amplifiers, but also as possible laser sources. A particularly promising device architecture is provided by the slot waveguide geometry, in which a thin SiO_2 slot is inserted into the silicon waveguide. Due to the refractive index contrast, the electric field amplitude polarized normal to the slot plane is enhanced inside the slot, which improves both absorption and emission efficiency of embedded luminescent structures. We incorporate both Erbium ions and size-controlled Silicon nanocrystals, used as Erbium sensitizers, into such a slot. Most efficient pumping of the 1.54 μm Erbium emission is found for small Si nanocrystals, in the range of 3 nm, and elevated post-Er-implantation annealing temperatures of 1000 °C. The sample structure is also demonstrated to induce a dependence on the polarization direction of the exciting laser light, where polarization normal to the slot layer enhances Erbium emission intensity.

HL 58: OFETs, OLEDs, and organic optoelectronics

Time: Wednesday 16:30–18:45 Location: EW 202

HL 58.1 Wed 16:30 EW 202

Light-matter interaction in protein microcavities — •Christof P. Dietrich, Anja Steude, Marcel Schubert, Sven Höfling, and Malte C. Gather — SUPA, School of Physics and Astronomy, University of St Andrews, KY16 9SS St Andrews, United Kingdom

There is an increasing interest in using biologically produced structures and materials for photonic applications. Recent research impressively illustrates the broad potential of biological materials for providing optical gain[1]. In particular, fluorescent proteins like eGFP retain a special position within the quickly growing family of biologically produced laser materials. eGFP has a barrel-like molecular structure that prevents concentration induced quenching of the fluorescence by suppressing Förster and Dexter energy transfer[2]. This allows the use of pure solid-state fluorescent protein as efficient optical gain material. We demonstrate highly efficient lasing from multiple photonic states in microcavities filled with self-assembled rings of recombinant eGFP in its solid state form. The lasing regime is achieved at very low excitation energies of 13nJ and occurs from cavity modes dispersed in both energy and momentum. The distribution of lasing states in energy is induced by the large spectral width of the gain spectrum of recombinant eGFP (FWHM = 25nm). Our results imply that there is considerable self-absorption in eGFP and that strong exciton-photon coupling may be observed in fluorescent proteins if suitably designed resonators are used.
[1] M.C. Gather and S.H. Yun, Nat. Photon. 5, 406 (2011).
[2] M.C. Gather and S.H. Yun, Nat. Comm. (in press).

HL 58.2 Wed 16:45 EW 202

Modulating 2D material optoelectronics through photochromic self-assembled monolayers — •Juan Li[1], Carlos-Andres Palma[1], Jakob Wierzbowski[1,2], Julian Klein[1,2], Filippo Nisic[3], Mahmoud M. Asmar[4], Sergio E. Ulloa[4], Claudia Dragonetti[3], Jonathan J. Finley[1,2], Emanuela Margapoti[1,2], and Johannes V. Barth Barth[1] — [1]Physik-Department,Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany — [2]Walter Schottky Institut,Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany — [3]Dipartimento di Chimica, Università degli Studi di Milano and UdR dell*INSTM di Milano, Via Golgi 19, I-20133 Milano, Italy — [4]Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany

The recent spotlight on highly crystalline natural-occurring and synthetic two-dimensional materials (2DMs) stands as a unique opportunity to accelerate atomically-precise technology made of complex 2DM and molecular architectures. Here we explore the modulation of the optoelectronic properties of graphene and molybdenum disulfide (MoS2) by means of azobenzene self-assembled monolayers platforms. We present (a) the emergence of photoswitchable bound states in graphene (b) photoswitchable rectification and (c) tuning of the photoluminescence yield on MoS2. Our results pave the way toward hybrid molecular/2DM (opto)electronic technology.

HL 58.3 Wed 17:00 EW 202

Time-resolved measurement of intramolecular photoinduced electron transfer processes in perylene diimides — •Robin Carl Döring[1], Eduard Baal[2], Jörg Sundermeyer[2], and Sangam Chatterjee[1] — [1]Faculty of Physics and Materials Science Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]Faculty of Chemistry and Materials Science Center, Philipps-Universität Marburg, Hans-Meerwein-Str., D-35043 Marburg, Germany

Perylene diimides (PDI) are commonly used as dyes but are also viable candidates for devices such as organic field-effect transistors and organic photovoltaics. We study a series of PDI samples by time-resolved photoluminescence and transient absorption measurements to identify the relaxation mechanisms following fs-optical excitation. Here, photoinduced electron transfer (PET) can occur. Following a high-energy excitation, an electron from the lone pair of the diimide is transferred

to the HOMO of the perylene core, hence disallowing radiative recombination. By introducing alkyle groups as spacer units the distance between electron donor and the fluorophore is increased. Therefore, the distant distance dependent PET is altered, leading to a reduced PET efficiency and hence changed decay rates.

HL 58.4 Wed 17:15 EW 202

Pressure Dependent Electronic Properties of Organic Semiconductors from First Principles — •Franz Knuth[1], Christian Carbogno[1], Volker Blum[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]MEMS Department, Duke University, Durham, NC 27708, USA

The electronic properties of organic semiconductors typically exhibit a significant dependence on the strain, stress, and pressure [1]. In this contribution, we present the theoretical background, assessment of approximations, and results of electronic and transport properties in the framework of density-functional theory. Our implementation considers the analytical strain derivatives (stress tensor) including the contributions that stem from (a) van-der-Waals interactions [2] and (b) the Fock-exchange in hybrid functionals. We validate our approach by investigating the geometric and electronic changes that occur in polyacetylene and anthracene under hydrostatic pressure. We show that the fraction of exact exchange included in the calculations is critical – and non-trivial to choose – for a correct description of these systems. Furthermore, we point out trends for the electrical conductivity under pressure and identify the dominant charge carriers and transport directions.

[1] J. H. Kim, S. Seo, and H. H. Lee, Appl. Phys. Lett. **90**, 143521 (2007); G. Giri *et al.*, Nature. **480**, 504 (2011)
[2] A. Tkatchenko and M. Scheffler, Phys. Rev. Lett. **102**, 073005 (2009).

HL 58.5 Wed 17:30 EW 202

A Transition from Vacuum Level Alignment to Fermi Level Pinning in Organic Semiconductors — •Mahdi Samadi Khoshkhoo[1], Alexander André[1], Thomas Chassé[1,2], and Marcus Scheele[1,2] — [1]Institute of Physical and Theoretical Chemistry, Universität Tübingen, Germany. — [2]Center for Light-Matter Interaction, Sensors & Analytics LISA+, Universität Tübingen, Germany

Coupled organic-inorganic nanostructures (COINs) have emerged as a promising class of materials for quantum dot-based optoelectronic devices. The architecture of these devices includes semiconductor quantum dots physically and electronically connected to each other through organic semiconductor bridges which can form a charge-transfer layer with the ability to pass only electrons or holes. In this way, the understanding of energy level alignment at 1) the organic/inorganic semiconductor or 2) the organic semiconductor/metal interface is essential in order to design charge-transfer layers with inherent rectification ability. In this presentation, we demonstrate the utilization UPS to investigate the interfaces between organic semiconductors and various metal substrates (which are chosen to span a wide range of work functions) in order to recognize the transition between two different alignment regimes. The substrates were chosen in a way that π-electronic molecular orbitals of ligands have an insignificant hybridization with substrate wave functions. This method provides valuable information for the design and fabrication of COIN optoelectronic devices, such as minimum hole and electron injection barriers, energy of polaronic states, polaronic relaxation energies, and the amount of interface dipole.

HL 58.6 Wed 17:45 EW 202

Extracting the emitter orientation in organic light-emitting diodes from external quantum efficiency measurements — •Tobias D. Schmidt[1], Lukas J. Reichardt[1], Andreas F. Rausch[2], Sebastian Wehrmeister[1], Bert J. Scholz[1], Christian Mayr[1], Thomas Wehlus[2], Rossa Mac Ciarnain[3], Norbert Danz[3], Thilo C. G. Reusch[2], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]OSRAM OLED GmbH, Wernerwerkstrasse 2, 93049 Regensburg, Germany — [3]Fraunhofer Institute for Applied Optics and Precision Engineering, 07745 Jena, Germany

Emitter orientation will play a major role in future applications of organic light-emitting diodes due to its strong impact on the efficiency of the devices. Up to now, determining the orientation of transition dipole moments required elaborate angular-dependent measurements of the light emission pattern. In this paper, we present a simplified and straightforward method to extract the emitter orientation from external quantum efficiency measurements. We demonstrate the validity of the method on three different dye-doped emitting systems.

HL 58.7 Wed 18:00 EW 202

Permeable Base Transistor - an Organic Thin-Film Transistor with High On/off Ratio and HF-operation — •Markus Klinger[1], Axel Fischer[1], Felix Kaschura[1,2], Bahman Kheradmand-Boroujeni[2,3], Daniel Kasemann[1], and Karl Leo[1] — [1]IAPP, TU Dresden, George-Bähr-Str. 1, 01069 Dresden — [2]cfAED, Flügelweg 20, 01157 Dresden — [3]CCN, TU Dresden, Helmholtzstraße 18, 01069 Dresden

Optimization of Organic Field-Effect Transistors (OFET) typically involves expensive structuring techniques in order to achieve small channel lengths in the micrometer range. Here, we show a Permeable Base Transistor (PBT), fabricated using thermal vapor deposition and shadow masks. These PBTs consist of a 'sandwich'-geometry with three parallel electrodes separated by two semiconducting C_{60} layers. The current flow between the upper and lower electrode is controlled by a thin perforated electrode in the middle [1]. Since electron transport is directed vertically, channel lengths in the range of 100 nm are achieved. By using insulating layers, we realize downscaled transistors with an active area of $(0,2\,\mathrm{mm})^2$. The PBTs reach a current density of $10\,\mathrm{A/cm^2}$, an on/off ratio greater than 10^6 and a gain of 1000 at a low driving voltage of 1.0 V. The transit frequency of 2.2 MHz is determined with an optimized measuring setup [2]. In comparison to agressively scaled horizontal OFETs [3], we present a device configuration realized at low cost, allowing for applications with high current and switching speed. [1] J. Appl. Phys., **111**(4), 044507; [2] IEEE Transactions on Electron Devices, **61**(5), 1423-1430; [3] Small, **8**(1), 73-79

HL 58.8 Wed 18:15 EW 202

Anisotropic electron mobility studies on Cl_2-NDI single crystals and the role of static and dynamic lattice deformations upon temperature variation — •N.H. Hansen[1], F. May[2], D. Kälblein[2], T. Schmeiler[1], C. Lennartz[2], A. Steeger[1], C. Burschka[3], M. Stolte[3], F. Würthner[3], J. Brill[2], and J. Pflaum[1,4] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]InnovationLab GmbH, Speyerer Strasse 4, 69115 Heidelberg, Germany and BASF SE, 67056 Ludwigshafen, Germany — [3]Institut für Organische Chemie and Center for Nanosystems Chemistry, Universität Würzburg, 97074 Würzburg, Germany — [4]ZAE Bayern, 97074 Würzburg

Recently, high mobility air-stable electron semiconductors have been synthesized to fill one of the major technological gaps in an all-organic circuitry. One of the promising candidates with a thin-film mobility of up to 1.3 $\mathrm{cm^2/Vs}$ at ambient conditions is Cl_2-NDI (naphthalene diimide) [Stolte et. al., Proc. of SPIE, Vol. 7778, 777804, 2010]. Yet little is known about its elementary carrier transport mechanisms on a molecular level. To address this lack of information, we performed anisotropic field effect transistor measurements on Cl_2-NDI single crystals and observe an increasing mobility at lower temperatures (1.5 $\mathrm{cm^2/Vs}$ at 300 K, 2.8 $\mathrm{cm^2/Vs}$ at 175 K), which hints at a band-like transport, as commonly assumed. However, as we will demonstrate the experimental data can be consistently described in the framework of a hopping-type model based on Levich-Jortner rates, which accounts for thermally induced lattice effects and electron-phonon interaction.

HL 58.9 Wed 18:30 EW 202

Ultra-high vacuum fabrication and characterization of organic thin film transistors: In-situ electrical and surface sensitive analysis on temperature effects and layer growth — •Roman Lassnig[1], Michael Hollerer[1], Bernd Striedinger[2], Alexander Fian[2], Barbara Stadlober[2], and Adolf Winkler[1] — [1]Institute of Solid State Physics, Graz University of Technology, Austria — [2]Materials Division, Joanneum Research, Austria

Many of the underlying principles affecting critical organic field effect transistor (OFET) parameters such as performance and lifetime are not fully understood to the present date. We present analysis on the formation, structure and stability of the semiconducting layer in pentacene OFETs, through a unique combination of in-situ layer deposition, real-time electrical and surface analytical characterization, during and subsequent to the deposition process itself. All investigations have been performed under ultra-high vacuum conditions at temperatures ranging from 125 K up to semiconductor desorption. In-situ Auger electron spectroscopy (AES) and thermal desorption spectroscopy (TDS) were performed parallel to the electrical investigations.

Ex-situ atomic force microscopy allowed direct connections to be made between growth mode, morphology and charge transport mechanisms. Of special interest was the onset of the OTFT functionality as a function of layer thickness in combination with sample pretreatment. In addition, the evaluation of, coverage and growth temperature dependent, linear and saturation charge carrier mobilities proved to be of great interest in regard to contact resistance assessments.

HL 59: Graphene: Applications, luminescence and spin relaxation (HL with O/TT)

Time: Wednesday 16:45–18:45 Location: ER 270

HL 59.1 Wed 16:45 ER 270

Fabrication and Growth of Three-dimensional Graphene Electrodes with Controllable Pore Size — •Simon Drieschner, Michael Weber, Evangelos Makrygiannis, and Jose A. Garrido — Walter-Schottky-Institut, Physik Department, TU München, Am Coulombwall 4, 85748 Garching

Three-dimensional graphene-based electrodes combine graphene's unique properties like high conductivity, chemical inertness, and mechanical stability with a high surface to volume ratio, which could be of great interest for energy applications. However, tuning the pore size of 3D graphene networks is a non-trivial challenge, since the growth of graphene depends on the shape and structure of the metal substrate. Here we demonstrate the fabrication of 3D electrodes by using metal powder providing an interconnected scaffold which serves as substrate for the growth of graphene by chemical vapor deposition. The pore size distribution is shown to be controlled by the used metal particles and the growth temperature. After wet chemical etching of the metal catalyst, a freestanding and stable graphene foam of low mass and high crystalline crystal quality as confirmed by Raman spectroscopy is obtained. Cyclic voltammetry and electrochemical impedance spectroscopy measurements are used to confirm its excellent electrochemical properties. Our work highlights the great potential of these 3D graphene electrodes for energy storage and sensing applications.

HL 59.2 Wed 17:00 ER 270

Graphene microelectrode arrays for the electrochemical detection of neurotransmitters — •Martin Lottner[1], Luis Batista-Pires[2], and Jose A. Garrido[1] — [1]Walter Schottky Institut, TU München, München, Deutschland — [2]Catalan Institute of Nanoscience and Nanotechnology, ICN2, Barcelona, Spain

Graphene has great potential for use as stimulation and sensing material in neural and cardiac implants. Its flexibility and chemical stability anticipate a good biocompatibility, which cytotoxicity studies have underlined. It is transparent to visible light and non-magnetic, which allows for unperturbed optical stimulation and post-implantation MRT imaging. In this contribution, we present graphene microelectrode arrays for the electrochemical detection of neurotransmitters. Vacancy defects were introduced by ozone exposure and growth conditions were varied to increase double layer content of the electrodes. The modifications were validated using Raman spectroscopy. Cyclic voltammetry studies show an electrochemical window of about 1V. Ferricyanide redox studies have been performed upon increasing defect density and double layer content, to investigate the transition from macro- to microelectrode behaviour. Further, a sensitivity for the detection of norepinephrine and dopamine below 1nM is demonstrated. This study shows that modified CVD graphene microelectrodes can be used for highly sensitive detection of neurotransmitters. Taking advantage of the high interfacial capacitance and large electrochemical window of graphene electrodes, we will discuss their use for safe extracellular stimulation.

HL 59.3 Wed 17:15 ER 270

Structural study of mono- and bilayer graphene nanoribbons directly grown on SiC(0001) — •Lauren A. Galves, Timo Schumann, João Marcelo J. Lopes, and Henning Riechert — Paul-Drude-Institut für Festkorperelektronik, 10117 Berlin, Germany

Graphene nanoribbons (GNR) are very promising for nanoelectronics, since they possess unique electronic properties which are dependent on their width, edges, as well as number of graphene layers [1-2]. Therefore, achieving the controlled and high-quality synthesis of GNRs is anticipated to be of great importance. One of the methods which show great potential is the growth of GNRs on surface facets of SiC(0001) by the graphitization method [3]. In this contribution we report on the controlled growth and characterization of epitaxial mono- and bilayer GNRs on SiC(0001) surfaces. They were synthesized by utilizing the surface graphitization method at high temperatures and a straightforward air annealing (for bilayer GNRs) [4]. The influence of the surface step heights (i.e. facet sizes) on the ribbon growth and properties was analyzed. A correlation between steps heights and ribbons width was established. The nanostructures were analyzed by AFM height and phase contrast images. This allowed the determination of the SiC surface morphology as well as ribbons width. Raman spectroscopy was employed to gain information about the thickness of the GNRs (i.e. mono- or bilayer graphene) and their preferential edge type.

[1] V. Barone et al., Nano Lett. 6, 2748 (2006); [2] T.S. Li et al., Eur. Phys. J. 64, 73 (2008); [3] M. Sprinkle et al. Nat. Nanotechnol. 5, 727 (2010); [4] M.H. Oliveira Jr. et al., Carbon 52, 83 (2013).

HL 59.4 Wed 17:30 ER 270

Correlation of the crystallite sizes and D band frequency of non-graphitic carbons — •Dominique B. Schuepfer[1], Kristin Faber[2], Bernd M. Smarsly[2], Roman V. Yusupov[3], and Peter J. Klar[1] — [1]Institute of Experimental Physics I, Justus-Liebig-University Giessen, Germany — [2]Institute of Physical Chemistry, Justus-Liebig-University Giessen, Germany — [3]Institute of Physics, Kazan Federal University, Russia

Raman spectroscopy is often used to determine the crystallite size L_a of non-graphitic carbons by taking into account the intensity ratio of the defect-induced D band and the G band. We present an analysis of soft pitches via Raman spectroscopy in comparison to wide-angle X-ray spectra revealing discrepancies for L_a. Significant errors can be caused by known issues, for example the superposition of certain bands while estimating the intensities. Therefore, we introduce an alternative approach: An analysis of the D band revealed a correlation between its position and the crystallite size in the range of crystallite sizes less than 2 nm. The Raman shift significantly increases for smaller L_a using an excitation wavelength in the visible range. UV light yields the opposite behavior of the D band position, probably because of resonant absorption processes. To further characterize the samples in different L_a-ranges ($L_a < 2$ nm and $L_a > 2$ nm) electron paramagnetic resonance spectroscopy (EPR) has been carried out. Isotropic shaped EPR spectra are observed up to a crystallite size of 2 nm and samples containing crystallite sizes larger 2 nm show anisotropic signals. This behavior correlates with the detected Raman shift.

HL 59.5 Wed 17:45 ER 270

Ultrafast photocurrents in back-gated graphene — •Felix Schade, Andreas Brenneis, Jose A. Garrido, Simon Drieschner, and Alexander W. Holleitner — Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, Garching, Germany

We present picosecond time-resolved photocurrent measurements of back-gated CVD grown graphene on sapphire substrates. We examine the optoelectronic dynamics with respect to (i) the thermal coupling of graphene to its environment [1], (ii) different doping levels by tuning the back-gate voltage with respect to the Dirac point, and (iii) thermoelectric, photovoltaic as well as bolometric contributions. To this end, the graphene sheets are contacted by a THz-stripline circuit, and the ultrafast response is read-out by an Auston-switch [2]. The back-gate is separated from the graphene by the help of ALD-grown sapphire.

The ERC grant NanoREAL is acknowledged.

[1] A. Brenneis, et al., Nature Nanotechnology, DOI: 10.1038/NNANO.2014.276 (2015). [2] L. Prechtel, et al. Nature Comm. 3, 646 (2012).

HL 59.6 Wed 18:00 ER 270

Coherent and Incoherent Photoluminescene from Photo-excited Graphene — •Torben Winzer[1], Richard Ciesielski[2], Matthias Handloser[2], Alberto Comin[2], Achim Hartschuh[2], and Ermin Malic[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany

— [2]Department Chemie, Ludwig Maximilians Universität München, Germany

Based on a microscopic theory and experimental measurements we investigate the ultrafast photoluminescence arsing from photo-excited graphene. Our calculations, performed within the density matrix formalism, allow for energy- and time-resolved insights into the radiative processes where two distinct microscopic mechanisms are distinguished: Beside the incoherent photoluminescence, which is driven by recombination of excited carriers, we find a coherent contribution induced by the microscopic polarization [1]. The incoherent spectrum mainly depends on the excitation strength. In contrast, the coherent photoluminescence spectrally shifts with the excitation energy, which is demonstrated for the first time and confirmed by our measurements.
[1] T. Winzer, R. Ciesielski, M. Handloser et al., arXiv:1411.0531v1 (2014)

HL 59.7 Wed 18:15 ER 270

Polarised Hot Carrier Photoluminescence in Graphene — •Thomas Danz, Andreas Neff, Reiner Bormann, Sascha Schäfer, and Claus Ropers — 4th Physical Institute, University of Göttingen, Göttingen, Germany

The thermalisation of photogenerated hot charge carriers in graphene leads to photoluminescence at wavelengths far away from that of the exciting pump laser [1,2]. To date, no polarisation properties of the photoluminescence have been reported, although recent numerical simulations show a strong anisotropy of the underlying relaxation processes in graphene [3]. This is in agreement with the results of transient pump-probe measurements showing a dependence of the transmissivity on the angle between pump and probe polarisations [4]. Here, we present polarisation- und time-resolved two-pulse excitation photoluminescence measurements with sub-30fs ultrashort laser pulses. We demonstrate an anisotropic nature of the emitted photoluminescence and use these findings to discuss complementary insights into the ultrafast carrier response in graphene.
[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] M. Mittendorff *et al.*, Nano Lett. **14**, 1504 (2014)

HL 59.8 Wed 18:30 ER 270

Spin Relaxation in Graphene — •Frank Ortmann[1], Dinh. V. Tuan[2], David Soriano[2], Sergio O. Valenzuela[2,3], and Stephan Roche[2,3] — [1]Institute for Materials Science and Dresden Center for Computational Materials Science, TU Dresden, Germany — [2]ICN2 Barcelona, Spain — [3]ICREA, Barcelona, Spain

Spin polarization of electrons in graphene has been under great attention in recent years due to intrinsically small spin-orbit coupling and hyperfine interaction and high carrier mobilities. However, experimental spin-relaxation times are 3-4 orders of magnitude too short compared to theoretical predictions. Such discrepancy, together with contradictory proposals for spin-relaxation mechanisms, triggered a debate about its behavior in clean and/or defective graphene.

We observe an intrinsic spin-dephasing mechanism in graphene that is most strongly impacting the Dirac point, which can be enhanced by the adsorption of heavy ad-atoms.[1] The extracted spin relaxation times (τ_s) from our simulations show good agreement with experimentally observed energy dependencies of τ_s.
[1] D. V. Tuan, F. Ortmann et al. Nature Phys. 10, 857 (2014).

HL 60: Quantum dots: Transport

Time: Wednesday 17:15–18:45 Location: EW 203

HL 60.1 Wed 17:15 EW 203

The Kondo resonance of a quantum dot in magnetic fields — •Alexander W. Heine[1], Daniel Tutuc[1], Gertrud Zwicknagl[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Institut für Mathematische Physik, Technische Universität Braunschweig, 38106 Braunschweig, Germany

The fingerprint of the Kondo effect in quantum dots is a peak of enhanced conductance at zero bias, the so-called zero bias anomaly. We examine experimentally the influence of magnetic fields on this zero bias peak. The measurements were performed in an ^{3}He/^{4}He dilution refrigerator with a base temperature of about 20 mK. A magnetic field B up to 6 T was applied parallel as well as perpendicular to the sample surface.

In a perpendicular magnetic field we analyze the splitting of the Kondo resonance in the so-called Kondo chessboard. Here a decrease of the splitting width with increasing magnetic field is observed. The data is compared to numerical renormalization group calculations by Hewson et al.[1], which show the relation between the effective splitting of the zero bias anomaly and B/T_K. Thereby we can show, that the quantum Hall effect in the two-dimensional leads affects the Kondo temperature and therefore the splitting of the zero bias anomaly.
[1] Hewson et al., Phys. Rev. B 73, 045117 (2006)

HL 60.2 Wed 17:30 EW 203

Optical detection of single-electron tunneling dynamics in self assembled quantum dots — •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, Lotharstr. 1, 47057 Duisburg, Germany — [2]Chair of Applied Solid State Physics, Ruhr-Universität Bochum, Universitätsstr. 150, 44780 Bochum, Germany

The tunneling dynamics of charge carriers into self-assembled quantum dots (QDs) have been studied using electrical measurements like transconductance spectroscopy. However, these techniques are still limited to measurements of an ensemble of QDs, i.e. the dynamics of single electron tunneling into a single QD has not been observed yet.

Here, for the first time, we demonstrate that we are able to study the electron tunneling between a single self-assembled QD and a 3D back contact, using resonance fluorescence as detection scheme. The QD is embedded in a diode structure, which allows controlled charging and discharging of the QD with single electron resolution. We apply voltage pulses to the top-gate contact and measure the resonance fluorescence signal, while electrons tunnel into or out of the QD. Using this new time-resolved measurement technique, we investigate the relation between the tunneling times into the QD and the chemical potential in the back gate. An even more detailed understanding of the tunneling processes between QDs and a charge carrier reservoir can be achieved by measuring the telegraph noise in the resonance fluorescence signal, when the states with occupation number 0 and 1 are degenerate.

HL 60.3 Wed 17:45 EW 203

All-electrical measurement of the spin-triplet relaxation time in self-assembled quantum dots — •A. Al-Ashouri[1], K. Eltrudis[1], A. Beckel[1], A. Ludwig[2], A. D. Wieck[2], A. Lorke[1], and M. Geller[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany — [2]Chair for Applied Solid State Physics, Ruhr-Universität Bochum, Universitätsstraße 150, 44780 Bochum, Germany

Devices for quantum computation require coherent access to qubits, which can be realized by a two level quantum system in quantum dots (QDs). Promising candidates for a suitable system include the excited spin triplet and its singlet ground state. A long lifetime is expected for an excited spin state, however, a desirable all-electrical read-out scheme for the qubit state has yet to be realized.

Here we use time-resolved transconductance spectroscopy[1] to electrically prepare and detect the triplet state in self-assembled InAs QDs and find a long spin relaxation time in the order of μs. The investigated QDs are embedded in a GaAs\AlGaAs matrix using a heterostructure FET. They are coupled to a two dimensional electron gas (2DEG) via a tunneling barrier. The 2DEG is used as a charge reservoir as well as a sensitive detector for the electron states in the QDs. After initialization of the spin-triplet state we observe the electron emission during read-out and in this way are able to record the temporal decay of the triplet state. The long timescale for the decay promises future coherent manipulation of such a spin-qubit.
[1] A. Beckel et al., Phys. Rev. B **89**, 155430 (2014).

HL 60.4 Wed 18:00 EW 203

Stochastic resonance in electron counting — •Timo Wagner, Johannes Bayer, Eddy P. Rugeramigabo, and Rolf J. Haug

— Institut für Festkörperphysik - Abteilung Nanostrukturen, Leibniz Universität Hannover, 30167 Hannover, Germany

We performed electron counting experiments on a double quantum dot (QD) as well as on a more advanced serial triple quantum dot structure. For both systems an adjacent quantum point contact (QPC) serves as sensitive charge detector to resolve time dependent single electron tunneling events. From the recorded time trace we extracted the waiting times for tunneling into and out of a quantum dot.

The two waiting time distributions reveal phase correlated oscillations. We identify those characteristic oscillations as stochastic resonance due to the superposition of a small harmonic signal and the bistable stochastic quantum dot signal. Further we studied and simulated the dependency of different system parameters on the resonance.

The quantum dots structures were defined by metallic topgates on a two dimensional electron gas on GaAs/AlGas. The measurements on the double quantum dot were performed in a He3 system at temperatures around 300mK and for the triple dot measurements we used a dilution refrigerator with base temperature around 20mK. Time resolved charge was archieved with a low noise DC setup.

HL 60.5 Wed 18:15 EW 203

Transport Measurements on a Triple Quantum Dot with Two Bias Voltages — •Monika Kotzian[1], Fernando Gallego Marcos[2], Gloria Platero[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, 30167 Hannover, Germany — [2]Instituto de Ciencia de Materiales, CSIC, Cantoblanco, 28049 Madrid, Spain

We present transport measurements on a lateral triple quantum dot with a star-like geometry [1] in dependence of two different bias voltages applied simultaneously. The structure is made with local anodic oxidation by AFM on a GaAs/AlGaAs heterostructure, the design allowing to simultaneously measure the conductance along two different paths with two quantum dots in each path. By controlling the potentials via the four gates of the device resonances of two and all three dots can be generated. [2,3] With one lead attached to each dot and using two of the leads as source contacts with two different bias voltages and one lead as a drain contact, novel possibilities arise to study the interaction between the transport paths. For characterization of the system and a better understanding of coupling effects and bias dependent behavior the transport near the triple dot resonance is simulated using the Born-Markov approximation.

[1] M. C. Rogge, R. J. Haug, Phys. Rev. B 77, 193306 (2008). [2] L. Gaudreau, et al., PRL 97, 036807 (2006). [3] M. C. Rogge, R. J. Haug, New Journal of Physics 11, 113037 (2009).

HL 60.6 Wed 18:30 EW 203

Electron Transport in a Quadruple Quantum Dot System — •Johannes Bayer, Timo Wagner, Eddy P. Rugeramigabo, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover

We successfully produced a tunable system of four tunnel-coupled quantum dots in series. The device was fabricated via electron beam lithography on an MBE-grown GaAs /AlGaAs heterostructure forming a 2DEG 110 nm beneath the surface with an electron density of $2.4 \cdot 10^{11}$ cm^{-2} and an electron mobility of $5.1 \cdot 10^5$ cm^2/Vs. We performed electronic transport measurements in a dilution refrigerator at a base temperature of about 10 mK. The quadruple quantum dot system (QQD) has been studied in terms of linear and nonlinear transport behavior. Additionally, two quantum point contacts are located near the quantum dots and used as sensitive charge detectors. We present a combination of transport measurements and charging diagrams in the many electron regime of the QQD.

HL 61: Posters III (Organic-inorganic perovskite semiconductors; Organic photovoltaics and electronics; Photovoltaics; Energy science; New materials and concepts)

Presenters are kindly requested to be near their poster for at least one hour in the time between 17:00-19:00 or to leave a note about their availability for discussions.

Time: Wednesday 15:00–20:00 Location: Poster F

HL 61.1 Wed 15:00 Poster F

Processing influence on structural and electronic properties of Lead Methylammonium Tri-Iodide films — •Christian Müller[1,2,3], Bernd Epding[1], Ilknur Yoldas[2], Robert Lovrincic[2,3], Hans-Hermann Johannes[2], and Wolfgang Kowalsky[2,3] — [1]Kirchhoff Institut für Physik, Universität Heidelberg — [2]Institut für Hochfrequenztechnik, TU Braunschweig — [3]InnovationLab GmbH, Heidelberg

Over the last few years the power conversion efficiency of organometal-halide perovskite (such as $CH_3NH_3PbI_3$) based solar cells has skyrocketed at an unprecedented rate to values around 18 %. This development is even more impressive if we take into account that such high efficiencies can be reached for very different cell, made from different precursor materials, and for both solution and vacuum processed absorber layers. All this approaches have in common that the exact role of the perovskite microstructure for the device performance is to date not well understood. We focus in this work on a comparison between solution vs. vacuum processed perovskite layers and solar cells based thereon. SPM and SEM measurements were performed for the different perovskite films. Thereby we were able to map electronic and structural properties with high spatial resolution. This enables us to directly correlate the obtained data to the device performance.

HL 61.2 Wed 15:00 Poster F

Charge Carrier Lifetime in methylammonium lead halide perovskite thin films — •Fabian Meier, Cornelius Krasselt und Carsten Deibel — Institute of Physics, Chemnitz University of Technology, 09126 Chemnitz, Germany

Thin film solar cells have shifted into the spotlight of current research and development because of their promising low-cost production resulting from high-throughout fabrication at low processing temperatures(1). Recently, hybrid perovskite structures on the base of lead halides have attracted considerable attention due to a tremendous increase in their power conversion efficiencies from 4 % to nearly 18 % within only a few years (2). Uncovering the recombination processes is of major importance for understanding and potentially circumventing the intrinsic losses in perovskite thin films. We performed absorption and photoluminescence (PL) meassurements of both mixed and pure methylammonium lead halides. The comparably sharp onsets of absorption and emission as well as the small Stokes shift between them are signs for the small energy losses of the charge carriers within corresponding solar cells. The charge carrier decay dynamics were investigated by performing time-resolved PL decay by time correlated single photon counting. We will discuss our results in view of the role of free carrier recombination and trap assisted recombination.

(1)*G.E. Eperon et all, Adv. Funct. Mater. 2014, 24, 151-157 (2)*N.G. Park, Mater. Today (2014), http://dx.doi.org/10.1016/j.mattod.2014.

HL 61.3 Wed 15:00 Poster F

Preparation and Charactarization of Methylammonium Lead Iodide Perovskite Absorber Layers — •David Grabowski, Andrea Jansen, Levent Gütay, Stephan J. Heise, Ingo Riedel, Jürgen Parisi, and Holger Borchert — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, 26129 Oldenburg, Germany

Since few years, perovskite thin films have attracted broad attention for application in solar cells: Without extreme efforts spent in technological developments, they already show strong electronic performance. In solar cells, the perovskite layer acts as a light absorber, that carries both electrons and holes. In this work we determine the significance of certain parameters during preparation on the emerging $CH_3NH_3PbI_3$ perovskite film. Through means of scanning electron microscopy (SEM) and x-ray diffraction (XRD) a one-step method and a two-step method have been compared and the latter proved to be more effective to achieve the desired morphology and crystal structure. Therefore we utilize a two-step method to first apply PbI_2 and later on CH_3NH_3I to create the perovskite, while systematically varying

crucial parameters. Through means of the aforementioned measuring equipment we verify advantageous parameters for mixing the solutions and the spin-coating process.

HL 61.4 Wed 15:00 Poster F

Evaluation of different layer sequences of perovskite solar cells — •Andrea Jansen, David Grabowski, Dorothea Scheunemann, Maria S. Hammer, Ingo Riedel, Jürgen Parisi, and Holger Borchert — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, 26129 Oldenburg, Germany

Since few years, perovskite solar cells have attracted a massive increase in research effort, which is due to their potentially very high efficiencies at low costs. In solar cells the perovskite layer functions as a light absorber and exhibits the ability to transport both electrons and holes. In this work, the deposition of the perovskite $CH_3NH_3PbI_3$ was implemented via a two-step coating method, in which a solution containing PbI_2 and another one containing CH_3NH_3I are deposited consecutively. Concerning photovoltaic performance, this method has shown to be advantageous compared to the one-step coating method, in which a solution containing both CH_3NH_3I and PbI_2 is deposited on the substrate. The perovskite layers were analyzed by scanning electron microscopy (SEM) and X-ray diffraction (XRD), in order to determine the film morphology and crystal structure, respectively. Different device concepts for implementing the solution-cast perovskite layers into solar cells will be presented and discussed.

HL 61.5 Wed 15:00 Poster F

First-principles study of tin-based hybrid organic-inorganic perovskites — •Jingrui Li and Patrick Rinke — COMP / Department of Applied Physics, Aalto University, Finland

Hybrid organic-inorganic perovskites have received rapidly growing interest in recent years as promising photoactive materials in emergent solar cell technologies [1]. While much experimental work is conducted on hybrid perovskite devices, a quantum mechanical understanding of the basic materials properties and fundamental processes is lagging behind. In this work we present a first-principles study of a series of methylammonium tin trihalide ($CH_3NH_3SnX_3$) perovskites employing relativistic density functional theory. We establish an all-electron reference for the ground state properties by benchmarking the local-atomic orbital code `FHI-aims` [2] and the full potential linear augmented plane wave code `exciting` [3] for the PBE exchange-correlation functional. The points of focus of our present study lie in (i) relativistic effects (more specifically, the scalar relativistic effects and the spin-orbit coupling) in the considered systems, (ii) improvement of electronic structure results by including exact exchange in the density functional, and (iii) changes in atomic and electronic properties due to the addition of chloride anions into the organo-tin triiodide perovskite.

[1] See, *e.g.*, M. A. Green *et al.*, *Nature Photon.*, **8**, 506 (2014).
[2] V. Blum *et al.*, *Comput. Phys. Commun.*, **180**, 2175 (2009).
[3] A. Gulans *et al.*, *J. Phys.: Condens. Matter*, **26**, 363202 (2014).

HL 61.6 Wed 15:00 Poster F

Improved interfaces in solution processed perovskite solar cells — •Florian Mathies[1,3], Julian Heusser[3,4], Aina Quintilla[1], Guillaume Gomard[1], Norman Mechau[1,3], and Uli Lemmer[1,2] — [1]Light Technology Institute, Karlsruhe Institute of Technology, Germany — [2]Institute of Microstructure Technology, Karlsruhe Institute of Technology, Germany — [3]InnovationLab, Heidelberg, Germany — [4]Kirchhoff-Institute for Physics, University Heidelberg, Germany

Perovskite semiconductor materials promise to have a massive impact in the field of photovoltaics. Perovskite solar cells with efficiencies up to 19% have been recently fabricated, demonstrating their capability to compete with state-of-the-art silicon solar cells.

A critical point for the electrical performance in perovskite solar cells is the perovskite/metal oxide blocking layer interface. Consequently, we investigated different metal oxides (TiO_2, ZnO, AZO and ZTO) with certain interfacial geometries, ranging from planar to nano- or mesoporous, with the perovskite layer. To make such solar cells compatible with flexible substrates and several industrially-relevant printing processes for a wide range of commercial applications, a reduction of process temperature is necessary. Using the previously described interfaces, the process temperature was reduced from 500°C to 120°C to determine its influence on the morphology at the interfacial layers by AFM and SEM studies, and on the electrical performance of the devices by IV-characteristic and IPCE measurements.

HL 61.7 Wed 15:00 Poster F

Electrical Characterization of Methyl Ammonium Lead Iodide — •Raffael Ruess, Martina Stumpp, Christoph Richter, Patrick Hofmann, and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen

Methyl ammonium lead iodide ($CH_3NH_3PbI_3$) is a trihalide perovskite semiconductor with promising and well-fitting parameters for the use as an absorber in hybrid solar cells. Homogeneous layers can be prepared by spin coating solutions of methyl ammonium iodide (CH_3NH_3I) and lead iodide (PbI_2) onto a substrate and annealing afterwards. In this work, the perovskite films were deposited via a two-step sequential deposition method. Current-voltage measurements were performed to determine the electrical conductivity of the perovskite film. An interesting hysteresis in the I-V measurements was observed corresponding to similar observations in perovskite solar cells and three possible reasons were discussed. Understanding the electrical behavior of perovskites, such as $CH_3NH_3PbI_3$, is important for finding further improvements on the efficiency of hybrid solar cells based on these materials.

HL 61.8 Wed 15:00 Poster F

Replacement of Lead in Organic-Inorganic Perovskite Absorber Layers — •Manuel Weiss, Christoph Richter, and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Heinrich-Buff-Ring 16, D-35392 Gießen

Perovskite solar cells are a very promising low-cost technology as efficiencies around 20 percent have been reported. One problem, however, is the presence of lead in the cells. Lead is known to be a toxic heavy metal which is, therefore, banned from a number of technical applications in various countries which represent, however, important global markets. The presence of lead can therefore be seen as one major obstacle that could prevent the commercial use of perovskite solar cells. Alternative metal ions that are less toxic and abundant in the earth crust are sought to replace lead at maintained functionality of the films. In this contribution, alternative metal ions were tested to form organic-inorganic perovskite layers. Films were characterized by Scanning Electron Microscopy, UV-visible absorption spectroscopy, X-ray diffraction and XPS to probe the elemental composition, structure, morphology and electronic coupling in the films. The different materials will be discussed in their applicability as new absorber layers in perovskite solar cells.

HL 61.9 Wed 15:00 Poster F

Current-Voltage Measurements on Perovskite Thin Films — •Jan Tinz, Martina Stumpp, Christoph Richter, Patrick Hofmann, and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen

The use of methyl ammonium lead iodide ($CH_3NH_3PbI_3$) as light absorbing material enables the production of efficient and low-cost solar cells due to its high charge carrier mobility. The direct band gap of the perovskite can be controlled by replacing the iodide with bromide to optimize the light absorption. Thin films of $CH_3NH_3Pb(I_{1-x}Br_x)_3$ were prepared in a one-step process by spin coating from solutions with different concentrations of lead iodide (PbI_2), methyl ammonium iodide (CH_3NH_3I) and methyl ammonium bromide (CH_3NH_3Br) on these substrates. Depending on the concentration of the solution, the thickness of the synthesized perovskite films varied. Current-voltage measurements were performed and the electrical conductivity of the synthesized perovskite thin films was determined. A basic understanding of the electrical characteristics of these thin layers is required for the development of more efficient hybrid solar cells based on $CH_3NH_3Pb(I_{1-x}Br_x)_3$.

HL 61.10 Wed 15:00 Poster F

Morphology of Methyl Ammonium Lead Iodide Thin Films Dependent on the Preparation Conditions — Martina Stumpp, •Jonas Horn, Raffael Ruess, Jan Tinz, and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen

Solar cells based on perovskites as absorbing material have attained large attention in the last two years due to the strong increase in the efficiencies of these cells. Perovskites have the great advantage of a high charge carrier mobility, low non-radiative carrier recombination and strong solar absorption. In this study, thin films of methyl ammo-

nium lead iodide ($CH_3NH_3PbI_3$) were prepared by one- or two-step solution-based processes on different substrates. Profilometry measurements were performed to attain an understanding of the roughness and the thickness of the perovskite films. The detailed morphology of the films was analyzed with the help of laser confocal and scanning electron microscopy. The dependence of the different preparation methods as well as the use of different substrates on the morphology of the ($CH_3NH_3PbI_3$) thin films is discussed.

HL 61.11 Wed 15:00 Poster F

Processing Optimization for Vacuum Deposited Perovskite Layers — Enkhtur Erdenebileg, Lauren E. Polander, Christian Körner, and •Karl Leo — Instutut für Angewandte Photophysik, Technische Universität Dresden, 01069 Dresden, Germany

Organic-inorganic hybrid perovskites currently attract considerable attention as promising light harvesting materials for solar cells due to their panchromatic absorption, excellent charge-transport characteristics, and ease of fabrication from inexpensive, commercially available materials. As a result of many recent advances related to changes in the stack design and processing conditions, the power conversion efficiency values for this new class of solar cells is increasing rapidly. Extremely uniform perovskite films can be formed using dual source vapor deposition of PbX2 and CH3NH3X (where X = I, Br, Cl) to yield high performance devices when used in combination with either solution-processed or vacuum-deposited transport layers. In this work, we optimize the vapor deposition of perovskite layers by investigating the effects of evaporation and annealing temperature on the properties of isolated perovskite films. The films are thoroughly examined using UV-vis absorption spectroscopy, grazing incidence X-ray diffraction, and scanning electron microscopy. The newly developed deposition conditions are then applied to fabricate optimized perovskite solar cells with vapor-deposited electron- and hole-transport layers.

HL 61.12 Wed 15:00 Poster F

Temperature-Dependence of a Perovskite-based Solar Cell — •Harald Hoppe — Langewiesener Str. 22, Institut für Physik, TU Ilmenau

The temperature dependence of a solar cell based on a hybrid perovskite material has been investigated. We find distinctive changes to occur within the photovoltaic parameters with temperature variation. The results are discussed in view of structural and electronic data.

HL 61.13 Wed 15:00 Poster F

Electroabsorption spectroscopy investigation of organic and perovskite solar cells — •Cheng Li[1,3], Yana Vaynzof[2,3], Tanaji Gujar[1], Dan Credgington[3], Zhi-Kuang Tan[3], Girish Lakhwani[3], Jianpu Wang[3,4], Mukundan Thelakkat[1], Neil Greenham[3], and Sven Hüttner[1,3] — [1]Macromolecular Chemistry I, University of Bayreuth, 95440 Bayreuth, Germany — [2]Centre for Advanced Materials, Im Neuenheimer Feld 227, Heidelberg University, Heidelberg, 69120, Germany — [3]Cavendish Laboratory, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom — [4]Institute of Advanced Materials, Nanjing Tech University, Nanjing, China 210009

In solution-processed photovoltaic devices, both organic and organic-inorganic perovskite based, the nanometer scale interfaces between the active material and electrodes play a crucial role on the device performance. In this poster, by using electroabsoption (EA) spectroscopy, combined with ultraviolet photoelectron spectroscopy (UPS), we investigate photovoltaic devices based on P3HT:PCBM, PBDTTT-CT:PC71BM and $CH_3NH_3PbI_{3-x}Cl_x$ systems. As a non-invasive method, EA provides unique information of the built-in potential (V_{BI}) in working devices. By characterizing the modulation of V_{BI}, we elucidate that the performance improvement of these solar cells utilizing interfacial engineering is mainly due to the shift of work function of electrodes, leading to an increase of the built-in potential in devices.

HL 61.14 Wed 15:00 Poster F

Charge-transfer states vs. triplet excited states in organic photovoltaics — •Johannes Benduhn, Donato Spoltore, Christian Körner, and Koen Vandewal — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden, Germany

Charge generation and recombination in organic solar cells occurs via the formation of charge-transfer (CT) states at the donor-acceptor interface. When the energy of the CT state is high, its formation can compete with the formation of triplet states on the donor or acceptor molecule, which can constitute an additional loss mechanism, reducing photo-voltaic performance.

With this work we aim to elucidate under which energetic and kinetic circumstances triplet state formation can be suppressed. Therefore we investigate material systems comprising of C_{60} as acceptor and a series of phthalocyanine dyes with slight variations in their molecular structure (ZnPc, F_4-ZnPc, CuPc, F_4-CuPc) as donor. The addition of fluorine allows tuning of the energy of the CT state, resulting in an increased open circuit voltage. Varying the central atom from Zn to Cu enhances inter-system crossing to a triplet excited state on the phthalocyanine molecule. The energy levels of all relevant electronic excited states are determined by sensitive measurements of the external quantum efficiency spectrum. The formation of triplets is quantified by steady state photo-induced absorption at various temperatures.

We find that in the system with a reduced inter-system crossing, charge generation for materials with a high energy CT state is still efficient, even though the triplet state is the lowest energy state.

HL 61.15 Wed 15:00 Poster F

Charge Transfer Absorption and Emission at ZnO/Organic Interfaces — •Fortunato Piersimoni[1], Raphael Schlesinger[2], Johannes Benduhn[3], Donato Spoltore[3], Sina Reiter[1], Ilja Lange[1], Norbert Koch[2], Koen Vandewal[3], and Dieter Neher[1] — [1]Institute of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Strasse 24-25, 14476 Potsdam, Germany — [2]Institut für Physik & IRIS, Adlershof Humboldt-Universität zu Berlin, Brook-Taylor-Strasse 6, 12489 Berlin, Germany — [3]Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Straße 1, 01069 Dresden, Germany

Here we investigate Hybrid Charge Transfer States (HCTS) at the planar interface based upon α-NPD and ZnO by means of spectrally resolved electroluminescence (EL) and external quantum efficiency (EQE) measurements. The appearance of a sub-gap signal in the EL and in the EQE spectra proves respectively the radiative decay and the absorption from direct excitation of HCTSs. By means of various phosphonic acid based self-assembled monolayers we tune the ZnO work function and the energy gap (Egap) between the ZnO conduction band and a-NPD LUMO level. We observe a correlation between Egap, the peak position of the NIR EL spectra and the open circuit voltage of photovoltaic devices, comprising these organic-inorganic interfaces. This unambiguously attributes the origin of the NIR emission to radiative recombination between an electron on the ZnO and a hole on α-NPD and confirms the relation between open circuit voltage and the energy of the charge-state, also for hybrid organic-inorganic interfaces.

HL 61.16 Wed 15:00 Poster F

Influence of electrical stress on the degradation of polymer solar cells — •Tobias Faber, Roland Rösch, and Harald Hoppe — Institute of Physics, Ilmenau University of Technology, Langewiesener Straße 22, 98693 Ilmenau, Germany

The stability of polymer solar cells is an ever-present topic in today's research on organic photovoltaics. While protocols for stability testing have been established within the course of the International Summits on Organic Solar Cell Stability (ISOS), there is no consensus on the voltage range within which solar cells should be characterized during degradation experiments. We show that this open parameter can result in different effects on the degradation path and the amount of degradation. In-situ measurements of IV-characteristics of continuously illuminated $PCDTBT:PC_{70}BM$ solar cells were conducted every 30 minutes for about 1600 hours. Three different potential regimes were realized by applying three different voltage ranges: "forward voltage" (-0.1 V ... 5 V), "basic voltage" (-0.1 V ... 1 V) and "reverse voltage" (-5 V ... 1 V). A strong influence of the applied voltages and currents running through the device on the initial exponential decrease of the power conversion efficiency, the so-called "burn-in", was revealed. The origin of the differences is discussed and degradation pathways are suggested.

HL 61.17 Wed 15:00 Poster F

Design of an energy-harvesting storage device based on organic solar cells and supercapacitor — •Lukas Hörlin[1], Andreas Baumann[1], Matthias Wiener[1], Gudrun Reichenauer[1], and Vladimir Dyakonov[1,2] — [1]Bayerisches Zentrum für Angewandte Energieforschung, Am Galgenberg 87, D-97074 Würzburg — [2]Experimentelle Physik 6, Julius-Maximilians-Universität Würzburg, Am Hubland, D-97074 Würzburg

A general problem of renewable energy system like photovoltaics and wind power is their volatility causing fluctations in the power grid.

Energy storage systems such as batteries or capacitors are promising candidates to overcome this fluctations making use of renewable energy more reliably. We designed a small-scale energy-harvesting storage device, which demonstrates the storage and use of the redundant energy by photovoltaic devices, namely organic bulk heterojunction (BHJ) solar cells, in a supercapacitor for a certain period of time. State-of-the-art organic BHJ solar cells were prepared by spin-coating and characterized by means of current-voltage characterisitics. The supercapacitor as the storage unit was analyzed by cyclic voltammetry. The energy harvesting system is realized by the ability to connect single organic solar cells in parallel and/or serial, which allowed us to vary the photocurrent and photovoltage of the unit and adapt it to the supercapacitor storage unit.

HL 61.18 Wed 15:00 Poster F

Material properties of organo-halide perowskites at different temperatures — •Gerhard Lackner[1], Irina Anusca[1], Vladimir Shvartsmann[1], Mehmet Sanlialp[1], Brahim Dhkil[2], and Doru C. Lupascu[1] — [1]Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg_Essen, Essen, Germany — [2]Ecole Centrale Paris, Structures, Properties and Modeling of Solids Laboratory, France

Recently, organo-halide perowskites have been attracted much interest by researchers due to their excellent performance as light absorbing material in solar cells. Certificated efficiencies of up to 20% have been reported [1]. Until now, the origins of their extremely well performance are not fully understood.

We investigated the material properties of methylammonium lead iodide (CH3NH3PbI3) and methylammonium lead bromide (CH3NH3PbBr3) for different temperatures. The results of this study confirm these achieved by Mitzi [2].

[1] Press release 17.11.2014, Wirtschaftswoche green, Andreas Menn, last visited on 01.12.2014, available online: http://green.wiwo.de/durchbruch-billig-solarzelle-erreicht-20-prozent-wirkungsgrad/

[2] D. B. Mitzi, in Progress in Inorganic Chemistry, Vol. 48 (Ed.: K. D. Karlin), John Wiley & Sons, Inc. Hoboken, NJ, USA 1999, p. 1.

HL 61.19 Wed 15:00 Poster F

Optoelectronic Interfaces for Restoration of Degenerated Retina — •Oliya Sadrillaevna Abdullaeva[1], Manuela Schiek[1], Karin Dedek[2], Matthias Schulz[3], Arne Lützen[3], and Jürgen Parisi[1] — [1]Energy and Semiconductor Research Laboratory, Department of Physics, Carl von Ossietzky University of Oldenburg, D-26111, Germany — [2]Department of Neurobiology, University of Oldenburg, 26111 Oldenburg, Germany — [3]Kekulé-Institut für Organische Chemie und Biochemie, Rheinische Friedrich-Wilhelms-Universität Bonn, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

A novel approach towards the development of artificial photoreceptors for diseases like retinitis pigmentosa and age-related macular degeneration is the employment of organic semiconducting thin films. These conditions eventually cause blindness due to photoreceptor degeneration. Ghezzi et al. have recently reported the restoration of light in explanted retinas from animal models of photoreceptor degeneration by a single-component organic film of poly(3-hexylthiophene) via a photo-excitation process. They were able to trigger neuronal firing upon illumination. Our work focuses on employment of a Squaraine dye 2,4-Bis[4-(N,N-diisobutylamino)-2,6-dihydroxyphenyl]squarain as potential organic material for neuronal stimulation. Squaraine dyes are characterized by their unique aromatic four membered ring system. This work is aimed at testing the biocompatibility of Squaraine dyes with different biological cell lines and if so exciting the cells by illumination.

HL 61.20 Wed 15:00 Poster F

Band-like electron transport and high mobility in F_2-TCNQ single-crystal field-effect transistors — •Yulia Krupskaya[1], Marco Gibertini[2], Nicola Marzari[2], and Alberto Morpurgo[1] — [1]University of Geneva, Geneva, Switzerland — [2]EPFL, Lausanne, Switzerland

It is believed that in organic single-crystal field-effect transistors (FET) of the highest quality, the electron transport occurs in the band-like regime, with the carrier mobility increasing upon lowering temperature. Neither the microscopic nature of this regime, nor why it occurs only in some materials but not in others is currently well understood. To address these issues, we performed a study of electron transport in single-crystal FET of different tetracyanoquinodimethane (F_x-TCNQ) molecules. We show that F_2-TCNQ devices exhibit the most pronounced band-like transport observed to date (a room-temperature electron mobility μ = 6-7 cm^2/Vs, increasing up to 25 cm^2/Vs at 150 K), whereas in TCNQ and F_4-TCNQ FET μ = 0.1-0.2 cm^2/Vs at room temperature and decreases upon cooling. Moreover, we present a comparative analysis of the crystal structure, electronic structure and the electron-phonon interactions for the three studied materials aimed on understanding of the microscopic mechanisms responsible for so different thransport properties.

Financial support: DFG KR 4364/1-1

HL 61.21 Wed 15:00 Poster F

Polycyclic aromatic hydrocarbons in organic charge-transfer complexes — •Sebastian Witt[1], Antonia Morherr[1], Martin Baumgarten[2], Achim Rippert[1], and Cornelius Krellner[1] — [1]Physikalisches Institut, Goethe-Universität Frankfurt am Main — [2]Max-Planck-Institut für Polymerforschung, Mainz

Polycyclic aromatic hydrocarbons were discovered to present a new class of organic superconductors [1]. The organic molecules, as e.g. Picene, takes the role of an acceptor, when intercalated with alkali metals. We present the results of new organic charge-transfer complexes, where the polycyclic aromatic hydrocarbons could be either the donor or the acceptor. Applying the horizontal vapor growth in vacuum or in an inert gas we succeeded to co-crystallize seven new complexes. These single crystals were characterized by x-ray powder diffraction, single crystal Laue-type diffraction, in reflection and transmission, uv/vis-spectrometry and atomic force microscopy. In this contribution, we present the structural and physical properties of these new charge transfer complexes.

[1] R. Mitsuhashi *et al.*, Nature **464**, 74 (2010).

HL 61.22 Wed 15:00 Poster F

Charge transfer and metallic conduction at the F_{16}CoPc - Rubrene interface — •Florian Rückerl[1], Yulia Krupskaya[2], Eni Dodbiba[1], Vasilis Nikolis[1], Alberto Morpurgo[2], and Martin Knupfer[1] — [1]IFW Dresden, Germany — [2]DPMC University of Geneva, Switzerland

We present the electronic properties of the F_{16}CoPc-Rubrene interface, studied by means of transport measurements and photoemission spectroscopy (PES). The interface (formed of F_{16}CoPc film evaporated on top of Rubrene single crystals) shows a slight metallic conductance at temperatures between 100 and 300 K with the resistivity of 300 kΩ, which is very low in comparison to previously studied organic interfaces [1] and lowest after the outstanding TTF-TCNQ interface [2]. Hall Effect measurements revealed the hole conductance in Rubrene with the hole density of $1.6 \cdot 10^{13}$ cm^2 and the mobility of 1.2 cm^2/Vs. PES measurements at the interface with various layer thicknesses give clear evidence for a charge transfer. We observe an oxidation of the Rubrene molecules and a reduction of the Phthalocyanine Cobalt center by filling the $3d_{z^2}$ orbital.

The very low resistivity and the fact that the magnetic Co ion is fully involved in the charge transfer process, makes this system especially interesting and promising in terms of organic electronics and molecular spintronics.

Financial support: KN 393/14, KR 4364/1-1

[1] I. Gutierrez Lezama et al. Nature Mat. 11, 588-794 (2012)
[2] H. Alves et al. Nature Mat. 7, 574-580 (2008)

HL 61.23 Wed 15:00 Poster F

Charge Transfer at the Rubrene/F_{16}CoPc Interface Studied by X-ray Photoemission Spectroscopy and Near Edge X-ray Absorption Fine Structure — •Jing Guo[1], Florian Rückerl[2], Francisc Haidu[1], Volodymyr Dzhagan[1], Georgeta Salvan[1], Martin Knupfer[2], and Dietrich R. T. Zahn[1] — [1]Semiconductor Physics, Technische Universität Chemnitz, D-09107 Chemnitz, Germany — [2]Leibniz Institute for Solid State and Materials Research Dresden, Electronic and Optical Properties Department, D-01069 Dresden, Germany

We studied the electronic properties of the F_{16}CoPc/rubrene interface using X-ray photoemission spectroscopy (XPS) and near edge X-ray absorption fine structure (NEXAFS). Due to the matching between the ionization potential of rubrene and the electron affinity of F_{16}CoPc, a charge transfer is expected to occur at the interface. Ferromagnetic LSMO layers were applied as substrates for the thin film growth due to potential spintronic application of such structures. The electron transfer from rubrene to the Co metal center is deduced from the lineshape of Co 2p band in the XPS spectra, resulting in a reduction of Co(II) to

Co(I). NEXAFS data show a filling of the Co $3_d{}^2$ orbital of $F_{16}CoPc$, confirming the charge transfer. Besides, NEXAFS spectra show that $F_{16}CoPc$ molecules have a tendency to stand on rubrene. The energy level alignment between rubrene and LSMO was also established using ultraviolet photoelectron spectroscopy and inverse photoemission spectroscopy

HL 61.24 Wed 15:00 Poster F

Optical Spectroscopy on Organic-Inorganic Hybrid Structures - Charge Transfer in Type-II Level Systems — •Ingo Meyenburg[1], Benjamin Heidelmeier[1], Matthias Weber[1], Nils Rosemann[1], Christian Prinzisky[2], Jane Falgenhauer[3], Derck Schlettwein[3], Jörg Sundermeyer[2], and Wolfram Heimbrodt[1] — [1]Philipps Universität Marburg Department of Physics and Material Sciences Centre, Renthof 5, D-35032 Marburg — [2]Philipps Universität Marburg department of chemistry, Hans-Meerwein-Straße, D-35032 Marburg — [3]Justus-Liebig-University, Institute of Applied Physics, Heinrich-Buff-Ring 16, 35392, Gießen, Germany

Understanding interface processes is crucial for improvements of existing and new functional materials based on organic-inorganic hybrid semiconductor structures. Exciton recombination of spatially indirect excitons across type-II organic-inorganic interface can give access to the level alignment and interface properties of the hybrids. In addition to this method the depletion of excited organic states as a consequence of charge transfer into the inorganic semiconductor, which can be revealed by time resolved photoluminescence, can precise the determination of the level alignment. Further optical measurements including Raman spectroscopy help to understand the properties of hybrids including the interface. Starting with the idea of material combinations known from dye sensitized solar cells which imply a charge transfer from organic to inorganic structure some promising hybrid systems are investigated. Besides Antrachinone derivates the indoline dye D149 on mesoporous ZnO is a recently studied hybrid structure.

HL 61.25 Wed 15:00 Poster F

Investigation of Recombination Processes in Organic Solar Cells — •Sascha Ullbrich, Donato Spoltore, Janine Fischer, Christian Körner, Koen Vandewal, and Karl Leo — Institut für Angewandte Photophysik, Dresden, Deutschland

Recombination of charge carriers is one of the most important loss mechanisms in a solar cell. In competition to generation, it defines the open-circuit voltage by setting the equilibrium charge carrier density. Thus, it is necessary to study and understand recombination mechanisms in order to tap the full potential of organic photovoltaics. In this work, non-geminate recombination mechanisms and recombination dynamics of organic solar cells based on small molecules with different active layer thicknesses are studied. Charge extraction measurements and intensity dependent current-voltage characteristics are used to determine charge carrier densities, recombination rates and the dominant recombination mechanism under steady state conditions. We observe a change from bimolecular to trap-assisted recombination towards lower carrier densities and a decreasing recombination order with increasing active layer thicknesses.

HL 61.26 Wed 15:00 Poster F

Effects of perfluorination on the electronic, optical, and transport properties of polyaromatic hydrocarbons: pentacene and pyrene in the molecular and solid phase — •Roberto Cardia[1], Giancarlo Cappellini[1], and Gian-Marco Rignanese[2] — [1]Università di Cagliari and Istituto Officina dei Materiali-CNR, Italy — [2]Institute of Condensed Matter and Nanoscience, Université Catholique de Louivain, Belgium

We report a comparative study on pentacene and pyrene polyaromatic hydrocarbons (PAHs) and their perfluorinated counterparts. The study has been performed for both the isolated molecule and their molecular solid phases. The former are investigated, performing all-electron calculations, using Density Functional Theory (DFT) and Time Dependent DFT with localized gaussian basis set and hybrid B3LYP exchange correlation functional, in order to quantify the effects of morphology and chemical modifications on their electronic, optical, and transport properties: in particular electron affinity, ionization energy, fundamental gap, optical absorption, exciton binding energy, and reorganization energies for holes and electrons. The molecular solids using DFT-LDA with plane-waves basis set and ionic pseudopotentials in order to determine and compare ground state properties. In contrast, different exchange-correlation functionals (LDA, PBE0) are considered to evaluate their electronic excitations.

HL 61.27 Wed 15:00 Poster F

Comparison of the polarization-resolved linear absorption and time-resolved photoluminescence properties of crystalline perfluoropentacene on various substrates — •David Leimbach, Robin Döring, Tobias Breuer, Gregor Witte, and Sangam Chatterjee — Faculty of Physics and Materials Science Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany

Perfluoropentacene (PFP) is the perfluorinated counterpart and hence n-type organic semiconductor to the prototypical p-type pentacene. It can be grown as highly crystalline thin films on various optically transparent substrates such as NaF, KCl, and graphene. While PFP forms in the typical herringbone motif on both NaF and KCl, it shows a *Brickwall*-like polymorphism on graphene. Structural analyses show a π-stacking distance of only 3.07 Å [1], promising far higher values for electron and hole mobility and therefore greatly improved vertical transport, a desirable feature in potential organic electronic applications. Here, we investigate the influence of the packing motif and hence of the intermolecular coupling on the optoelectronic properties. Making use of polarization-resolved linear-absorption spectroscopy with sub-*m spatial resolution we identify the corresponding exciton transition energies and correlate them with the orientation of crystalline domains and the substrate. Furthermore, we find altered carrier recombination dynamics using time-resolved micro-photoluminescence spectroscopy.

HL 61.28 Wed 15:00 Poster F

Imaging the electric potential distribution of thin film solar cells — •Michael Scherer[1,2], Robert Lovrincic[1,2], and Wolfgang Kowalsky[1,2] — [1]InnovationLab GmbH, Heidelberg — [2]TU Braunschweig, Institut für Hochfrequenztechnik, Braunschweig

Huge research efforts on second to fourth generation solar cells lead to a tremendous growth in the power conversion efficiency of thin film solar cells, competing silicon based photovoltaics.

Charge generation and transport in these devices occur in layered stacks containing thin films of different functional materials. Because of layer thicknesses on the nano- to microscale, a complex interplay of interface and bulk effects determines the performance of the devices. This interplay can hardly be predicted from simulations or interface experiments only, highlighting the role of cross-sectional studies with high lateral resolution. We perform a correlated scanning Kelvin probe microscopy (SKPM) and electron beam induced current (EBIC) study on solar cell cross sections to image the electronic properties of entire solar cell devices.

Our scanning probe station is placed within the vacuum of a combined scanning electron microscopy (SEM)/focused ion beam (FIB) cross beam system. We prepare cross sections of different types of solar cells and characterize them with SKPM and EBIC on the same spot. The samples are illuminated and contacted in a defined manner and studied in vivo within the vacuum of our cross beam station.

HL 61.29 Wed 15:00 Poster F

Influence of ZnO doping in ALD deposited Al_2O_3 on Q_{fix} and charge carrier lifetime — •Johannes Ziegler[1], Thomas Schneider[1], Alexander N. Sprafke[1], and Ralf B. Wehrspohn[1,2] — [1]Institute of Physics Martin Luther University Halle-Wittenberg — [2]Fraunhofer Institute for Mechanics of Materials IWM Halle

Thin Al_2O_3 films deposited by thermal ALD on Si surfaces are known to provide an excellent passivation quality. Beside the chemical passivation of recombination active dangling bonds on the silicon surface by saturation, the field effect passivation generated by a high density of fixed negative charges in the Al_2O_3 is responsible for the reduction of parasitic charge carrier recombination in silicon solar cells [1]. In this work the influence of ZnO on the fixed negative charges in the Al_2O_3 layers and on their passivation quality on p-type silicon is studied by CV and QSSPC measurements.

[1] B.Hoex, J.Schmidt, R.Bock, P.P. Altermatt,M. C. M. van de Sanden and W. M. M. Kessels, Appl. Phys. Lett, 89:042112 (2006)

HL 61.30 Wed 15:00 Poster F

Investigation of order–disorder related band gap changes in $Cu_2ZnSn(S,Se)_4$ solar cells using electroreflectance — Christoph Krämmer[1], Christian Huber[1], Christian Zimmermann[1], Mario Lang[1], •Alexander Opolka[1], Thomas Schnabel[2], Tobias Abzieher[1,2], Erik Ahlswede[2], Heinz Kalt[1], and Michael Hetterich[1] — [1]Institute of Applied Physics, Karls-

ruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg, 70565 Stuttgart, Germany

$Cu_2ZnSn(S,Se)_4$ (CZTSSe) has attracted attention in thin-film photovoltaics due to its similarity to the well-established $Cu(In,Ga)(S,Se)_2$. However, the use of the low-cost and earth-abundant constituents Zn and Sn promise to overcome the weak point of the $Cu(In,Ga)(S,Se)_2$ system, although up to now the gap in efficiency between these two systems could not be closed. Among other things a high amount of point defects is made responsible for this deficit. In this contribution we demonstrate reversible band gap shifts which are induced by post-annealing of finished CZTSSe solar cells and are attributed to changes in the disorder within the Cu–Zn lattice planes. These changes follow the stochastic Vineyard model which further predicts a critical temperature above which the kesterite structure is entirely Cu–Zn disordered.

HL 61.31 Wed 15:00 Poster F

Photoluminescence investigation of the order–disorder effect in $Cu_2ZnSn(S,Se)_4$ solar cells — Christian Zimmermann[1], •Mario Lang[1], Christoph Krämmer[1], Thomas Schnabel[2], Tobias Abzieher[1,2], Angelika Schulz[1], Heinz Kalt[1], and Michael Hetterich[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70565 Stuttgart, Germany

Due to its composition of low-cost and earth-abundant elements, $Cu_2ZnSn(S,Se)_4$ (CZTSSe) is a promising material system for thin-film photovoltaics. Yet, a lack of efficiency compared to the well-established thin-film technology $Cu(In,Ga)(S,Se)_2$ is present, and therefore further improvements have to be realized. Recently, an order–disorder transition accompanied by a band gap shift has been reported. In this contribution the influence of this transition on the photoluminescence spectra is investigated as a function of sample temperature and excitation power. The results are analysed with reference to the fluctuating potential model.

HL 61.32 Wed 15:00 Poster F

Solution-based fabrication of kesterite $Cu_2ZnSnSe_4$ absorber layers and solar cells — •Markus Neuwirth[1], Huijuan Zhou[1], Chao Gao[1], Mario Lang[1], Christian Zimmermann[1], Christoph Krämmer[1], Christian Huber[1], Alexander Schiele[1], Thomas Schnabel[2], Tobias Abzieher[2], Erik Ahlswede[2], Michael Powalla[2,3], Heinz Kalt[1], and Michael Hetterich[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70565 Stuttgart, Germany — [3]Light Technology Institute, KIT

In the race for new energy sources, $Cu_2ZnSnSe_4$ (CZTSe) thin-film solar cells play a promising role since the absorber only comprises environmentally friendly and earth-abundant elements. Our fabrication approach for CZTSe consists of a cheap and simple solution-based two-step process that spares toxic solvents such as hydrazine. Utilizing a doctor-blading process we are able to form reproducible homogeneous precursors that transform into CZTSe by subsequent thermal annealing in a Se atmosphere. An automated buffer layer deposition process also increases the reproducibility of the overall sample quality. X-ray diffraction, Raman spectroscopy and external quantum efficiency measurements provide a better understanding of the kesterite absorber properties and their influence on cell performance.

HL 61.33 Wed 15:00 Poster F

Two-step fabrication process for $Cu_2ZnSnSe_4$ layers and solar cells on GaAs and molybdenum-coated glass substrates — •Alexander Schiele[1], Chao Gao[1], Mario Lang[1], Christoph Krämmer[1], Thomas Schnabel[2], Tobias Abzieher[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

$Cu_2ZnSnSe_4$ (CZTSe) is a promising thin-film absorber material due to its earth-abundant, low-cost and non-toxic components. Despite these advantages, CZTSe solar cells have not yet achieved the required efficiency for practical application. Therefore, high-quality absorber layers are necessary in order to perform fundamental material studies and further improve device performance. One way of fabricating such high-quality CZTSe layers is to utilize a precursor layer stack consisting of (epitaxial) ZnSe, Cu, and Sn deposited in a molecular-beam epitaxy system. A subsequent annealing process leads to the formation of CZTSe with large grains which in case of a GaAs(001) substrate inherits the preferential orientation of the monocrystalline ZnSe layer. The influence of GaAs as a substrate compared to molybdenum-coated glass is investigated by X-ray diffraction, Raman spectroscopy, and conversion efficiency measurements of finished solar cells.

HL 61.34 Wed 15:00 Poster F

Development and Characterization of an Ultrathin Hybrid p-n Interface for Solar Cell Applications — •Mahfujur Rahaman, Raul D. Rodriguez, Jacek Gasiorowski, and Dietrich R. T. Zahn — Halbleiterphysik,Technische Universität Chemnitz, Germany

In this work ultra-thin hybrid p-n interfaces were developed and characterized for photovoltaic application using inorganic 2-dimensional p-type GaSe as well as F16CoPc and PCBM n-type organic semiconductors. Due to the layered structure of GaSe, it is possible to deposit nano flakes by means of mechanical exfoliation. The F16CoPc thin film was deposited by thermal evaporation and PCBM by spin coating on a metal substrate. The properties of p-n interfaces were determined using a wide spectrum of techniques. Optical properties were characterized using spectroscopic ellipsometry (SE) and photoluminescence, while the surface morphology and electrical studies were performed using atomic force microscopy (AFM) and Kelvin probe force microscopy (KPFM) methods. The photovoltaic effect was investigated by means of I-V measurements in the dark and under illumination using 514.7 nm laser excitation.

HL 61.35 Wed 15:00 Poster F

Time-resolved Photoluminescence in thin film semiconductors - experiment and simulation — Matthias Maiberg, Conrad Spindler, Torsten Hölscher, Enrico Jarzembowski, Stefan Hartnauer, and •Roland Scheer — Martin-Luther-University Halle-Wittenberg, Photovoltaics Group, Von-Danckelmann-Platz 3, 06120 Halle, Germany

Time-resolved photoluminescence (TRPL) often is used to measure the effective lifetime of minority carriers in a semiconductor. However, there are several reasons for the TRPL decay not equal the decay of the minority carrier density: Bimolecular recombination, charge carrier drift and diffusion, shallow defects in the band gap, and varying defect densities.

By computer simulation we can explain most of the experimental findings. A curved decay for excitation with high injection levels can be assigned to bimolecular recombination. Contrary, a curved decay for low injection levels can be related to minority carrier capture and reemission from shallow defects in the band gap as well as to defect densities that vary on the lateral scale.

In bias voltage dependent TRPL on pn junctions (solar cells), the decay time increases with increasing voltage. This can be explained by a reduction of charge carrier drift in the space charge region and may be used to determine the charge carrier mobility.

HL 61.36 Wed 15:00 Poster F

Optical Imaging of $Cu(In,Ga)Se_2$ Solar Cells with Consideration of Material Homogeneity as a Quality Control Tool for Photovoltaic Devices — •Steffen Kretzschmar, Oliver Nagel, Dieter Greiner, Christian A. Kaufmann, and Thomas Unold — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, D-14109 Berlin

The luminescence yield of $Cu(In,Ga)Se_2$ solar cells or absorber layers can be used as a quality control indicator of the photovoltaic performance, in particular the open circuit voltage, of these devices. Here we present a study of electroluminescence and photoluminescence imaging on $Cu(In,Ga)Se_2$ solar cells using an InGaAs detection system with a good spectral match to the chalcopyrite luminescence emission. The results are compared to current-voltage and external quantum efficiency analyses on the same devices. In accordance with theory we find a linear dependence of the open circuit voltage on the logarithm of the luminescence yield. However, when not taking lateral inhomogeneities into account, a large spread in the correlation of solar cell parameters to imaging results is observed. We find that using an analytical homogeneity correction model leads to a distinct improvement of the correlation between the luminescence data and the device parameters open-circuit voltage and conversion efficiency which allows the use of luminescence imaging as a predictive tool for inline monitoring and quality control.

HL 61.37 Wed 15:00 Poster F

First-principles calculation of the band alignment of CuGaS2 chalcopyrite for photovoltaic purpose — Jesus Eduardo Castellanos[1,2], •Pablo Palacios[1,3], Jesus J. Arriaga[2], and Perla Wahnón[1] — [1]Instituto de Energía Solar, ETSI Telecomunicación, Universidad Politécnica de Madrid, 28040 Madrid, Spain. — [2]Instituto de Física, Benemérita Universidad Autónoma de Puebla, Av. San Claudio y 18 Sur. C.U. 72570. Puebla, México — [3]Dpt. Física Aplicada a las ingenierías Aeronáutica y Naval, ETSIAE, Universidad Politécnica de Madrid, 28040, Madrid, Spain.

The study of interfaces between two materials semiconductors, being one of them the CuGaS2 chalcopyrite, and the processes that occurs in the interfaces are necessary for a better understanding of how these proposed materials operate in the entire structure of the solar cell. In our study we considered the effect of the lattice mismatch between each pair of contact materials. We search for surface orientations which can reduce as most as possible the lattice mismatch, but strained layer have appeared. This strain has an important effect on the electronic structure, mainly in the band-gap. Alignments are calculated using the electrostatic potential as reference . Using the periodic slab model we calculated the minimum-energy structure and band offset for the three specific interfaces. Some of these interfaces have shown band alignments which are suitable for potential applications in photovoltaics and optoelectronics.

HL 61.38 Wed 15:00 Poster F

Microstructure Investigation of Lithiated Silicon — •Wenlong Zhao, Lukas Diekmeyer, Eike Epler, Burkhard Roos, Vladimir Roddatis, Cynthia A. Volkert, and Carsten Nowak — Insitute for Materials Physics, Göttingen, Germany

Because of its theoretically high gravimetric capacity, silicon receives a lot of attention as potential anode material for lithium-ion batteries. Experimentally, the expected capacity is usually not observed which is attributed to the high volume change of silicon on lithiation and the accompanying amorphization of the silicon.

In this work, we present results on the microstructure investigation of lithiated silicon. Single crystalline silicon pillars of micrometer dimension where electrochemically lithiated in an organic electrolyte. After subsequent delithiation and focused ion beam based sample preparation, the samples were characterized with high resolution transmission electron microscopy and laser assisted atom probe tomography. The observed formation of atomic scale defects on {111} and {113} planes and the formation of amorphous channels in the volume of the material are discussed.

HL 61.39 Wed 15:00 Poster F

Transport Measurements on Thermoelectric $CoSb_3$ and Partially-Filled $Yb_xCo_4Sb_{12}$ Skutterudites — •Martin Lonsky[1], Sven Heinz[1], Marcus Daniel[2], Manfred Albrecht[2,3], and Jens Müller[1] — [1]Physikalisches Institut, Goethe-Universität, Frankfurt (M), Germany — [2]Institut für Physik, TU Chemnitz, Chemnitz, Germany — [3]Institut für Physik, Universität Augsburg, Augsburg, Germany

Semiconducting $CoSb_3$ is a member of the skutterudite family of compounds and a promising candidate for thermoelectric applications. Its thermoelectric properties can be improved by filling void space in its crystal structure with foreign atoms such as Yb or La. These loosely bound atoms serve as phonon-scattering centers and thereby reduce thermal conductivity drastically.

The aim of our study is a systematic investigation of the electronic transport properties for different filling factors on thin films of thermoelectric $CoSb_3$ and partially filled $Yb_xCo_4Sb_{12}$ skutterudites. Transport parameters as resistivity $\rho(T)$, effective charge carrier density $n(T)$ and Hall mobility $\mu(T)$ have been determined in a broad temperature range from 20 to 250 K. In contrast to $CoSb_3$, which is close to compensation of hole- and electron-like carriers, $Yb_xCo_4Sb_{12}$ clearly shows an n-type semiconductor behavior. Apart from resistance and Hall-effect measurements, we applied fluctuation (noise) spectroscopy in order to gain a deeper insight into the charge carrier dynamics of the investigated materials.

HL 61.40 Wed 15:00 Poster F

In situ Raman investigation of silicene — •Dmytro Solonenko[1], Patrick Vogt[2], Ovidiu D. Gordan[1], and Dietrich R. T. Zahn[1] — [1]Halbleiterphysik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany — [2]Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin, Germany

Silicene, the silicon counterpart of graphene, possesses unique electronic and structural properties. Its inherent buckling leads to an opening of the bandgap and presence of polarized spin-states under an external electric field[1]. Moreover, its implementation into Si-based technology is considered to be less challenging than in the case of graphene. Silicene does not exist in nature and can be obtained only by synthesis on a supporting substrate. Only recently silicene could be synthesized on Ag(111) and characterized in terms of its structural and electronic properties[2]. However, some questions regarding the structural aspects and the interaction with the Ag substrate remain. Raman spectroscopy was employed to answer some of the open questions. Here, we report in situ Raman measurements of mono- and multilayer silicene obtained for a broad range of excitation wavelengths. Silicene layers were grown under UHV-conditions on a Ag (111) substrate and the formation of different silicene phases was verified by LEED. The temperature and chemical stability of silicene was tested by in situ temperature-dependent measurements and ex situ oxidation.

1. N.D. Drummond et al., Physical Review B 85, (2012).
2. P. Vogt et al., Physical Review Letters 108, (2012).

HL 61.41 Wed 15:00 Poster F

Coulomb oscillations in improved metal nanoparticle field-effect transistors — •Svenja Willing, Mirjam Volkmann, Sandra Möller, Hauke Lehmann, and Christian Klinke — Institut für Physikalische Chemie, Universität Hamburg, Grindelallee 117, 20146 Hamburg, Germany

Following the current down-scaling trend in electronic device fabrication, transistors based on nanoparticles represent a great possibility for further miniaturization. The small self-capacitance of the individual metal nanoparticles results in a Coulomb energy gap [1] that is influenced not only by the particles' size and interparticle distance but also by electrical fields. The transport through arrays of metal nanoparticles separated by tunnel barriers can thus be tuned through the application of a gate voltage in the manner of a conventional semiconductor field-effect transistor.

We synthesize monodisperse CoPt nanoparticles by colloidal chemistry [2] and deposit them onto silicon substrates as highly-ordered monolayers via the scalable Langmuir-Blodgett method. Using standard lithography steps, we implement different gate geometries and define the shape of the nanoparticle array to improve the gate-voltage influence in the resulting metal nanoparticle based transistor. Electrical transport measurements show a broad Coulomb blockade regime and Coulomb oscillations in the output and transfer characteristics respectively. We find that the oscillations can be measured at temperatures of up to approximately 100 K.

[1] Phys. Rev. B **44**, 1646 (1991) [2] Nano Lett. **10**, 964 (2010)

HL 61.42 Wed 15:00 Poster F

Study of CIS/ZnO heterojunction solar cells by electrical characterization — •Jairo Cesar Nolasco, Dorothea Scheunemann, Holger Borchert, and Jürgen Parisi — Energy and Semiconductor Research Laboratory, Department of Physics, Carl von Ossietzky University of Oldenburg, D-26111, Germany

Colloidal quantum dot (CQD) photovoltaics, using solely solution-processed semiconductor nanocrystals as light-harvesting material, have seen rapid advances in recent years. The use of highly toxic Pb and Cd compounds used in absorber films, such as PbSe and PbS might limit the possible application of CQD photovoltaics. It has been demonstrated, that one less toxic alternative is the use of CuInS2 (CIS) as absorber material. Initial studies on CIS/ZnO heterojunction solar cells indicated that their performance is limited by an interface barrier. In this contribution, by using electrical characteristics (e.g., capacitance-voltage measurements) and device modeling, the existence of such heterojunction interface barrier is investigated.

HL 62: Invited Talk Rolf Haug

Time: Thursday 9:30–10:00 Location: ER 270

Invited Talk HL 62.1 Thu 9:30 ER 270

Folded Graphene - Solid State Physics in a Nutshell — •Rolf J. Haug[1], Johannes C. Rode[1], Hennrik Schmidt[1,2], and Dmitri Smirnov[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Centre for Advanced 2D Materials and Graphene Research Centre, National University of Singapore, Singapore

The folding of a monolayer of graphene results in a stack made up from two single layers of graphene. The atomic lattices are arranged one on top of the other with a certain twist angle between the crystallographic directions of the two layers. Depending on this twist angle the electronic properties of the produced system can be quite different leading to a variety of well known effects of solid state physics. For large twist angles the two layers are actually electronically decoupled [1]. For such twist angles screening effects and variations in Fermi velocities can be observed [2]. For small twist angles much more interesting electronic structures appear. Depending on the twist angle the two atomic lattices give origin to a moiré superstructure resulting in a new electronic band structure of the system [3]. In addition the coupling between the two layers is modulated leading to even more complex electronic effects. In the talk the expected physics of such systems and some recent experimental results will be reviewed. [1] H. Schmidt et al., Appl. Phys. Lett. 93, 172108 (2008) [2] H. Schmidt, T. Lüdtke, P. Barthold, R.J. Haug, Phys. Rev. B 81 121403 (2010) [3] H. Schmidt, J. C. Rode, D. Smirnov, R.J. Haug, Nature Comm. 5, 5742 (2014)

HL 63: Group IV elements and compounds

Time: Thursday 9:30–11:30 Location: EW 015

HL 63.1 Thu 9:30 EW 015

Selective formation of nano-GeSn(Si) structures on nano-patterned-Si(001) — •V. Schlykow[1,2], N. Taoka[1], M. Zöllner[1], O. Skibitzki[1], Y. Yamamoto[1], G. Niu[1], P. Zaumseil[1], G. Capellini[1,3], and T. Schroeder[1,4] — [1]IHP, 15236 Frankfurt (Oder), Germany — [2]University Leipzig, Germany — [3]Università degli Studi Roma Tre, Italy — [4]BTU Cottbus, Germany

The GeSn(Si) alloy is one of the key materials to link electrical and optical devices. Sn introduction makes it possible to change the energy band structure, making group IV materials suitable for optical device applications. However, crystalline defects due to lattice mismatch between GeSn(Si) and Si are a crucial problem hindering the realizing of optical devices. Recently, we have established an advanced heteroepitaxy approach to achieve fully coherent, dislocation-free Ge/SiGe/Si structures formed on nano-patterned Si(NP-Si) substrates. In this study we form nano-GeSn(Si) structures at low temperature with hydrogen plasma(HP). To confirm the possibility of selective MBE growth of Ge and Sn on Si or SiO2 surface, deposition rates of Ge and Sn on Si or SiO2 surfaces were investigated. RHEED and XPS clarified that the Ge deposition rate on the Si surface in HP at 300 °C is much higher than that on the SiO2 surface. A Sn signal in XPS could not be detected after Sn deposition on the SiO2 surface in HP. These results indicate that a window for (nearly) selective MBE growth can be achieved in HP to form nano-GeSn(Si) crystals on NP-Si. Post treatments for selective deposition of the alloy are part of ongoing investigations.

HL 63.2 Thu 9:45 EW 015

Valence band offset in heterojunctions between crystalline silicon and amorphous silicon (sub)oxides — •Martin Liebhaber, Mathias Mews, Tim Schulze, Lars Korte, and Klaus Lips — HZB, Institute Silicon Photovoltaics, Kekuléstr. 5, 12489 Berlin

The heterointerface between amorphous silicon (sub)oxides (a-SiO_x:H, 0<x<2) and crystalline silicon (c-Si) is investigated.

By varying SiH_4/CO_2 precursor gas mixtures, the stoichiometry of chemical-vapor-grown a-SiO_x:H layers was controlled, starting from pure a-Si:H to near-stoichiometric a-SiO_2. *In-system* photoelectron spectroscopy was employed to measure the valence band offset ΔE_V, while the defect density D_{it}, at the a-SiO_x/c-Si interface was determined using photoconductance decay.

We measure a systematic increase of ΔE_V starting from the established value of 0.3 eV for a-Si:H/c-Si to 4.3 eV for the a-SiO_2/c-Si heterojunction. Concomitantly the electronic quality (D_{it}) of the heterointerface deteriorates. For carrier transport across the a-SiO_x:H/c-Si heterojunction ΔE_V determines the barrier height for thermionic emission and/or tunneling of holes. Therefore the application of silicon suboxides in high-efficiency heterojunction solar cells seems to be unsuitable, mainly due to electronic transport hindrance resulting from the large ΔE_V, as also predicted by modeling studies [1].

The established analysis scheme can be readily applied to other types of heterojunctions, e.g. to promising silicon/metal oxide junctions [2].

[1] A. Kanevce et al., J. Appl. Phys. 105, 094507 (2009).

[2] C. Battaglia et al., Appl. Phys. Lett. 104, 113902 (2014).

HL 63.3 Thu 10:00 EW 015

Understanding 3C-SiC/SiO_2 interfaces in SiC-nanofiber based solar cells from *ab initio* theory — •Taufik Adi Nugraha and Stefan Wippermann — Max-Planck-Institute for Iron Research, Düsseldorf, Germany

Nanostructured materials – such as e. g. hybrid nanocomposites consisting of inorganic semiconducting nanofibers and organic surfactants – provide genuinely novel pathways to exceed the Shockley-Queisser limit for solar energy conversion. The synthesis of such functionalized nanofibers can be performed completely using only inexpensive wet chemical solution processing. However, the synthesis conditions often lead to complex interfacial structures involving thin oxide layers between the nanofiber and surfactants, whose atomistic details are poorly understood at best. Here we present a combined density functional theory and tight binding investigation of interfaces between 3C-SiC nanofiber surfaces and SiO_2. Considering a wide variety of possible interfacial structures we utilize a grand canonical approach to generate a phase diagram and predict the structural details of the interface as a function of the chemical potentials of Si, O and H. This study provides directions about how the synthesis conditions lead to specific types of interfacial structures and their impact on the electronic properties of the interface. The authors wish to thank U. Gerstmann, S. Greulich-Weber and W. G. Schmidt for helpful discussions. S. W. acknowledges BMBF NanoMatFutur Grant No. 13N12972.

HL 63.4 Thu 10:15 EW 015

Band offsets at the crystalline / hydrogenated amorphous silicon interface from first-principles — •Ebrahim Hazrati, Karol Jarolimek, and Gilles A. de Wijs — Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands

The heterojunction formed between crystalline silicon (c-Si) and hydrogenated amorphous silicon (a-Si:H) is a key component of a new type of high-efficiency silicon solar cell. Since a-Si:H has a larger band gap than c-Si, band offsets are formed at the interface. A band offset at the minority carrier band will mitigate recombination and lead to an increased efficiency.

Experimental values of band offsets scatter in a broad range. However, a recent meta-analysis of the results (W. van Sark et al. (Eds.): Physics & Tech. of Amorphous-Crystalline Heterostructure, pp. 405, Springer 2012) gives a larger valence offset (0.40 eV) than the conduction offset (0.15 eV).

In light of the conflicting reports our goal is to calculate the band offsets at the c-Si/a-Si:H interface from first-principles. We have prepared several atomistic models of the interface. The crystalline part is terminated with (111) surfaces on both sides. The amorphous structure is generated by simulating an annealing process at 1100 K, with DFT molecular dynamics. Once the atomistic model is ready it can be used to calculate the electronic structure of the interface. The position of band edges in the amorphous part is obtained by fitting the calculated density of states to a square root dependence. Our preliminary

results show that the valence offset is larger than the conduction band offset.

HL 63.5 Thu 10:30 EW 015

Iron segregation at dislocations in silicon: a combined first-principles and kinetic Monte Carlo study — •Benedikt Ziebarth[1,2], Matous Mrovec[2], Christian Elsässer[2], and Peter Gumbsch[1,2] — [1]Karlsruher Institute of Technology, Karlsruhe, Germany — [2]Fraunhofer IWM, Freiburg, Germany

The efficiency of silicon based solar-cells is strongly affected by internal defects and impurities. Metallic impurities, in particular interstitial iron, result in a large loss of electric power production as they act as recombination centers for photo-induced charge carriers. It is known that metallic impurities like iron atoms are influenced by stress fields inside the silicon crystal. Here, we present a systematic study on how iron impurities are influenced by stress fields of dislocations in silicon using first-principles methods based on density functional theory. In a first step, the formation energies of iron impurities in bulk silicon has been investigated for hydrostatic, uniaxial and shear strain. Surprisingly, the most stable configuration of interstitial iron – the tetrahedral site – seems to be unaffected by any deformation of the crystal. Other configurations, however, are affected by deformations which results in a different diffusivity of Fe. The first-principles results from the formation energies are carried over to a kinetic Monte Carlo simulation in order to understand the effect on diffusion by a stress field induced by a screw dislocation or a 60° mixed dislocation. The kinetic Monte Carlo simulations reveal an effective segregation of iron atoms to the compressive-strain region of the mixed dislocation.

HL 63.6 Thu 10:45 EW 015

Structural and electrical properties of sulfur doped Si by ion implantation — •Fang Liu[1,2], Slawomir Prucnal[1], Kun Gao[1,2], Muhammad Khalid[1], Wolfgang Skorupa[1], Manfred Helm[1,2], and Shengqiang Zhou[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany

Hydoping Si with chalcogens is one of the effective approaches to form an intermediate band (IB). This IB material is a candidate of infrared photodetectors and intermediate band solar cells. However, the chalcogens have relatively low solid solubility limit in Si. We prepared sulfur doped silicon to above the Mott insulator concentration by ion implantation followed by pulsed laser annealing. The degree of crystalline lattice recovery in implanted layers and the lattice location of sulfur in Si were analyzed by Rutherford backscattering spectrometry / Channeling. Our results show that S atoms are occupying substitutional lattice sites in Si. We also observe an insulator-to-metal transition in silicon hyperdoped with sulfur to concentrations well above the maximum solubility limit of about 3*1016 cm-3. Analyzing temperature-dependent conductivity data, we find that a transition from insulating to metallic conduction occurs at a peak sulfur concentration of around 1*1021 cm-3.

HL 63.7 Thu 11:00 EW 015

Observation of Nitrogen Vacancy Center Fluorescence from Levitated Diamonds — •Alexander Kuhlicke, Andreas W. Schell, Joachim Zoll, Heather Partner, and Oliver Benson — Humboldt-Universität zu Berlin, Institut für Physik, AG Nanooptik, Newtonstraße 15, 12489 Berlin

Nitrogen vacancy (NV) defect centers in diamonds show remarkable optical properties and have emerged as perfect candidates for several different applications. Stabilization of diamond crystals in free space allows for particle isolation and is an important step towards optomechanical experiments on diamond nanoparticles. We report trapping of submicron diamonds in a linear quadrupole ion trap [1]. We discuss particle stability and the influence of surface charges, which are required for the electrodynamic confinement. The NV fluorescence of individual levitated clusters with diameters from micro- down to a few hundred nanometers can be observed. Optically characterized particles can be stored in the trap or deposited on photonic structures like fiber facets. Subsequently, an atomic force microscope can be used for precise size measurements.

[1] A. Kuhlicke et al., Nitrogen vacancy center fluorescence from a submicron diamond cluster levitated in a linear quadrupole ion trap, Appl. Phys. Lett. 105, 073101 (2014)

HL 63.8 Thu 11:15 EW 015

A low-loss, broadband antenna for effcient photon collection from a coherent spin in diamond — •Daniel Riedel, Dominik Rohner, Marc Ganzhorn, Timo Kaldewey, Patrick Appel, Elke Neu, Richard J. Warburton, and Patrick Maletinsky — Departement of Physics University of Basel, Basel, Switzerland

Light extraction from emitters in high-index, solid-state hosts is intrinsically difficult, but key to performance of applications in quantum-sensing, -metrology or -computing. We present a novel solution to this problem in form of a broadband, metal-free, low-loss optical antenna giving highly directed output for such emitters [1].

We engineer our device around individual nitrogen vacancy (NV) electronic spins in thin ($< 1\ \mu$m), single-crystalline diamond membranes. We demonstrate the functionality of our antenna by measuring the emission patterns for different diamond layer thicknesses. Our findings show excellent agreement with an analytical theory and confirm that the NV emission is channeled preferentially into a medium-angle cone (NA < 0.75) in one direction. For broadband (640-750 nm), single NV fluorescence we report photon count rates approaching one MHz. Importantly, our photonic structure preserves the high spin coherence of NVs in single-crystalline diamond ($T_2 > 100\ \mu$s).

Our results pave the way for near-unity photon collection efficiencies and unprecedented detection rates for not only NV centers, but a broad class of quantum emitters in high-index, solid-state systems.

[1] D. Riedel et al., accepted at Physical Review Applied

HL 64: Focus Session: Optical interconnects - Materials, devices, and integration

Optical interconnects across optical fiber are rapidly replacing metal-based interconnects at short reach (up to 300 m) to medium reach (up to 2 km) distances in data centers, supercomputers, and at across a few meters in homes, aircraft, and automobiles. The concepts of Ubiquitous Connectivity, Big Data, and Natural/Organic User Interfaces all depend on advances in materials, devices, and integrated systems concepts for applications in optical interconnects whether across optical fiber, photonic waveguides, or free-space. Furthermore, a true paradigm shift in systems designs based on the use of optical interconnects at very short reach ($<$ 2m) and ultrashort reach ($<$ 2 mm) distances is underway as there are potentially huge advantages in energy efficiency, bandwidth density, purchase and operating cost, and performance. Presentations are solicited on all aspects of basic and applied research on materials, optoelectronic and photonic devices, and integrated systems for the realization of the next several generations of optical interconnects.

Organizer: James A. Lott (TU Berlin)

Time: Thursday 9:30–12:45 Location: EW 202

Invited Talk HL 64.1 Thu 9:30 EW 202

Energy efficient optical interconnects for datacom and HPCs — •Dieter Bimberg — Center of NanoPhotonics, TU Berlin

Vertical-cavity surface-emitting lasers (VCSELs) are emerging to be the decisive cost-effective, energy-efficient, and reliable light sources for short-reach (up to ˜1000 m) optical interconnects in data centers

and supercomputers. To viably replace copper interconnects and to advance to on-chip integrated photonics, VCSELs ideally should be able to operate at high energy efficiency, at large bit rates, and without cooling at up to 85 °C with immunity to temperature variations, which seem to be contradictions. We demonstrate that VCSELs with narrow 3-5 *m oxide apertures and ~ 15 nm shift between gain peak and maximum mirror transmission can achieve temperature-stable, energy-efficient and high-speed operation coincidently. Detailed theoretical and systematic experimental temperature- and oxide aperture-diameter-dependent characterization including static characteristics, small-signal analysis, and data transmission experiments are presented, for a variety of wavelengths. With contributions by: Connie Boldt, Günther Larisch, Hui Li, James Lott, Philip Moser, Philip Wolf, Maya Volwasen

Invited Talk HL 64.2 Thu 10:00 EW 202

Plasmonic and Metallic Cavity Semiconductor Nanolasers for Ultimate Miniaturization — •C.Z. Ning — Arizona State University, Tempe AZ, USA — Tsinghua University, Beijing, China

Miniaturization has been an eternal theme for electronics and photonics since the dawn of the semiconductor era. Size reduction of photonic devices has been driven both by the rich physics and by promising applications in future integrated nanophotonic systems. Micro cavity lasers have been topics of great interests for several decades due to their interesting photonic and quantum optical properties and their potential applications. However, further size reduction of such dielectric/semiconductor-cavity laser becomes exceedingly challenging when the wavelength becomes the eventual roadblock.

In this talk, we will present a summary overview of efforts in the last few years in developing metallic cavity or plasmonic nanolasers. Recent progress in theoretical and experimental studies will be presented, including the demonstration of the first nanolaser with a below-diffraction limit size, our recent efforts in raising the operating temperature of such nanolasers, and the eventual realization of the first room temperature subwavelength size nanolasers. Through the presentation, special emphasis will be placed on the unique features of such nanolasers that distinguish them from the conventional semiconductor lasers. We will also discuss some of attracting features that are yet to be realized experimentally. Finally, we will discuss new designs and current research towards further miniaturization and performance improvement.

Invited Talk HL 64.3 Thu 10:30 EW 202

Polymer waveguides for electro-optical integration in data centers — •Roger Dangel, Jens Hofrichter, Folkert Horst, Daniel Jubin, Antonio La Porta, Norbert Meier, Jonas Weiss, and Bert Jan Offrein — IBM Research - Zurich, Säumerstrasse 4, 8803 Rüschlikon, Switzerland

Tba

Coffee break

Invited Talk HL 64.4 Thu 11:15 EW 202

Silicon Photonics for Optical Interconnects — •Roel Baets — Ghent University - imec, Photonics Research Group, Ghent, Belgium

Silicon photonics is maturing very rapidly into an industrial technology platform for high datarate transceivers for optical data- and telecommunication. Nevertheless there is a rich landscape of exploratory research in this field in which new material combinations are being developed with a view of performance improvements (bandwidth, power dissiption, footprint, cost,...). Furthermore silicon photonics is also gearing towards other applications and markets, even if this means that the conventional telecom bands have to be left. In this talk some recent examples of these developments will be discussed.

Invited Talk HL 64.5 Thu 11:45 EW 202

Long wavelength VCSELs for optical interconnects — •Markus Amann — Walter Schottky Institut, TU München, 85748 Garching, Am Coulombwall 4

Wird nachgereicht

HL 64.6 Thu 12:15 EW 202

Temperature-dependent modulation and impedance characteristics of 980 nm VCSELs — •Hui Li[1], Philip Wolf[1], Philip Moser[1], Gunter Larisch[1], James A. Lott[1], and Dieter Bimberg[1,2] — [1]Institut für Festkörperphysik und Zentrum für Nanophotonik, Technische Universität Berlin, Hardenbergstraße 36, D-10623, Berlin, Federal Republic of Germany — [2]King Abdulaziz University, Jeddah, Kingdom of Saudi Arabia

Multimode optical fibre interconnects based on vertical-cavity surface-emitting lasers (VCSELs) are a key enabling technology for short-reach data communication. Considering cost, long-term system sustainability, and reliability, optical interconnects must operate without extra cooling, implying the VCSELs must operate at much elevated temperatures. By introducing a -15 nm QW gain-to-cavity etalon wavelength offset, the temperature-stability, the maximum bit rate at high temperature, and the energy efficiency of our VCSELs are simultaneously improved. We present temperature stable 980 nm VCSELs capable of operating error-free at 38 Gb/s at 25 up to 85 °C without any change of working point and modulation conditions. A small-signal equivalent circuit model is fitted to measured scattering parameters to extract the circuit elements, -3 dB modulation bandwidth, D-factor, and parasitic cutoff frequency. Showing large values of -3 dB modulation bandwidth and D-factor both at room temperature and elevated temperatures, our VCSELs achieve high-speed, temperature-stable and energy-efficiency operation simultaneously, which makes these VCSELs well suited for very-short-reach and ultra-short-reach optical interconnects.

HL 64.7 Thu 12:30 EW 202

Characterisation of Hybrid VCSEL and DFB Organic Microlasers — •Tim Wagner, Markas Sudzius, Andreas Mischok, Hartmut Fröb, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr Str. 1, 01069 Dresden

Microlasers based on organic small molecules have shown great potential as coherent light sources [1,2]. Two important types of resonators being under investigation are the vertical-cavity surface-emitting laser (VCSEL) and the distributed-feedback laser (DFB). The gain medium in all structures produced is a blend of the red laser dye DCM doped by 2 wt% into the host material Alq_3. Although based on entirely different concepts, the two resonators exhibit comparable lasing thresholds and confinement factors.

In this work, we design a hybrid device combining both resonators in one compound structure, where second-order Bragg diffraction couples vertical modes of the VCSEL and lateral modes of the DFB. Using optical spectroscopy techniques, we analyse the emission properties and lasing characteristics to control the balance between the different mechanisms on positive optical feedback inside the composite system. Based on the results obtained, a novel structure is simulated and designed to optimise the performance of the hybridised microlaser device.

[1] I. Samuel and G. Turnbull *Chemical Reviews* **107**, 1272 (2007)
[2] A. Mischok et al. *Advanced Optical Materials* **2**, 802 (2014)

HL 65: Focus Session (DS with HL): Oxide semiconductors I

Time: Thursday 9:30–12:45 Location: H 2032

Invited Talk HL 65.1 Thu 9:30 H 2032

Growth, properties and devices of gallium-oxide-based wide-gap semiconductors — •Shizuo Fujuta — Kyoto University, Kyoto, Japan

Recently, high-power devices with orthorhombic α-Ga_2O_3 have attracted increasing interest supported by solution-grown highly-crystalline substrates. However, orthorhombic crystals are rare in semiconductor family, hence there hardly are other semiconductors of the same crystal structure for alloys or multilayer structures with α-Ga_2O_3. On the other hand we have developed the growth of corundum-structured α-Al_2O_3, α-Ga_2O_3, α-In_2O_3 and their alloys achieving the band gap engineering from 3.8 to 8.8 eV, overcoming metastable phases of α-Ga_2O_3 and α-In_2O_3. For the growth we can apply a low-cost and environmental-friendly mist CVD method, which allowed highly-crystalline films as evidenced by FWHM of ω-scan XRD curves as small as <50 arcsec for α-Ga_2O_3 and <500 arcsec for others. The author will report crystal qualities, electrical properties, doping and preliminary device performances with MOS structures at the conference. In addition, alloying with transition-metal oxides such as α-Fe_2O_3 or α-Cr_2O_3 achieves addition of magnetic properties to semiconductors, as evidenced by magnetization hysteresis at >300K. This can also develop new multifunctional materials and devices with function engineering.

HL 65.2 Thu 10:00 H 2032

Growth-Kinetics Study and Doping the Group-III Sesquioxide β-Ga2O3 — •Patrick Vogt and Oliver Bierwagen — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5 - 7, 10117 Berlin, Germany

In the present talk, a comprehensive study of the growth-kinetics of β-Ga2O3 (-201) on Al2O3 (0001) is given. The growth was performed by plasma-assisted molecular beam epitaxy. Under ultra-high vacuum conditions atomic gallium and oxygen plasma were reacting amongst others to form β-Ga2O3. Besides the growth-kinetics studies for undoped Ga2O3 we also doped this material with tin. Under different growth conditions we investigated the carrier concentration depending on different growth parameters like growth temperature (Tgrowth) and metal fluxes, Ga and Sn flux, respectively.

This study shows the variation of the growth-rate depending on various growth-parameter such as the gallium beam equivalent pressure, Tgrowth and the oxygen flux. It turned out, that in the gallium-rich regime the formation of the volatile suboxide Ga2O reduce the growth-rate of β-Ga2O3 and result in an etching of the film when no oxygen is supplied. In order to investigate the carrier concentration of the Ga2O3 : Sn transport measurements were performed.

HL 65.3 Thu 10:15 H 2032

Au-Schottky contact on In2O3 single crystals — •Maryam Nazarzadehmoafi[1], Christoph Janowitz[1], Mattia Mulazzi[1], Stephan Machulik[1], Zbigniew Galazka[2], and Recardo Manzke[1] — [1]Institut für Physik, Humboldt Universität zu Berlin, Newtonstraße 15, 12489 Berlin, Germany — [2]Leibniz Institut für Kristallzüchtung, Max Born Str. 2, 12489 Berlin, Germany

Au contacts on melt-grown-In2O3 (111) single crystals were studied using angle-resolved photoemission spectroscopy to monitor the band bending by core level and valence band spectra, with correction for the photovoltage effect. The measurement was performed through stepwise Au evaporation onto the (111) surface of In2O3 at room temperature (RT) as well as low temperature (LT). A small Schottky barrier on RT-samples and a larger one on LT-samples were observed. The comparison of the experimental barrier height with the predicted one from the Schottky-Mott rule shows a discrepancy. It implies that the complexity of the atomic structure of the present metal-semiconductor interface is beyond the applicability of the Schottky-Mott rule. The results indicate that an explicit reference to the surface electron accumulation layer is not necessary when discussing the Schottky character of the Au/In2O3 contact. In addition, the results reveal the epitaxial growth of Au on In2O3 and also the chemical reaction and formation of an Au-In alloy at RT.

HL 65.4 Thu 10:30 H 2032

Schottky contacts and pn-heterojunctions on heteroepitaxial In_2O_3 thin films grown by pulsed laser deposition — •Daniel Splith, Florian Schmidt, Steffen Lanzinger, Stefan Müller, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Leipzig, Germany

Oxide semiconductors like In_2O_3 are promising materials for a new generation of transparent electronic devices. While the properties of highly tin-doped In_2O_3 (ITO) for use as a transparent conductive oxide (TCO) are well investigated, interest in the semiconducting properties of In_2O_3 for the investigation of material properties and application in devices arose recently. In order to create devices like diodes or field-effect transistors, the creation of a space charge region is required, which can be done either by a Schottky contact (SC) or a pn-junction.

In this contribution we discuss the fabrication of rectifying contacts based on SCs [1] and pn-heterojunctions with an amorphous p-type oxide like NiO or $ZnCo_2O_4$ [2]. To optimize the performance of the rectifying contacts different approaches were used: By introducing a Mg-doped In_2O_3 layer, the reverse current was decreased by several orders of magnitude since Mg acts as an acceptor in In_2O_3 and therefore increases the width of the space charge region. Also, a tin doped back contact layer was employed in order to decrease the series resistance of the contacts. Further, different substrates were used to investigate the influence of the crystal quality on the rectifying properties.

[1] H. von Wenckstern *et al.*, APL Mat. 2, 046104 (2014)
[2] F.-L. Schein *et al.*, Appl. Phys. Lett. 104, 022104 (2014)

HL 65.5 Thu 10:45 H 2032

Temperature-dependent thermal conductivity in Mg-doped and undoped β-Ga_2O_3 bulk-crystals — •Martin Handwerg[1,2], Rüdiger Mitdank[1], Zbigniew Galazka[3], and and Saskia F. Fischer[1] — [1]AG Neue Materialien, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH,Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [3]Leibniz Institute for Crystal Growth, Max-Born-Strasse 2, 12489 Berlin, Germany

Transparent semiconducting insulators like Ga_2O_3 are important materials for high power electronics and optoelectronics. For β-Ga_2O_3 only little information exist concerning the thermal properties, especially the thermal conductivity λ. Here, the thermal conductivity is measured by applying the electrical 3ω-method on Czochralski-grown β-Ga_2O_3 bulk crystals, which have a thickness of 200 μm and 800 μm. At room temperature the thermal conductivity along the [100]-direction in Mg-doped electrical insulating and undoped semiconducting β-Ga_2O_3 is confirmed as 13 ± 1 $Wm^{-1}K^{-1}$ for both crystals [1]. The phonon contribution of λ dominates over the electron contribution below room temperature. The observed function $\lambda(T)$ is in accord with phonon-phonon-Umklapp scattering and the Debye-model for the specific heat at $T \gtrsim 90$ K which is about 0.1 fold of the Debye-temperature θ_D. Here a detailed discussion of the phonon-phonon-Umklapp scattering for $T < \theta_D$ is carried out. The influence of point defect scattering is considered for $T < 100$ K.

[1] Martin Handwerg et al. , 2014, SST, accepted (arXiv 1407 4272)

30 min. break.

Invited Talk HL 65.6 Thu 11:30 H 2032

$BaSnO_3$; The next generation of transparent conducting oxide? — •David Scanlon — Department of Chemistry, University College London, UK — Diamond Light Source Ltd., Harwell, UK.

La-doped cubic perovskite $BaSnO_3$ has been reported to possess electron mobilities as high as 320 $cm^2\,V^{-1}\,s^{-1}$ for carrier concentrations of $8 \times 10^{19}\,cm^{-3}$, comparable to the very best transparent conducting oxides (TCOs). In this presentation we will examine the electronic structure and defect chemistry of $BaSnO_3$, and use this information to explain why La-doped $BaSnO_3$ possesses all the qualities needed to be the next generation $n-$type TCO.

HL 65.7 Thu 12:00 H 2032

Nitrogen doping in tin dioxide thin film grown by chemical vapor deposition — •Jie Jiang, Yinmei Lu, Benedikt Kramm, and Bruno K Meyer — I. Physics Institute, Justus-Liebig-University Giessen, Giessen, Germany

As a direct band gap semiconductor, tin dioxide (SnO2) is a promising

candidate for next generation ultraviolet light emitting diodes (LEDs) and photo detectors, due to its large band gap of 3.6 eV, and high carrier mobility of about 250 cm2/Vs at room temperature. An essential step to fabricate SnO2-based optoelectronic devices is to obtain high quality p-type SnO2 films. Nitrogen could be an excellent p-type dopant in SnO2 owing to its suitable electronegativity and ion size, high solubility limit, and non-toxicity. At the same time, only a few experimental investigations were performed on N-doped SnO2. For this reason, we deposit the N-doped SnO2 thin films on c-sapphire substrates via chemical vapor deposition (CVD), using SnI2 powder and O2 and NH3 gas as source materials. Both undoped and N-doped samples are annealed at different temperature for a short time using a rapid thermal processing. The crystal structure, electrical properties and optical properties of the films were measured and investigated by X-ray diffraction (XRD), Hall effect measurements, optical transmittance, secondary ion mass spectrometry (SIMS) and X-ray photoelectron spectroscopy (XPS), respectively. The effect of short-time annealing on structural, optical and electrical properties is also analyzed.

HL 65.8 Thu 12:15 H 2032

Dopant clustering in p-type transparent semiconducting Cr_2O_3:Mg — •Karsten Fleischer, David Caffrey, Leo Farrell, Emma Norton, Daragh Mullarkey, Elisabetta Arca, and Igor V. Shvets — School of physics and Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin, Dublin 2, Ireland

We present an analysis of the Raman spectra of p-type transparent conducting Cr_2O_3:Mg grown by various techniques including spray pyrolysis (SP), pulsed laser deposition (PLD), molecular beam epitaxy (MBE) and reactive magnetron sputtering (RMS). The best performing films show a distinct broad range Raman signature related to defect-induced vibrational modes not seen in stoichiometric, undoped material. Our comparative study demonstrates that Raman spectroscopy can quantify unwanted dopant clustering in the material at high Mg concentrations, while also being sensitive to the Mg incorporation site. By correlating the Raman signature to the electrical properties of the films, growth processes can be optimised to give the best conducting films and the local defect structure for effective p-type doping can be studied.

HL 65.9 Thu 12:30 H 2032

Annealing effects on electrical properties of room-temperature deposited zinc oxynitride thin films — •Anna Reinhardt, Heiko Frenzel, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Semiconductor Physics Group

Amorphous oxide semiconductors have attracted much attention as channel material for thin-film transistors (TFT) due to their comparatively large electron mobility ($>$ 10 cm^2/Vs) achieved already by low-temperature fabrication. In order to further increase channel mobilities while maintaining the stability of oxide-based TFTs the alloying of ZnO by nitrogen was suggested [1].

We have investigated the electrical properties of semiconducting zinc oxynitride (ZnO_xN_y) thin films depending on annealing temperature and doping. Therefore we conducted annealing experiments in air and N_2 atmosphere up to 400°C. The ZnO_xN_y thin films were deposited on glass substrates by reactive radio-frequency magnetron sputtering of a metallic zinc target at room-temperature. Electrical properties were examined using the four-probe van der Pauw technique. The as-deposited films show n-type semiconducting behaviour with carrier concentrations of $1 \times 10^{17} - 3 \times 10^{18}$cm^{-3} and Hall mobilities ranging from 10 to 20 cm^2/Vs. With increasing annealing temperature the resistivity decreases whereas the mobility increases. In addition, possible structural changes due to annealing were analyzed using x-ray diffraction.

[1] Y. Ye *et al.*, J. Appl. Phys., 106, 074512 (2009)

HL 66: Focus Session (CPP with HL): Hybrid photovoltaics and perovskites I

Time: Thursday 9:30–13:00 Location: C 130

Invited Talk HL 66.1 Thu 9:30 C 130

Advances in hybrid solar cells: From hybrid organic/inorganic to perovskite photovoltaics — •Lukas Schmidt-Mende — University of Konstanz

In this presentation we will discuss the path from solid-state dye sensitized solar cells over extremely thin absorber cells towards perovskite solar cells. Hybrid solar cells have been investigated for some time and a lot of knowledge gained in this field has helped to increase the power conversion efficiencies of recently discovered perovskite solar cells from 2.2% when first reported in 2006 to over 20% in 2014. Going from liquid electrolyte cells to solid-state hybrid solar cell architecture had a major influence on this performance step. Many structures previously used in hybrid solar cells have been now implemented very successfully in perovskite solar cells. We will give some examples of such knowledge transfer from conventional hybrid solar cells to perovskite solar cells. A discussion of the similarities as well as the differences of the described solar cell types will help to understand possible limitations.

HL 66.2 Thu 10:00 C 130

Electron tomography of interpenetrating polymer:nanocrystal networks as photoactive layers in hybrid solar cells: correlations between the morphology and device performance — •Holger Borchert, Christopher Krause, Dorothea Scheunemann, and Jürgen Parisi — Carl von Ossietzky University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, 26111 Oldenburg, Germany

Hybrid bulk heterojunction solar cells use as absorber layer an interpenetrating network of conductive polymer and inorganic semiconductor nanocrystals. Thereby, the nanomorphology of the blend layers plays an important role for the functionality of the devices. On the one hand, the absorber layer should have a large interface between both material components in order to enable efficient separation of electron-hole pairs. On the other hand, continuous pathways for electrons through the nanoparticle phase and holes through the polymer phase are required in order to enable efficient transport of the charge carriers towards the electrodes. A unique technique to investigate the three-dimensional morphology of such hybrid material layers is electron tomography, where three-dimensional images are reconstructed from a series of transmission electron micrographs recorded under different angles. In the present contribution, we investigated active layers consisting of poly(3-hexylthiophene) and colloidally prepared copper indium disulfide nanocrystals. Correlations between the morphology of the blend layers and the electrical performance of hybrid solar cells are analyzed in dependence of varied preparation parameters.

HL 66.3 Thu 10:15 C 130

Laser-ablated titania nanoparticles for aqueous processed hybrid solar cells — •Volker Körstgens[1], Stephan Pröller[2], Christoph Mayr[1], Gonzalo Santoro[3], Stephan V. Roth[3], Hristo Iglev[4], Reinhard Kienberger[4], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85848 Garching — [2]TU München, Munich School of Engineering, James-Franck-Str. 1, 85748 Garching — [3]DESY Photon Science, Notkestr. 85, 22607 Hamburg — [4]TU München, Physik-Department, LS Laser- und Röntgenphysik, James-Franck-Str. 1, 85748 Garching

Hybrid solar cells are produced by applying a new water-based processing method. The active layer consists of titanium dioxide nanoparticles produced by laser ablation in liquid and the water-soluble hole-conducting polymer poly[3-(potassium-6-hexanoate)thiophene-2,5-diyl] (P3P6T). The production of TiO_2 nanoparticles via laser ablation in liquid is tested with two approaches, using TiO_2 powder as target and a solid titanium target. The crystallinity of both components of the active layer, laser-ablated TiO_2 and P3P6T is investigated with X-ray diffraction (XRD) and grazing incidence wide angle X-ray scattering (GIWAXS). A key factor for the performance of the active layer is the functionalization of TiO_2 with the polymer P3P6T, which is probed with spectroscopic methods. The hybrid solar cells show high fill factors and open circuit voltages underlining the potential of the novel material and the environment-friendly processing method.

HL 66.4 Thu 10:30 C 130

Junction formation and current transport mechanisms in hybrid n-Si/PEDOT:PSS solar cells — •Sara Jäckle[1], Matthias Mattiza[2], Manuela Göbelt[1], and Silke Christiansen[1,2] — [1]Max-Planck-Institute for the Science of Light, Erlangen, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Hybrid photovoltaics combining a transparent highly conductive polymer and an absorbing inorganic semiconductor promise efficient charge carrier separation and transport. We present solar cells with the 'metal'-like wide-gap polymer PEDOT:PSS and n-doped silicon archiving an open-circuit voltages up to 640mV and a power conversion efficiencies of 12%. The hybrid charge separating interface is commonly treated as a majority carrier dominated Schottky junction. Capacity- and current-voltage characteristics proof by investigating n-Si/PEDOT:PSS solar cells with varying silicon substrate doping concentrations that an inversion layer is created on the silicon surface and the charge transport is dominated by minority carriers. We will present a hybrid junction schematic explaining the promising solar cell characteristics. Furthermore possible degradation mechanisms of these hybrid solar cells under ambient conditions and the effect of encapsulation with low temperature deposited metal oxides will be discussed.

HL 66.5 Thu 10:45 C 130

A Comparative Study of Polythiophene/c-Si Hybrid Solar Cells and Inorganic a-Si:H/c-Si Devices — •M. Zellmeier[1], T. Brenner[2], S. Janietz[3], N. H. Nickel[1], and J. Rappich[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium Photovoltaik, Kekulèstr. 5, 12489 Berlin — [2]University of Potsdam, Institute of Physics & Astronomy, Karl-Liebknecht-Straße 24-25, 14476 Potsdam-Golm — [3]Fraunhofer-Institut für Angewandte Polymerforschung (IAP), Abteilung Polymere und Elektronik, Geiselbergstr. 9, 14476 Potsdam

Non-excitonic polymer/silicon heterojunction solar cells regularly exceed power conversion efficiencies (PCE) of 10%. In combination with the possibility to use solution processing to form an electron-hole separating junction, this device type becomes highly attractive due to its potential for low cost processing. Here, we present a study in which P3HT/c-Si hybrid devices are compared to a-Si:H/c-Si heterojunctions. The advantages of the narrow absorption band of P3HT are pointed out using quantum efficiency measurements. Furthermore, the influence of the intrinsic interlayer (SiOx, Methylgroups) in the final device is investigated and directly compared to equivalent structures (SiOx, intrinsic a-Si:H) in the inorganic devices. The wafer lifetime with and without polymer was examined using quasi steady state photoconductance measurements (QSSPC) and interpreted regarding their influence on the open circuit voltage. The obtained results were used to improve the hybrid devices, leading to a high-performance hybrid solar cell with an open circuit voltage of 659 mV and a PCE of 11%.

HL 66.6 Thu 11:00 C 130

High efficiency hybrid triple junction solar cells comprising of amorphous silicon and low band gap polymers exceeding 11 % Power Conversion Efficiency. — •Steffen Roland[1], Sebastian Neubert[2], Steve Albrecht[1], Bernd Stannowski[2], Mark Seger[3], Antonio Facchetti[3], Rutger Schlatmann[2], Bernd Rech[2], and Dieter Neher[1] — [1]University of Potsdam, Institute of Physics and Astronomie, Potsdam, Germany — [2]PVcomB/Helmholtz-Zentrum Berlin für Materialien und Energie GmBh, Berlin, Germany — [3]Polyera Corporation, Illinois, USA

Merging inorganic and organic solar cells in a series connected hybrid multi-junction is shown to be an elegant approach to prepare efficient solar cells with a total active layer thickness well below 1 μm. Complementary absorption, high absorption coefficients, and the ease of fabrication make organic low band-gap (LBG) materials, mixed with $PC_{61}BM$, suitable for the use in multi-junction solar cells in combination with amorphous silicon (a-Si:H). Transfer matrix based optical modeling was employed to predict the optimum layer thicknesses of each. External quantum efficiency measurements show that all planar hybrid multi-junctions are current limited by the a-Si:H middle junction. Light scattering front contacts are used to increase the absorption and thereby currents in the amorphous silicon sub-cells. The presented multi-junction solar cells are highly efficient, showing high open circuit voltages and high fill factors up to 80 %. Therefore, merging inorganic/organic sub-cells in multi-junction devices bears great potential as efficient, truly thin film solar cells.

15 min. break.

Invited Talk HL 66.7 Thu 11:30 C 130

The solid state physics of hybrid perovskites — •Jarvist Moore Frost[1], Federico Brivio[1], Keith Butler[1], Aurelien Leguy[2], Artem Bakulin[3], Piers Barnes[2], and Aron Walsh[1] — [1]University of Bath, Bath, United Kingdom — [2]Imperial College London, London, United Kingdom — [3]Cambridge University, United Kingdom

Hybrid perovskites offer rich solid state physics. Here we apply electronic structure techniques to develop an understanding of their intrinsically dynamic behaviour. We study the rich kinetics of the rotation of the organic cation by applying careful analysis to ab-initio molecular dynamics simulations [1]. Informed by observations of the dynamics, a on-lattice model model is developed to access far longer length and timescales of the dynamic system. Parameterisation of the Hamiltonian is from electronic structure calculations. This model shows columnar anti-ferroelectric and ferroelectric ground states, as a function of strain and lattice distortion energetics. The transition from short range to long range order as a function of temperature is analysed by defining & measuring correlation functions. The electrostatic potential is reconstructed from dipole orientation. A model for polaronic transport and recombination in the material is developed, where the low electron recombination rates in these materials is related to the columnar structure of the electrostatic potential leading to electron and hole segregation.

1. J.M. Frost, K. Butler, A. Walsh, APL Materials 2 (8), 081506 (2014).

HL 66.8 Thu 12:00 C 130

Quantum-Chemical Calculations of Hybrid Perovskites — •Wichard J. D. Beenken, Ksenia Korschunova, Mezhoura Oussadou, Lars Winterfeld, and Erich Runge — Institut für Physik und Institut für Mikro- und Nanotechnologie, Technische Universität Ilmenau, Germany

Hybrid perovskites possess a multitude of structural phases depending on temperature and the organic cations. Thus a deeper understanding of the various crystal structures and their influence on the electronic bandstructure is necessary to control the quality of these materials for solar cells. Though there exist already several structure analyses of perovskites by X-ray diffraction, the severe problem remains that the contrast of organic light atoms (C, N, H) and inorganic heavy atoms (Pb, I) is several magnitudes. This makes it difficult to determine the exact positions of the organic cations within the perovskite lattice spanned by a network of octahedral Lead-Iodid anions. Consequently, most of the published structures for hybrid perovskites do only provide guesses for the organic part, in particular for the H-atoms. Their positions, however, may be important for understanding the electronic band structure, which is also difficult to be determined experimentally, e.g. by angle resolved UPS, for the polycrystallinity of the samples. Therefore, we have done DFT calculations using the quantum-chemical package VASP 5.3for crystal structure optimization and band structure determination of low-temperature and metastable phases of several organic-inorganic hybrid perovskites.

HL 66.9 Thu 12:15 C 130

Radiative efficiency of perovskite solar cells — •Kristofer Tvingstedt[1], Olga Malinkiewicz[2], Andreas Baumann[3], Carsten Deibel[1], Henry J. Snaith[4], Vladimir Dyakonov[1,3], and Henk J. Bolink[2] — [1]Experimental Physics VI, Julius-Maximillian University of Würzburg, 97074 Würzburg, Germany — [2]Instituto de Ciencia Molecular, Universidad de Valencia, 46980 Paterna, Valencia, Spain — [3]Bavarian Center for Applied Energy Research, 97074 Würzburg, Germany — [4]University of Oxford, Clarendon Laboratory, Parks Road Oxford, OX1 3PU, United Kingdom

Perovskite PVs have reached significant power conversion efficiency in a very short time period. Apart from providing a rather high photocurrent, they also retain a comparatively high open circuit voltage. We here address the upper limit to open circuit voltage and power conversion efficiency for the novel type of photovoltaic cells based on methylammonium lead iodide perovskites. By accurate determination of the present solar cells radiative efficiency, that is their ability to emit light, we conclude how far these solar cells are from their own thermodynamic limit. We explain the reason for the high voltage and put it in relation to those of earlier generation photovoltaic technologies. We further highlight that, as the perovskite steady state photoluminescence is rather strong at open circuit conditions, and substantially

quenched only at short circuit, they perform just as good solar cells should do, and in this respect also rather different from most OPVs or DSSC cells studied so far.

HL 66.10 Thu 12:30 C 130

Recombination behaviour of hybrid perovskite thin films studied by low temperature photoluminescence — Sergej Levcenco, Amrita Mandal Bera, Dan Wargulski, Ibrahim Simsek, and •Thomas Unold — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner Platz 1, 14109 Berlin

Hybrid organometal perovskites recently have been successfully implemented as absorber layers in high efficiency thin film solar cells. In particular the CH3NH3PbI3 based materials show long minority carrier recombination lifetimes, implying a minor role of non-radiative recombination even at room temperature. In order to better understand the radiative recombination properties we have studied hybrid perovskite layers on glass, which where pepared by immersion of polycrystalline PbI2- thin films into methylammoniumiodide dissolved in isopropanol. The perovskite layers show high luminescence efficiencies at room temperature with a broad peak centered at around 1.6eV. At low temperature, several additional transitions are observed, which shift with temperature and show significant thermal quenching. Changes in the radiative emission caused by degradation of the layers under ambient conditions will also be reported.

HL 66.11 Thu 12:45 C 130

Transient electrical studies probing charge carrier recombination in methylammonium lead iodide perovskite solar cells — •Andreas Baumann[1], Stefan Väth[2], Kristofer Tvinstedt[2], Michael C. Heiber[2], Cristina Momblona[3], Henk J. Bolink[3], and Vladimir Dyakonov[1,2] — [1]Bayerisches Zentrum für Angewandte Energieforschung, Am Galgenberg 87, D-97074 Würzburg — [2]Experimentelle Physik 6, Julius-Maximilians-Universität Würzburg, Am Hubland, D-97074 Würzburg — [3]Universidad de Valencia, Paterna, Spain

Organo-metal halide perovskites like methylammonium lead iodide show extraordinary photovotlaic performance with power conversion efficienies exceeding 20%. However, a fundamental understanding of the physical processes in perovskite solar cells is still lacking but is essential for further development in this quickly emerging research field. Here, we present our recent studies on the charge carrier recombination in methylammonium lead iodide perovskite solar cells in a planar configuration without porous transport layers by means of open circuit voltage decay measurements. The results are compared with the recombination behavior in reference state-of-the-art polymer-fullerene bulk heterojunction solar cells.[1] We observed two very different time domains in the transients of the perovskite solar cells in contrast to the organic reference solar cells. We will discuss potential origins of these unique behavior and compare the results for various device configurations.[1] A. Baumann et al., APL Mater. 2, 081501 (2014)

HL 67: Topological insulators I (MA with HL/TT)

Time: Thursday 9:30–12:00 Location: EB 202

HL 67.1 Thu 9:30 EB 202

DETECTION OF SURFACE SPIN CURRENT IN 3-DIMENSIONAL TOPOLOGICAL INSULATOR, BiSbTeSe — •Masashi Shiraishi[1], Yuichiro Ando[1], Takahiro Hamasaki[1], Kohji Segawa[2], Satoshi Sasaki[2], Feng Yang[2], Mario Novak[2], and Yoichi Ando[2] — [1]Kyoto Univ., Japan — [2]ISIR, Osaka Univ., Japan

Topological insulators (TIs) attract tremendous attention in recent years, since topologically-protected edge current is a persistent pure spin current. The first detection of the edge current was achieved by using 2-dimensional TI, HgTe quantum well [1], and the next challenge is to detect the edge current in 3-dimensional TIs, because a number of spin channel can be dramatically increased. Whereas Li et al. claimed that they successfully detected the surface spin current in Bi2Se3 by using an electrical spin accumulation method [2], the polarity of the spin signals is not accordance with the direction of magnetization of a detector ferromagnet. Thus, there is still open for discussion how to detect the edge spin current. Here, we present the detection of the edge spin current of BiSbTeSe, which is a bulk insulative TI [3]. The spin signal due to the spin accumulation was detected electrically, and was observed up to 150 K [4].

[1] M. Koenig et al., Science 318, 766 (2007). [2] C. Li et al., Nature Nanotech. 9, 218 (2014). [3] T. Arakane, Yo. Ando et al., Nature Commun. 3, 636 (2011). [4] Yu. Ando, M. Shiraishi et al., Nano Lett., in press.

HL 67.2 Thu 9:45 EB 202

First-principles calculation of quasiparticle spin interference and scattering processes on 3D topological insulators — •Philipp Rüssmann, Phivos Mavropoulos, Nguyen H. Long, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

We present density-functional calculations of the quasiparticle interference (QPI) due to scattering of electrons off magnetic and non-magnetic impurities at the surface of the strong topological insulator Bi_2Te_3. The focus of our work is the calculation and analysis of possible spin-dependent scattering processes and their relation to the QPI pattern observed in experiment. The presence of an impurity magnetic moment leads to broken time-reversal symmetry and the protection against back-scattering is lifted. Therefore, we investigate magnetic transition-metal adatoms as well as non-magnetic Bi and Te adatoms on Bi_2Te_3. Finally, we compare the QPI pattern and scattering processes at different energies around the Fermi energy and discuss the importance of the hexagonal warping of the constant energy contours.

The electronic structure calculations are carried out with our KKR-Green function method for scattering properties at defects [1]. We acknowledge financial support from the DFG (SPP-1666), from the VITI project of the Helmholtz Association and computational support from the JARA-HPC Centre at the RWTH Aachen University.

[1] N. H. Long, P. Mavropoulos, B. Zimmermann, D. S. G. Bauer, S. Blügel, and Y. Mokrousov, Phys. Rev. B **90**, 064406 (2014).

HL 67.3 Thu 10:00 EB 202

Momentum resolved spin dynamics of bulk and surface excited states in the topological insulator Bi_2Se_3 — C Cacho[1], A Crepaldi[2], M Battiato[3], J Braun[5], H Ebert[5], K Hricovini[4], •Jan Minar[5,6], and F Parmigiani[2] — [1]Central Laser Facility, STFC Rutherford Appleton Laboratory, Harwell, United Kingdom — [2]Elettra - Sincrotrone Trieste, Italy — [3]Institute of Solid State Physics, Vienna University of Technology — [4]Universite de Cergy-Pontoise, France — [5]LMU München, Germany — [6]University of West Bohemia, Plzen, Czech Rep.

The prospective of optically inducing a spin polarized current for spintronic devices has generated a vast interest in the out-of-equilibrium electronic and spin structure of topological insulators (TIs). In this presentation we prove that only by measuring the spin intensity signal over several order of magnitude in spin, time and angle resolved photoemission spectroscopy (STAR-PES) experiments is it possible to comprehensively describe the optically excited electronic states in TIs materials. The experiments performed on Bi2Se3 reveal the existence of a Surface-Resonance-State in the 2nd bulk band gap interpreted on the basis of fully relativistic ab-initio spin resolved photoemission calculations. Remarkably, the spin dependent relaxation of the hot carriers is well reproduced by a spin dynamics model considering two non-interacting electronic systems, derived from the excited surface and bulk states, with different electronic temperatures. For more details see: Cacho et all.,
http://arxiv.org/abs/1409.5018

HL 67.4 Thu 10:15 EB 202

Spin structure of the Dirac state of the topological insulator Bi_2Te_3(0001) — •Christoph Seibel[1], Henriette Maass[1], Hendrik Bentmann[1], Jürgen Braun[2], Jan Minár[2], Taichi Okuda[3], and Friedrich Reinert[1] — [1]Experimentelle Physik VII, Universität Würzburg, D-97074 Würzburg — [2]Department Chemie, Physikalische Chemie, Universität München, Butenandtstrasse 5-13, D-81337 München — [3]Hiroshima Synchrotron Radiation Center, Hiroshima

University, Higashi-Hiroshima 739-0046, Japan

Three-dimensional topological insulators feature non-trivial surface states in the fundamental band gap of the bulk. In particular, the spin texture of these topological surface states (TSS) attracts attention in the context of possible applications in spintronics. We have performed angle- and spin-resolved photoemission measurements to analyze the three-dimensional spin texture of the TSS of the topological insulator Bi_2Te_3. The measured photoelectron spin-polarization is found to significantly deviate from the anticipated ground-state spin texture of the TSS, as derived e.g. on the basis of first-principles calculations. Possible origins of our observations are discussed in terms of the influence of spin-orbit coupling on the photoemission process. We compare our experimental data to the results of fully relativistic one-step photoemission calculations.

HL 67.5 Thu 10:30 EB 202

Atomic relaxations in Bi_2Se_3 (0001) — Sumalay Roy[1], •Holger L. Meyerheim[1], Katayoon Mohseni[1], Arthur Ernst[1], Mikhail Otrokov[2,3], Maia G. Vergniory[1,2], Gregor Mussler[4], Christian Tusche[1], Evgueni Chulkov[2,3], and Jürgen Kirschner[1,5] — [1]MPI f. Mikrostrukturphysik, D-06120 Halle, Germany — [2]DIPC, San Sebastian, Spain — [3]Tomsk St. Univ. , Russia — [4]FZ Jülich, Germany — [5]MLU Halle-Wittenberg, Germany

Surface x-ray diffraction analysis of the Bi_2Se_3(0001) surface reveals an expansion of the top Se-Bi interlayer spacing in the range between 2 and 17% relative to the bulk. It is directly related to the concentration of surface contaminants like carbon and is observed in both, single crystals and MBE grown ultrathin films. Deeper layers and the first van der Waals gap remain unrelaxed. Ab-initio calculations which are in agreement with angular resolved photoemission experiments reveal that carbon acts as an n-dopant, while the top layer expansion induces a shift of the Dirac point towards the bulk conduction band of Bi_2Se_3 [1,2].

[1] S. Roy, H.L. Meyerheim, A. Ernst et al., PRL **113**, 116802 (2014); [2] S. Roy, H.L. Meyerheim, K. Mohseni et al., PRB **90**, 155456 (2014)

This work is supported by SPP1666 (Topological Insulators) of the DFG.

HL 67.6 Thu 10:45 EB 202

Spin resolved momentum microscopy of the topological insulator Bi_2Se_3 — •Christian Tusche[1], Martin Ellguth[1], Shigemasa Suga[1,2], Holger L. Meyerheim[1], and Jürgen Kirschner[1,3] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [2]Institute of Scientific and Industrial Research, Osaka, Japan — [3]Institut für Physik, Martin-Luther-Universität, Halle, Germany

Topological insulators are a new class of materials that attracted wide interest by their electronic structure with unusual relations of electron spin and momentum, leading to highly spin polarized "Dirac-cone" surface states. Recently, comprehensive experimental access to such band structures became feasible by spin resolved momentum microscopy. This novel concept combines high resolution imaging of photoelectrons in two-dimensional (k_x, k_y) sections with a highly efficient imaging spin filter. Electron reflection at a Au/Ir(100) mirror allows us to measure 5000 spin-resolved points in the surface Brillouin zone, simultaneously.

We show that the band-structure of Bi_2Se_3 is characterized by highly spin polarized states within the complete Brillouin zone, beyond the "Dirac cone" surface state. For the latter we find that the spin polarization of photoelectrons can reach up to 90%, the highest value reported so far. A direct conclusion on the ground state polarization in these systems is complicated by the peculiar interplay between spin- and light-polarization in the photoemission, as directly observed in spin-resolved (k_x, k_y) images.

This work is supported by SPP1666 (Topological Insulators) of the DFG. M.E. acknowledges support by the BMBF (05K12EF1).

HL 67.7 Thu 11:00 EB 202

The magnetism of Ni adatoms adsorbed on the TI Bi_2Te_2Se — Jan Honolka[1], Martin Vondráček[1], •Lasse Cornils[2], Malte Schüler[3], Markus Dunst[4], Jonas Warmuth[2], Lihui Zhou[2], Anand Kamlapure[2], Alexander Ako Khajetoorians[2,5], Matteo Michiardi[6], Lucas Barreto[6], Philip Hofmann[6], Jian-Li Mi[6], Martin Bremholm[6], Bo B. Iversen[6], Cinthia Piamonteze[7], Hubert Ebert[4], Jan Minar[4,8], Tim Wehling[3], Roland Wiesendanger[2], and Jens Wiebe[2] — [1]Inst. of Physics ASCR, Prague, Czech Republic — [2]INF, University of Hamburg, Germany — [3]Inst. of Theo. Physics, University of Bremen, Germany — [4]LMU München, Germany — [5]IMM, Radboud University Nijmegen, The Netherlands — [6]iNano, Aarhus University, Denmark — [7]PSI, Switzerland — [8]New Technologies-Research Center, University of West Bohemia, Pilsen, Czech Republic

The predicted gap opening in the surface state of topological insulators (TIs) induced by surface magnetic doping, and the associated novel electron phases, have recently caught strong interest of the scientific community. However, the experimental evidence of an induced gap opening is still controversial [1] and calls for a detailed investigation of the magnetism of different adatoms. Here, we show by a combined XMCD, ARPES and STS study, that Ni adatoms on the TI Bi_2Te_2Se reveal a surprising behaviour: While there is no detectable XMCD signal at the Ni $L_{2,3}$-edges, the XAS spectrum unveils a considerable resonant absorption of the d-shell. The results are analyzed by *ab-initio* calculations. [1] J. Honolka *et al.*, PRL **108**, 256811 (2012).

HL 67.8 Thu 11:15 EB 202

Fe-induced stress on Bi_2Se_3(0001) — •Kenia Novakoski Fischer, Safia Ouazi, Dirk Sander, and Jürgen Kirschner — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle

The topological insulator Bi_2Se_3 has attracted intense research activity since its discovery 5 years ago [1]. Here we present the first experimental study of the stress change induced by sub-monolayer deposition of Fe on Bi_2Se_3. Deposition of 0.2 ML Fe at 300 K induces a stress change of -2.3 N/m. On the contrary, deposition of Fe at 150 K leads to negligible stress change of less than -0.2 N/m. The growth of Fe at 473 K induces a stress of -3.4 N/m. LEED reveals that the hexagonal diffraction pattern of the substrate gets blurred for deposition at 150 K, whereas deposition at higher temperature induces faint diffraction spots indicative of precursor of possible FeSe formation. We discuss these results in view of a recent STM study [2], where the authors suggest thermally activated sub-surface doping of Bi_2Se_3 by Fe.

[1] H. Zhang, C.X. Liu, X.L. Qi, X. Dai, Z. Fang, and S. C. Zhang, Nat. Phys. 5 (2009) 438; W. Zhang, R. Yu, H.J. Zhang, X. Dai, and Z. Fang, New Journal of Physics 12 (2010) 065013. [2] T. Schlenk, M. Bianchi, M. Koleini, A. Eich, O. Pietzsch, T. O. Wehling, T. Frauenheim, A. Balatsky, J.-L. Mi, B. B. Iversen, J. Wiebe, A. A. Khajetoorians, Ph. Hofmann, and R. Wiesendanger, Phys. Rev. Lett. 110 (2013) 126804

HL 67.9 Thu 11:30 EB 202

Atomic structure and magnetism of Fe on Bi_2Se_3 — •Andrey Polyakov[1], Holger L. Meyerheim[1], E. Daryl Crozier[2], Robert A. Gordon[3], Maia G. Vergniory[4], Arthur Ernst[1], Evgueni V. Chulkov[4], and Jürgen Kirschner[1,5] — [1]MPI f. Mikrostrukturphysik, D-06120 Halle, Germany — [2]SFU, Burnaby, V5A 1S6 BC, Canada — [3]CLS at APS Sector 20, Argonne, IL, USA — [4]DIPC, San Sebastian, Spain — [5]MLU Halle-Wittenberg, Germany

We have carried out extended x-ray absorption fine structure (EXAFS) and surface x-ray diffraction (SXRD) experiments in combination with ab-initio calculations to investigate the geometric and magnetic properties of iron deposited on the (0001) surface of the topological insulator Bi_2Se_3 in the coverage range between about 0.2 and 1.5 monolayers (ML). For iron deposited at T=170 K in the low coverage limit no polarization dependence of the EXAFS amplitude (electric field vector parallel vs. perpendicular to the surface of the bulk crystal) could be observed. In combination with the nearest neighbor distance of 2.42 Å this suggests that Fe atoms substitute bismuth atoms involving a local relaxation of the neighboring selenium atoms. Ab-initio calculations support this structural model and predict antiferromagnetic ordering of iron [1]. SXRD data collected at 1.5 ML indicate that iron atoms also occupy threefold hollow surface sites. Mild annealing leads to the formation of a bulk FeSe like structure. [1] M. G. Vergniory et al. PRB 89, 165202 (2014); This work is supported by SPP 1666 (Topological Insulators). Work at APS sector 20 is supported by the CLS and by US DOE under Contract No. DE-AC02-06CH11357

HL 67.10 Thu 11:45 EB 202

Signatures of Dirac fermion-mediated magnetic order — •Paolo Sessi[1], Felix Reis[1], Thomas Bathon[1], Konstantin Kokh[2], Oleg Tereshchenko[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Novosibirsk State University, 630090 Novosibirsk, Russia

The spin-momentum locking of topological states offers an ideal plat-

form to explore novel magneto-electric effects. These intimately depend on the ability to manipulate the spin texture in a controlled way. Although numerous studies aimed to shed light on the role played by magnetic perturbations, contradictory results have been obtained and a clear picture is still missing. The interaction of surface magnetic moments with topological states has predominantly been performed by using spatial averaging techniques such as angle-resolved photoemission spectroscopy and x-ray magnetic circular dichroism. Here, we combine low-temperature scanning tunneling microscopy with single-adatom deposition to directly map the evolution of the electronic properties of topological states under the influence of different magnetic perturbations. By analyzing energy-resolved quasi-particle interfer- ence maps, we reveal signatures of Dirac fermion-mediated surface magnetic order for extremely dilute adatom concentrations. By using different magnetic elements and coverages, we find that this striking observation crucially depends on two parameters: single adatoms mag- netic anisotropy direction and energy-level alignment [1].

[1] P. Sessi et al., Nature Comm. 5, 5349 (2014).

HL 68: Low-dimensional systems: Molecular conductors (TT with CPP/HL/MA/O)

Time: Thursday 9:30–11:00 Location: H 3010

HL 68.1 Thu 9:30 H 3010

Nature of the empty electronic states of TCNQ and their thermal evolution due to the CDW instability of TTF-TCNQ revealed by NEXAFS — •Alisa Chernenkaya[1], K. Medjanik[1,2], P. Nagel[3], M. Merz[3], S. Schuppler[3], E. Canadell[4], J.-P. Pouget[5], and G. Schönhense[1] — [1]JGU, Mainz, Germany — [2]MAX-lab, Lund, Sweden — [3]KIT, Karlsruhe, Germany — [4]ICMAB, Bellaterra, Spain — [5]Uni Paris-Sud, Orsay, France

The electronic structure of TTF-TCNQ was studied by near-edge x-ray absorption fine structure (NEXAFS) to detect a signature of the Peierls transition at 54 K [1]. All experimental unoccupied TCNQ orbitals predicted by first-principles calculations are clearly resolved, the $\sigma^*(\pi(a_g,\ b_3u))$ orbital was observed for the first time [2]. The temperature dependence of NEXAFS peak intensities gives evidence of a subtle modification of the electronic structure when the charge density wave (CDW) fluctuations develop as the Peierls transition of the TCNQ stacks is approached from higher temperatures. These changes are explained on the basis of the charge transfer, the shape of the lower empty TCNQ molecular orbitals and the deformation of TCNQ during the pre-transitional CDW fluctuations. Finally the data suggest that the internal stack deformation consisting in a substantial out of plane displacement of the central ring with respect to the cyano-groups allows to gain C-C bonding energy which helps the stabilization of the Peierls transition on the TCNQ stack.

[1] J.P. Pouget, Z. Kristallogr. 219, 711, 2004.
[2] A. Chernenkaya et al., EPJB, accepted.

HL 68.2 Thu 9:45 H 3010

Observation of charge localization and the charge ordering transition in $(TMTTF)_2AsF_6$ using NEXAFS — •Katerina Medjanik[1], Alisa Chernenkaya[2], Sergej Nepijko[2], Gunnar Öhrwall[1], Pascale Foury-Leylekian[3], Pere Alemany[4], Enric Canadell[5], Gerd Schönhense[2], and Jean-Paul Pouget[3] — [1]Lund University, MAX IV Laboratory, 22100 Lund, Sweden — [2]Institut für Physik, JOGU, 55099 Mainz, Germany — [3]Laboratoire de Laboratoire de Physique des Solides, Université Paris-Sud, 91405 Orsay, France — [4]IQTCUB, Universitat de Barcelona, 08028 Barcelona, Spain — [5]ICMAB-CSIC, 08193 Bellaterra, Spain

High-resolution near-edge X-ray absorption fine structure (NEXAFS) measurements at MAX II, Lund (beamline I1011 [1]) were performed on a $(TMTTF)_2AsF_6$ [2] single crystal upon cooling from room temperature to 90 K. Systematic shifts of different spectral features of the F 1s and S 2p signal by up to 0.8 eV to opposite sides on the photon-energy scale with respect to the spectra at room temperature have been detected. Most likely, the shift of the S 2p signal is connected with the breakdown of itinerant conductivity and loss of screening when entering the charge-localization regime.The appearance of a new F 1s pre-edge signal upon entry into the charge ordering (CO) phase at 90 K is a clear fingerprint of the reorganization of the anions in the layered material and changing in the dimerization of molecular orbitals with respect to room temperature.Project funded by DFG through SFB Transregio 49.

[1] I. A. Kowalik et al., J. Phys.: Conf. Ser. 211, 012030 (2010);
[2] M. de Souza et al., Physica B, 405, 92 (2010).

HL 68.3 Thu 10:00 H 3010

Low-Energy Excitations in the Quantum Spin Liquid κ-$(BEDT\text{-}TTF)_2Cu_2(CN)_3$ — •Andrej Pustogow[1], Elena Zhukova[2], Boris Gorshunov[2], Marko Pinteric[3,4], Silvia Tomic[4], John Schlueter[5], and Martin Dressel[1] — [1]1. Physikalisches Institut Universität Stuttgart — [2]Moscow Institute of Physics and Technology, Russia — [3]Faculty of Civil Engineering, Maribor, Slovenia — [4]Institut za fiziku, Zagreb, Croatia — [5]Argonne National Laboratory, USA

The suppression of long range magnetic order due to geometrical frustration gives rise to the quantum spin liquid state. Theoretical considerations predict enhanced absorption within the Mott gap caused by spinons, which results in a low-frequency power-law behaviour of the optical conductivity, i.e. for $\hbar\omega_c < J \approx 250K$. To verify this hypothesis, the optical conductivity of the spin liquid candidate κ-$(BEDT\text{-}TTF)_2Cu_2(CN)_3$ was measured, where the dimerized organic molecules are arranged on a triangular lattice. An extremely wide energy range from radio frequencies up to the near infrared ($10^{-13}eV - 1eV$) was covered by dielectric spectroscopy, THz absorption and optical reflectivity measurements. We could indeed identify a power-law behaviour $\sigma(\omega) \propto \omega^{\beta}$ where two distinct exponents β change from 0.9 to 1.7 at low temperatures, with the corresponding crossover scaling with temperature: $\hbar\omega_c \approx k_BT$. While our results agree well with $(ZnCu)_3\ (OD)_6\ (Cl)_2$, another spin liquid candidate, theory predicts exponents of 2 and 3.33, respectively. Hence, these experimental findings may motivate a refinement of the theoretical framework.

HL 68.4 Thu 10:15 H 3010

Mott criticality in organic charge-transfer salts κ-$(BEDT\text{-}TTF)_2X$ studied by thermal expansion under He-gas pressure — •E. Gati[1], R. S. Manna[1], U. Tutsch[1], B. Wolf[1], L. Bartosch[2], T. Sasaki[3], H. Schubert[1], J. A. Schlueter[4], and M. Lang[1] — [1]Physikalisches Institut, Goethe Uni, SFB/TR49, D-60438 Frankfurt — [2]Inst. für Theoretische Physik, Goethe Uni, D-60438 FfM — [3]IMR, Tohoku University, Sendai 980577, Japan — [4]Materials Science Division, National Laboratory, Argonne, Illinois 60439, USA

The Mott transition and the underlying universality class have been intensively studied in the past. The proposal of a hitherto unknown *unconventional* universality class for the quasi 2D organic charge-transfer salt κ-$(BEDT\text{-}TTF)_2Cu[N(CN)_2]Cl$ (κ-Cl) [1], based on resistivity measurements, has attracted particular interest. In this compound, the Mott transition can be accessed by chemical pressure or the application of very small hydrostatic pressures of 300 bar. We will present measurements of the thermal expansion of κ-Cl under ^{4}He-gas pressure [2], an unique technique, which provides a very sensitive tool to investigate critical phenomena [3,4], including effects of coupling of electrons to the crystal lattice [5]. A comparison of our results with theoretical predictions of a scaling theory [4] shows that the critical properties are incompatible with the proposed unconventional universality class.

[1] F. Kagawa et al., Nature 436, 534 (2005).
[2] R. S. Manna et al., Rev. Sci. Instrum. 83, 085111 (2012).
[3] M. de Souza et al., PRL 99, 0370031 (2007).
[4] L. Bartosch et al., PRL 104, 245701 (2010).
[5] M. Zacharias et al., PRL 109, 176401 (2012).

HL 68.5 Thu 10:30 H 3010

Electronic structure and superconductivity of multi-layered organic charge transfer salts — •Harald O. Jeschke, Michaela Altmeyer, Daniel Guterding, and Roser Valenti — Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt

We examine the electronic properties of polymorphs of $(BEDT\text{-}TTF)_2Ag(CF_3)_4(TCE)$ (1,1,2-trichloroethane) within density functional theory (DFT). While a phase with low superconducting transition temperature $T_c = 2.6$ K exhibits a κ packing motif, two high

T_c phases are layered structures consisting of α' and κ packed layers. We determine the electronic structures and discuss the influence of the insulating α' layer on the conducting κ layer. In the κ-α'_1 dual-layered compound, we find that the stripes of high and low charge in the α' layer correspond to a stripe pattern of hopping parameters in the κ layer. Based on the different underlying Hamiltonians, we study the superconducting properties and try to explain the differences in T_c.

HL 68.6 Thu 10:45 H 3010

New Charge Transfer Systems based on PAHs — •Antonia Morherr[1], Sebastian Witt[1], Martin Baumgarten[2], Harald O. Jeschke[3], and Cornelius Krellner[1] — [1]Physikalisches Institut, Goethe Universität Frankfurt, D-60438 Frankfurt am Main — [2]MPI für Polymerforschung, D-55128 Mainz — [3]Institut für Theoretische Physik, Goethe Universität Frankfurt, D-60438 Frankfurt am Main

The Polycyclic Aromatic Hydrocarbons (PAHs) Picene, Coronene and Phenanthrene attracted strong attention in the last years as first superconducting PAHs when intercalated with potassium [1]. K_3Picene shows a T_c of 18 K and the T_c of intercalated Coronene lies between 3.5 K and 15 K [2].
Here, we present charge transfer complexes with PAHs representing donor or acceptor molecules of these complexes. The knowledge of different crystallization modes of these systems, e.g. mixed stack or alternating stack configuration, are important for the physical properties. The complexes were grown by horizontal vapor growth technique or by growth from solution. Crystal structures, electrical transport measurements and spectroscopical investigations are presented in this contribution. In addition to the experimental data, we present band-structure calculations, which were performed by density functional methods. The interpretation of both is one approach to understand growing conditions of different stack configurations and an important step towards the design of new charge transfer complexes.

[1] R. Mitsuhashi et al., Nature 464, 76 (2010)
[2] Y. Kubozono et al., Phys. Chem. Chem. Phys. 13, 16476, (2012)

HL 69: GHz Dielectrics - Materials for mobile communication I (DF with HL/MM)

The world wide amount of wireless data exchange doubles roughly every year. In addition the individual data rates increase and the efficiency of the data exchange needs improvements. Antenna and filter elements are key components for such a development and are subject to intense research efforts. Impulses for innovation also originate from materials while new antenna and filter concepts influence material development. Two Focused Sessions are addressing the subject.

Organizer: Martin Letz (Schott AG Mainz)

Time: Thursday 9:30–13:00 Location: EB 407

Topical Talk HL 69.1 Thu 9:30 EB 407

New application scenarios for dielectric materials in mobile communication systems of the 5th generation — •Roland Gabriel — Kathrein-Werke KG, Anton-Kathrein-Straße 1-3, D-83004 Rosenheim / Germany

The worldwide data volume in mobile communication systems double nearly every year. To address this challenge, higher frequency bands will be used and broadband and multiband equipment are required. The new standard LTE-A and the standardization process for the 5th generation of the mobile communication systems enforces changes in the technology of antennas and filters. Beside the usage of new and higher frequency bands up to 60 GHz the broadband and multiband approach increase the requirements for the linearity of the components. For the use in FDD (frequency division duplexing) - systems this means an extreme low level of the active and passive intermodulation. In this contribution the extendend requirements for passive intermodulation are discussed. Different available solutions for the filter technology will be compared regarding the usage for different system solutions of the 4th and 5th generation. In addition the use of dielectric radiators in antennas will be reconsidered with respect to the multiband approach and the required inter- and intra-band isolation.

HL 69.2 Thu 10:00 EB 407

Impedance matching for high power transistors based on printed ceramics — •Alex Wiens, Daniel Kienemund, and Rolf Jakoby — Technische Universität Darmstadt, Institut für Mikrowellentechnik und Photonik

The multitude of standards in modern tele-communication systems, such as GSM, UMTS, LTE and WiFi make the hardware of a radio front end face a variety of frequencies and bands. Generally, each element of the front end is optimized to perform best at a certain frequency band and signal type. Power amplifiers can be considered as the most critical components of RF/microwave communication systems, as they dominate the power consumption and hence the efficiency of the whole system. They are therefore consequently the focus of intense research to achieve improved linearity and increased power efficiency. Barium-Strontium-Titanate (BST) varactors offer an alternative to semiconductor and MEMS technologies in the design of tunable matching networks for reconfigurable multi-band RF-power amplifiers, and for load modulation applications, where the varactor tuning is used to maintain high efficiency over a large dynamic range of the input signal. Recent advances in fabrication of high power tunable RF varactors based on BST are presented and discussed. Measurement results of a BST-based tunable matching network, implemented inside a GaN HEM Transistor show promissing performance for telecommuncation frequency range.

HL 69.3 Thu 10:20 EB 407

Enhanced magnetooptic Kerr effect and magnetic properties of Ce:YIG thin films — •Andreas Kehlberger[1], Kornel Richter[1], Gerhard Jakob[1], Mehmet C. Onbasli[2], Gerald F. Dionne[2], Dong Hun Kim[2], Taichi Goto[2], Gerhard Götz[3], Günter Reiss[3], Timo Kuschel[3], Caroline A. Ross[2], and Mathias Kläui[1] — [1]Universität Mainz, Mainz, Germany — [2]Massachusetts Institute of Technology, Cambridge, USA — [3]CSMD, Physics Department, Bielefeld University, Germany

Yttrium iron garnet (YIG) is a ferrimagnetic and electrically insulating garnet oxide that has low intrinsic magnetic damping. These properties make YIG a functional layer for spin-wave generation and filtering for telecommunication devices operating at microwave bands. The substitution of Y by Ce allows for an enhancement of the magnetooptic properties and to further influence the magnetic material properties. Our work presents an extensive study of high quality epitaxial Ce:YIG thin films and reveals that not only the magnetooptic properties but also the magnetic anisotropy can be tailored by the Ce substitution. For the first time we show that beside the Faraday rotation also the magnetooptic Kerr effect is enhanced compared to pure YIG, making a broader range of wavelength, including the fibreoptics band, accessible. We present growth methods for polycrystalline Ce:YIG films, which allow the development of integrated on-ship devices.[1,2] Our results show the suitability of Ce:YIG thin film for future magnetooptic and spintronic applications. [1] Lei Bi et al., Nature Photon. 5, 758-762 (2011) [2] Taichi Goto et al., J. Appl. Phys. 113, 17A939 (2013)

HL 69.4 Thu 10:40 EB 407

Design of miniaturized antennas for GNSS applications using a high DK dielectric material — •Stefano Caizzone — Institute of Communications and Navigation, German Aerospace Center (DLR), Wessling, Germany

The use of high dielectric constant (high DK) materials is particularly appealing for a vast number of Radio Frequency (RF) applications, including antenna design. In this field, in fact, high DK low-loss dielectric materials could enable consistent improvements in antenna miniaturization. To the present day, however, common high-DK materials suffer from relatively large manufacturing tolerances, implying remarkable frequency shifts in the antenna radiation and need for retuning. This work, on the other hand, shows the use of a new dielectric

material with diminished tolerances for antenna design purposes, both through preliminary tests with a simple antenna structure and through the enhanced design of a miniaturized antenna for GNSS applications. The initial tests were performed in order to validate the usability of the material in the RF area: it was used as a substrate for a microstrip patch antenna. The results show a good behavior of the high DK material and its aptitude for RF antenna design. As a consequence, a Dielectric Resonator Antenna (DRA), fully exploiting the dielectric properties of the material, was designed for use in the lower L-Band of the Global Navigation Systems, allowing for good performance over a wide bandwidth, covering E5, L2 and E6 bands.

Topical Talk HL 69.5 Thu 11:00 EB 407

Dielectric-loaded antennas for circular polarisation: their contribution to the information capacity of wireless terminals — •Oliver Leisten — Maruwa Europe Ltd, UK

Dielectric-loaded multi-filar helix antennas offer solutions as miniature circular polarised antennas in small devices with the advantage that body-loading can suppress reflections from the device: improving circular polarisation discrimination. This is an example of materials-science enabling the design of antennas providing relatively predictable performance in a cluttered and changing near environment. Modern wireless systems typically operate with complex scattering from objects in the indoor environment which can be scaled in frequency to be compared to the Rayleigh scattering of light from the particles of dense smoke. Indeed modern MIMO devices exploit the low spatial autocorrelation of such fields invoking the principle of spatial multiplexing to multiply the information capacity per unit of spectral bandwidth. Such systems use multiple receiving antennas to receive scattered signals summing by superposition, at those discrete antenna locations, of information streams transmitted from multiple transmitting antennas. The small resonance volume dielectric-loaded antennas, together with platform independent polarisation, enhances statistical independence of signals, improving system data-capacity by reducing interference between datastreams. The use of right and left hand circular polarised antennas to invoke polarisation diversity is interesting as Rayleigh scattering develops spin-turbulent fields.

20 min Coffee Break

HL 69.6 Thu 11:50 EB 407

$Ba_4Al_2Ti_{10}O_{27}$ glass-ceramics as dielectric materials for antenna elements in wireless communications — •Martun Hovhannisyan[1], Hubertus Brauna[1], Yuliang Zheng[2], Arshad Mehmood[2], Martin Letz[1], and Rolf Jakoby[2] — [1]Material & Technology Development, SCHOTT AG, Hattenbergstrasse 10, Mainz, 55122, Germany — [2]Technical University of Darmstadt, Darmstadt, D-64283 Darmstadt, Germany

Dielectric glass-ceramics with $Ba_4Al_2Ti_{10}O_{27}$ as the main crystalline phase are obtained by controlled heat-treatment of a non-porous bulk-glass phase. Such a non-porous material has advantages over ceramics with residual porosity wherever metallization steps are applied to the material. Depending on the details of heat-treatment profile the $Ba_4Al_2Ti_{10}O_{27}$ is formed as a main phase with secondary phases $BaTi_4O_9$ or $BaAl_2Si_2O_8$. Microstructural observation using scanning electron microscopy (SEM) shows nanometer-sized crystals (40nm) grown in a true glass phase. The microwave dielectric characterization using Hakki-Coleman setup shows a Qf from 2000 GHz to 10.000 GHz, dielectric constant from 19 to 33 and |tf| of <20 ppm/K. Balancing between different crystalline phases allows to adjust |tf| to zero. To our knowledge the present work is the first one emphasizing the attractiveness of the microwave dielectric properties of the phase $Ba_4Ti_{10}Al_2O_{27}$. Such glass-ceramics are well suited for antenna and filter applications in microwave electronics.

HL 69.7 Thu 12:10 EB 407

Highly conducting $SrMoO_3$ thin films for microwave applications — •Aldin Radetinac[1], Arzhang Mani[1], Sergiy Melnyk[2], Mohammad Nikfalazar[2], Jürgen Ziegler[1], Yuliang Zheng[2], Rolf Jakoby[2], Lambert Alff[1], and Philipp Komissinskiy[1] — [1]Institute for Materials Science, TU Darmstadt, Germany — [2]Institute for Microwave Engineering and Photonics, TU Darmstadt, Germany

We have measured the microwave resistance of highly conducting perovskite oxide $SrMoO_3$ thin film coplanar waveguides. The epitaxial $SrMoO_3$ thin films were grown by pulsed laser deposition and showed low mosaicity and smooth surfaces with a root mean square roughness below 0.3 nm. Layer-by-layer growth could be achieved for film thicknesses up to 400 nm as monitored by reflection high-energy electron diffraction and confirmed by X-ray diffraction. We obtained a constant microwave resistivity of 29 $\mu\Omega$cm between 0.1 and 20 GHz by refining the frequency dependence of the transmission coefficients. Our result shows that $SrMoO_3$ is a viable candidate as a highly conducting electrode material for all-oxide microwave electronic devices. This work was supported by the DFG project KO 4093/1-1.

[1] A. Radetinac, A. Mani, S. Melnyk, M. Nikfalazar, J. Ziegler, Y. Zheng, R. Jakoby, L. Alff, and P. Komissinskiy, Appl. Phys. Lett. **105**, 114108 (2014)

Topical Talk HL 69.8 Thu 12:30 EB 407

Tunable GHz-components with ferroelectric and liquid crystal technologies for mobile terrestrial and satellite-based systems — •Rolf Jakoby — Institute of Microwave Engineering and Photonics, Technische Universität Darmstadt, Merckstr. 25, 64283 Darmstadt, Germany

Recent progress in Liquid Crystal (LC) technology made in Darmstadt is very promising for next-generation reconfigurable/tunable microwave and millimeter wave devices because they exhibit excellent properties at high frequencies above 15 GHz, since LC losses generally decrease with increasing frequency. This opens up new low-cost LC applications beyond optics. In contrast, ferroelectric material, particularly Barium Strontium Titanate (BST), is well suited at frequencies below 15 GHz, using screen and inkjet printing of BST layers. Hence, with these two material classes, we can cover a frequency range from 1 GHz up to 1 THz for tunable components such as varactors, tunable delay and loaded lines, phase shifters, tunable filters, adaptive matching networks, tunable frequency selective surfaces, tunable multiband antennas, polarization-agile antennas, phased-scanning reflect- and phased arrays. This contribution presents an overview of the both technologies, BST and LC, including basic principles, tuning mechanisms, processing technologies, device concepts and design, packaging and integration issues as well as functional tests with focus on frequency-agile multiband antennas and filters as well as electronically beam-steering antennas for mobile terrestrial and satellite-based applications.

HL 70: Spintronics: Mobile electrons and holes (with MA/TT)

Time: Thursday 10:00–12:30 Location: ER 164

HL 70.1 Thu 10:00 ER 164

Conserved Spin Quantity in Strained Hole Systems with Rashba and Dresselhaus Spin-Orbit Coupling — •Michael Kammermeier[1], Paul Wenk[1], John Schliemann[1], Klaus Richter[1], and Roland Winkler[2] — [1]Universität Regensburg, D-93040 Regensburg, Germany — [2]Northern Illinois University, IL 60115 DeKalb, US

We investigate conditions for the existence of a conserved spin quantity in two-dimensional hole gases in zincblende type semiconductor heterostructures. It is shown that in the presence of shear stress, a symmetric in-plane strain, and both Rashba and Dresselhaus spin-orbit coupling one can find such a conserved quantity. The found optimal parameter-space, for strain and spin-orbit coupling strength, gives the possibility to an experimental access. This is in contrast to previous works which require restrictions on the band model parameters (here the Luttinger parameters) which are either difficult to realize in real materials or even singular ($\gamma_3 = 0$).

* * *

[1] Schliemann *et al.*, PRL **90** 146801 (2003)
[2] Bernevig *et al.*, PRL **97** 236601 (2006)
[3] Kohda *et al.*, PRB **86** 081306 (2012)
[4] Dollinger *et al.* Phys. Rev. B **90**, 115306 (2014)

HL 70.2 Thu 10:15 ER 164

Quantum transport and response with spin-orbit coupling in magnetic fields — •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

Electronic transport in spin-polarized systems with impurity interactions and spin-dependent meanfields is discussed. The coupled quantum kinetic equations for the scalar and spin components for SU(2) are derived with special consideration of spin-orbit coupling and magnetic fields. Linearizing, the RPA spin and density dynamical responses to electric fields (polarized light) are preseented for arbitrary magnetic fields, Several known effects are described: spin-Hall, anomalous Hall and optical Hall effect, spin-heat coupling. New transport coefficients occur due to the selfconsistent precession direction. Clarifying the relative importance of meanfield and scattering correlations, new modes due to magnetic fields and spin-orbit coupling are found. (EPL, 104 (2013) 2700)

HL 70.3 Thu 10:30 ER 164

Spin injection through Fe/GaAs Schottky contacts — •Lennart-Knud Liefeith, Rajkiran Tholapi, Max Hänze, Ann-Kathrin Michel, Taras Slobodskyy, and Wolfgang Hansen — Institut für Festkörper- und Nanostrukturphysik, Hamburg, Hamburg

The understanding of the dominant mechanism of spin injection through the Fe/GaAs interface is crucial for spintronics applications. It was suggested that the spin injection process is controlled by thermal activation of surface states at the ferromagnet/semiconductor interface [1]. To test this theory we investigated the bias dependence of the spin injection efficiency as well as the electrical properties of the interface. The measurements were carried out using non-local spin detection devices at liquid helium temperatures and backed up by magneto optical Kerr effect and magnetic force microscopy measurements on the electrodes. We found that the post growth annealing strongly influences the spin injection efficiency and a notable asymmetry of the spin injection efficiency depending on the applied bias was observed.

[1] Q. U. Hu et. al., „Spin accumulation near Fe/GaAs(001) interfaces: The role of semiconductor band structure“, Physical Review B 84, 085306 (2011)

HL 70.4 Thu 10:45 ER 164

Electric control of spin transport in GaAs (111)B quantum wells — •Alberto Hernández-Mínguez, Klaus Biermann, and Paulo Santos — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

The main challenge towards the use of electron spins in semiconductors is the control of the dephasing mechanisms that reduce the spin lifetime below the spin manipulation time. In III-V semiconductors, the main relaxation processes are related to the spin-orbit interaction (SOI). In the case of GaAs(111) quantum wells (QWs), the SOI can be efficiently suppressed for out-of-plane spins by applying an electric field, E_z, transverse to the QW plane. In this case, the contribution to the SOI induced by E_z compensates the intrinsic SOI due to the zinc-blende lattice and spin lifetimes of tenths of ns are observed.

In this contribution, we show experimental studies of both carrier and spin diffusion in a GaAs(111) QW under the effect of vertical electric fields. Spin polarized electron-hole pairs are optically generated in the QW by a tightly focused laser beam. The carrier and spin dynamics are studied by spatially and time-resolved photoluminescence. We show that the enhancement of the spin lifetime due to SOI compensation allows the transport of out-of-plane electron spins over distances exceeding 10 μm. In addition to the spin lifetime, the spin diffusion coefficient D_s also depends on E_z. For the carrier densities and temperatures studied, D_s shows a maximum of approx. 50 cm^2/s at SOI compensation, where it approaches the values observed for the carrier diffusion coefficient under the same experimental conditions.

HL 70.5 Thu 11:00 ER 164

Time and space resolved visualization of spin diffusion and drift in GaAs based two-dimensional electron gases — •Markus Schwemmer[1], Roland Völkl[1], Tobias Korn[1], Sergey Tarasenko[2], Dieter Schuh[1], Dominique Bougeard[1], Mariusz Ciorga[1], Werner Wegscheider[3], and Christian Schüller[1] — [1]Institute of Experimental and Applied Physics, Faculty of Physics, University of Regensburg, Germany — [2]A. F. Ioffe Physical-Technical Institute, Russian Academy of Sciences, St. Petersburg, Russia — [3]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 resident two-dimensional electron gas based on a modulation-doped AlGaAs/GaAs quantum well. The interplay between the Dresselhaus and Rashba fields according to crystallographic orientation and layer structure of the sample determines the electron spin dynamics. On one hand we present diffusive and current-driven motion of a spin packet in a sample in which the orientation of the optically injected spins point along the effective spin orbit field. Therefore D'yakonov-Perel spin dephasing is suppresed and a long spin coherence time can be attained. On the other hand the diffusive spreading of the initial spin packet in a sample with a spin-orbit interaction close to the spin helix regime is monitored, whereby a direct visualization of the helix pattern is achieved. Financial support by the DFG via SFB 689 and SPP 1285 is gratefully acknowledged.

Coffee break

HL 70.6 Thu 11:30 ER 164

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

We performed time-resolved Kerr rotation (TRKR) measurements on an undoped [113]-grown double quantum well (QW) structure to resolve the spin dynamics of hole ensembles at low temperatures. Our gated system consists of two QWs with different well widths, which we use for the spatial separation of the optically excited electron-hole pairs. Thus, we are able to create hole ensembles with spin dephasing times of several hundreds of picoseconds in the broader QW without any doping.

This allowed an unexpected observation of a non-precessing component in the TRKR signal in the presence of an applied magnetic field perpendicular to the spin polarization. These measurements also show the non-precessing component to be a part of the optically generated hole spin polarization. This effect might arise from a tilting of the quantization axis with respect to the applied magnetic field due to a large anisotropy between the in- and out-of-plane hole g factor.

HL 70.7 Thu 11:45 ER 164

Inelastic light scattering in a two-dimensional electron gas under external magnetic fields — •Christoph Schönhuber, Di-

eter Schuh, Dominique Bougeard, Tobias Korn, and Christian Schüller — Universität Regensburg, 93040 Regensburg, Germany

We present inelastic light scattering measurements of a 12-nm-wide (001)-oriented GaAs/AlGaAs QW under external magnetic fields. The investigated system is single-side Si doped to reach a balanced Rashba and Dresselhaus SOI contribution.

The performed measurements on intrasubband transitions of the conduction band reveal for B=0 a double peak structure for the [1-1] direction due to spin splitting, while the [11] direction features only a single peak. For small magnetic fields, the wave vector appears to be conserved in the scattering process while both directions aim to assimilate the excitation with increasing field strength. At higher perpendicular magnetic fields, the anisotropic behaviour has vanished and the spectra are characterized by inter-Landau excitations.

HL 70.8 Thu 12:00 ER 164

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

Several theoretical works treat the spin dynamics in zinc-blende semiconductors. We present extremely low excitation Hanle depolarization measurements on well characterized n-doped MBE grown GaAs in the vicinity of the metal-to-insulator transition (MIT). The doping concentrations range from the MIT at $2 * 10^{16}$ cm^{-3}, where extremely long spin lifetimes are experimentally observed [1], up to the merging of impurity and conduction band at $8 * 10^{16}$ cm^{-3}, where for conduction band electrons the spin relaxation is typically dominated by the Dyakonov-Perel mechanism (DP). We conclude from our measurements that DP is also dominating the impurity band regime in slightly metallic samples. Furthermore the measurements show no indication of spin relaxation by hopping transport (HT) that has recently been predicted as the main mechanism of relaxation for the impurity band regime [2]. In contrast our measurements of the spin dynamics indicate a metal-like behavior of the electrons in the impurity band.

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

HL 70.9 Thu 12:15 ER 164

Boundary dependent spin manipulation via Rashba-SOC — •Phillipp Reck and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

Besides spin injection, controlled spin manipulation is a major aspect of active spintronic devices such as spin transistors. In a two dimensional electron gas (2DEG), this manipulation is often achieved by Rashba spin orbit coupling (SOC).

We study numerically the effects of a non-trivial deformation of a wire (quasi 1DEG) on the spin evolution of an initially spin polarized wave packet exposed to Rashba SOC. To make sure that the wave packet follows the deformation, we apply additionally a magnetic field to get edge states, which are resistant to impurity scattering. The benefit of the deformation is the higher variability of the spin state: Without the deformation, the spin precesses on the Bloch sphere around one fixed axis, whereas the deformation changes continuously the orientation of the precession axis leading to a more complex spin evolution. Thus, it is possible, e. g., to create either a x-, y- or z-spin polarization by only changing the Rashba SOC, but not the geometry.

A generalization is a wire with a periodic deformation. Because of the constant out-of-plane magnetic field and an in-plane rotating effective magnetic field due to SOC, one could engineer spin resonance effects.

HL 71: New concepts and new materials

Time: Thursday 10:15–12:30 Location: EW 201

HL 71.1 Thu 10:15 EW 201

$YMnO_3$ - based MIS structure with a selective, capacitive photo-detecting properties — •Agnieszka Bogusz[1,2], Om S. Choudhary[2], Ilona Skorupa[1], Danilo Bürger[2], Alexander Lawerenz[3], Oliver G. Schmidt[2,4], and Heidemarie Schmidt[2] — [1]Institute Of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf — [2]Department of Materials for Nanoelectronics, Chemnitz University of Technology — [3]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik GmbH — [4]Institute for Integrative Nanosciences, IFW-Dresden

This work investigates the $YMnO_3/Si_3N_4/p-Si$ structures in terms of novel, capacitance-based photo-detecting properties. Photocapacitance-voltage (C-V) characteristics of the $YMnO_3/Si_3N_4/p-Si$ structures have been determined at room temperature for a wide spectral range (λ= 300-980 nm). C-V characteristics indicate a charge trapping process which is used as the basis for novel approach to photodetectors. Our model discusses the immobilization of otherwise mobile charges in Si_3N_4 when the negative polarization charge of the multiferroic $YMnO_3$ [1] is at the $YMnO_3/Si_3N_4$ interface. The observed capacitance minima are well-defined by the direction of bias ramp. Voltages corresponding to these minima were further used as a reference point for a read out of capacitance in retention and optical selectivity tests. Results indicate that investigated structures exhibit a good photo-sensitivity of red light and the retention properties are non-volatile for one capacitance branch. [1]B.B. Van Aken et al. Nature Mater.3,164(2004)

HL 71.2 Thu 10:30 EW 201

Coulomb blockade in metal nanoparticle field-effect transistors — •Hauke Lehmann, Svenja Willing, Sandra Möller, Mirjam Volkmann, and Christian Klinke — Institut für Physikalische Chemie, Universität Hamburg, Grindelallee 117, 20146 Hamburg, Germany

Metallic nanoparticles offer possibilities to build and improve basic electrical devices. The role of a semiconductor's bandgap is adopted by the Coulomb energy gap [1] due to the charging of the single particles' capacities. Thus, it is required to keep the nanoparticles individualized by tunnel barriers, while a merging of the particles would render them metallic again.

We synthesize monodisperse CoPt nanoparticles by colloidal chemistry [2]. Those particles are deposited via the Langmuir-Blodgett technique as highly-ordered homogeneous monolayers onto substrates with predefined gold electrodes. Additional structuring of the films yields stripes from individual nanoparticles. Such a defined channel can be controlled through a carefully adjusted gate voltage much more precisely compared to former experiments on whole nanoparticle films [3]. An insulating layer on top of the nanoparticles enables the application of a local top-gate electrode instead of using the global back gate. We find oscillations indicating the Coulomb blockade at temperatures of up to approximately 100 K.

[1] C. W. J. Beenakker, Phys. Rev. B **44**, 1646 (1991)
[2] S. Lim et al., Nano Lett. **10**, 964 (2010)
[3] Y. Cai et al., J. Appl. Phys. **114**, 034311 (2013)

HL 71.3 Thu 10:45 EW 201

Thermal rectification in asymmetric MoS_2 nanoribbons: a non-equilibrium molecular dynamics study — •Leonardo Medrano Sandonas[1,2], Rafael Gutierrez[1], Arezoo Dianat[1], and Gianaurelio Cuniberti[1,3,4] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [3]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — [4]Dresden Center for Computational Materials Science (DCCMS), TU Dresden, 01062 Dresden, Germany

We provide insights into the design and understanding of thermal rectifiers based on asymmetric MoS_2 nanoribbons. Non-equilibrium molecular dynamics (NEMD) simulations are used to study the influence of geometrical shapes on the thermal rectification. Our results point out that asymmetric MoS_2 nanoribbons can display considerable thermal rectification. Moreover, this rectifier effect increases with the asymmetry degree of the device but, as expected, it weakens with increasing linear dimensions. Among the geometrical shapes studied in the present work, T−shaped MoS_2 nanoribbons present the highest thermal rec-

tification for each asymmetry degree. We also found that vibrational modes for frequencies greater than 380 cm^{-1} are almost fully localized and spatially distributed on the edges of the asymmetric nanoribbons. Thus, similar to asymmetric and defective nanostructures made of a single material, we find that lateral confinement of the vibrational modes is a mechanism of thermal rectification in MoS_2 nanoribbons.

HL 71.4 Thu 11:00 EW 201

Full two-dimensional band-mapping of Ni-intercalated TiS2 by momentum microscopy — •Shigemasa Suga[1,2], Christian Tusche[1], Yuichiro Matsushgita[1], Martin Ellguth[1], Akinori Irizawa[2], and Jürgen Kirschner[1,3] — [1]Max-Planck-Institute of Microstructure Physics, Weinberg 2, Halle 06120, Germany — [2]Institute of Scientific & Industrial Research, Osaka University, 8-1 Mihogaoka, Ibaraki, Osaka 567-0047, Japan — [3]Institut für Physik, Martin-Luther-Universität, Halle, Germany

Atom intercalation into the van der Waals gap of a layered semiconductor TiS2 can effectively modify its electronic properties in the bulk and surface. In order to probe the changes of its surface electronic structure on Ni intercalation, we have performed high-resolution and simultaneous two-dimensional photoelectron spectroscopy of Ni1/3TiS2 by use of a momentum microscope. Full (kx,ky) band dispersions are revealed up to 2.0 Å-1. Small electron Fermi surfaces (FSs) with noticeable dispersion observed near the M points in TiS2 became much stronger in Ni1/3TiS2, in which a very small hole FS pocket with clear dispersion is additionally observed near Γ point. Detailed new experimental results are compared with first principles theoretical band calculations. Differences between these materials are dominated by the contribution of the Ni 3d states of the surface Ni atoms positioned at the C3v site, being different from its D3d site beneath the surface. The use of a momentum microscope is demonstrated to be inevitable for clarifying detailed electronic structures of many solids under hot debates. M.E. acknowledges support by the BMBF (05K12EF1).

HL 71.5 Thu 11:15 EW 201

Determination of Optical and electronic structure properties studied for Sr[LiAl3N4]:Eu+2 as a next-generation LED-phosphor material. — •Sikander Azam[1], Robin Niklaus[2], Wolfgang Schnick[2], and Jan Minar[1,2] — [1]New Technologies-Research Center, University of West Bohemia, Univerzitni 8, 306 14 Pilsen, Czech republic — [2]Dept. of Chemistry, University of Munich, Germany

Recently, Sr[LiAl3N4]:Eu+2 has been shown to be a promising LED-phosphor material with a great potential for industrial application [1]. Using density functional theory (DFT) within the local density approximation (LDA), the generalized gradient approximation (GGA) and the modified Becke*Johnson (mBJ) form we investigated the structural, electronic and optical properties of Sr[LiAl3N4]:Eu+2. The total energy has been optimized as a function of the unit cell volume. All other parameters like the density of state (DOS), the band structure and the linear optical susceptibility are calculated for the relaxed structure applying the optimized lattice constant. We show that our calculated band structure agrees quantitatively very well with corresponding experimental data. It will be shown that for the calculation of optical properties, which are closely related to the corresponding electronic structure our results are an essential precondition. [1] P. Pust et al., Nature Mat. 13, 891 (2014)

HL 71.6 Thu 11:30 EW 201

Coupled organic-inorganic nanostructures: Size dependent carrier transport in tetrathiafulvalenedicarboxylate capped PbS nanocrystals — •Alexander André[1,2], Mahdi Samadi Khoshkoo[1,2], and Marcus Scheele[1,2] — [1]Institute of Physical and Theoretical Chemistry, University of Tübingen, Auf der Morgenstelle 18 72076 Tübingen — [2]Center for Light-Matter Interactions, Sensors&Analytics (LISA+), Auf der Morgenstelle 15 72076 Tübingen

Both, inorganic semiconductor quantum dots (QD) and organic semiconductors (OSC), are emerging classes of materials for optoelectronic applications. QDs provide the possibility of size tailored optical and electronic properties all the while keeping sufficiently high charge carrier mobilities and diffusion lengths. OSCs however, offering high material purity and a large degree of ordering in thin films, have already been successfully implemented as transistors and light emitting devices. In our work we aim to combine these two material classes in order to get the best of both worlds. To that end we prepare coupled organic-inorganic nanostructures, so called COINs. Thin films of PbS nanocrystals, with different diameters, functionalized with tetrathiafulvalenedicarboxylate were fabricated via spin coating or superlattice self-assembly at a liquid-liquid interface. The morphology of the resulting samples was investigated with SEM, FT-IR and AFM. The conductivity and charge carrier mobility was measured using a field effect transistor setup. We can show the successful formation of highly ordered nanocrystal superlattices with charge carrier mobilities on the order of $10^{-4}\ cm^2/V*s$.

HL 71.7 Thu 11:45 EW 201

Nanointerfaces in InAs-Sn_2S_6 nanocrystal-ligand networks: atomistic and electronic structure from *first principles* — •Emilio Scalise[1], Stefan Wippermann[1], and Giulia Galli[2] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [2]University of Chicago, Chicago, United States

Semiconducting nanocomposites – consisting of nanocrystals (NCs) embedded in a host matrix – offer exciting prospects for solar energy conversion, light emission and electronic applications. Recent advances in wet chemical synthesis techniques allow for the synthesis of nanocrystals, their assembly into superlattices and embedding into a host matrix completely using only inexpensive solution processing. However, the atomistic details of the resulting nanocomposites are poorly understood, due to the complexity of the synthesis conditions and the unavailability of robust experimental techniques to probe nanointerfaces at the microscopic level. Here we present a density functional theory investigation of the interaction of Sn_2S_6 ligands with InAs NCs. Employing a grand canonical approach, we considered a multitude of structural features possibly realized at the NC-ligand interface, such as surface termination, reconstructions and passivation, substitution of subsurface atoms, ligand dissociation, NC core-shell formation and the adsorption of the ligands on NCs with different structures. This study provides guidance about the experimental conditions which lead to specific structural motifs and highlights the impact of structural details on the electronic properties of the composite.

HL 71.8 Thu 12:00 EW 201

Graphene 3D Electrodes for Energy Storage Applications — •Evangelos Makrygiannis, Simon Drieschner, Michael Weber, and Jose A. Garrido — Walter-Schottky-Institut, Physik Department, TU München, Am Coulombwall 4, 85748 Garching

Due to its unique properties like high conductivity, chemical stability, and high surface to volume ratio, graphene meets the most essential requirements for fabricating electrodes with high electrical double layer capacitance for supercapacitor applications. Here we present the fabrication and characterization of graphene foam based electrodes for energy storage applications. Chemical vapor deposition (CVD) is used to grow graphene foam samples with nickel foam as a substrate. Different growth parameters are investigated in order to obtain stable three-dimensional structures as well as to achieve high graphene quality, which is confirmed by Raman spectroscopy. To decrease the equivalent series resistance and to have a highly inert contact, multilayer CVD graphene sheet was used to connect the foam to the current collector. Cyclic voltammetry, electrochemical impedance spectroscopy, and charge discharge measurements in various electrolytes are performed to assess the potential of these three-dimensional graphene electrodes for energy storage applications.

HL 71.9 Thu 12:15 EW 201

Conductive polymers on microporous graphene based electrodes for supercapacitor applications — •Michael Weber, Simon Drieschner, Evangelos Markrygiannis, and Jose A. Garrido — WSI,Physik-Departement,Technische Universität München,James-Franck-Str.1,85748 Garching,Germany

Conductive polymers have been studied as pseudocapacitive electrode material owing to their high specific capacitance and high reaction rates. In order to increase the surface area and to have a efficient charge tranfer, a highly conductive three-dimensional current collector is required for supercapacitors providing high power density. Graphene-based electrodes have a high specific area, a high conductivity and are chemical inert, which makes them a promising current collector material for supercapacitor applications.

Here we present three dimensional graphene electrodes coated with conductive polymers by electropolymerization and chemical polymerization for supercapacitor electrodes. As conductive polymers polyaniline, polypyrrole and polyphenylene were polymerized with different polymerization parameters like temperature and concentration. Polyaniline and polypyrrole are moderate conductive p-doped polymers, chemically stable in aqueous solutions and can be polymerized

out of inexpensive precursers. Polyphenylene is a p- or n-doped conductive polymer which enables it to be operated in a high potential window in non-aqueous electrolytes. Their potential for supercapacitors is confirmed by cyclic voltammetry, electrochemical impedance spectroscopy and charge-discharge measurements.

HL 72: Quantum wires

Time: Thursday 10:15–11:45 Location: EW 203

HL 72.1 Thu 10:15 EW 203

Random Distribution of Phase Domains in Single Nanowires — •Arman Davtyan, Otmar Loffeld, and Ullrich Pietsch — Naturwissenschaftlich-Technische faculty, University of Siegen, Siegen, Germany

Investigation of the polytype structure of single GaAs nanowires grown on GaAs(111) have been performed using Coherent x-ray Diffraction Imaging (CDI) at the ID1 beamline of ESRF. The high number of twin defects gives rise to the complex speckle pattern instead of expected zinc blende (ZB), twin zinc blende (TZB) or wurtzite (WZ) structural peaks. Because the phase information is lost in the experiment it has to be retrieved by means of Phase Retrieval (PR) procedure. Although fast convergence of retrieved amplitudes the use of different trail phases provides different solutions for the phase pattern. Therefore no unique solution of the stacking fault distribution can be obtained. Here we show that the set of retrieved phase pattern contains hidden statistical information about the average number of the twin defects within the NW. In order to get more inside into the problem we simulated various polytype distributions in highly defective NWs and calculated the resulting speckle pattern. It turned out that already a stack of 2-3 perfect ordered zinc-blende and twinned zinc-blende units provides Bragg like intensity maxima. Therefore the measured speckle pattern can only be interpreted by a completely random distribution of these phase units.

HL 72.2 Thu 10:30 EW 203

Electrical properties of freestanding GaAs nanowires investigated by a multi-tip STM — •Matthias Steidl[1], Stefan Korte[2], Weihong Zhao[1], Hubertus Junker[2], Werner Prost[3], Vasily Cherepanov[2], Bert Voigtländer[2], Peter Kleinschmidt[1], and Thomas Hannappel[1] — [1]Photovoltaics Group, Institute for Physics, Technische Universität Ilmenau, D-98684 Ilmenau — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, D-52425 Jülich and JARA-Fundamentals of Future Information Technology — [3]CeNIDE and Center for Semiconductor Technology and Optoelectronics, University of Duisburg-Essen, D-47057 Duisburg

We have grown undoped and p-type Zn-doped GaAs-Nanowires (NW) on GaP(111)B using the Au-assisted vapor-liquid-solid growth mode in a metal-organic vapor phase apparatus with different growth procedures. For the electrical characterization we applied a multitip STM as a nanoprober and conducted four-point probe measurements on single free-standing NWs. The doped NWs show highly non-linear I-V curves with diode like behavior. This reveals the existence of a space charge region along the NW axis, which we attribute to variations in the doping concentration. Furthermore, spatially resolved measurements of electron beam induced current (EBIC) indicate the width and localization of this space charge region. These measurements reveal that both the resistivity and the localization of the space charge region is dependent on the growth condition.

HL 72.3 Thu 10:45 EW 203

Optical properties of ultrathin GaAs-AlGaAs core-shell nanowires — •Julia Winnerl[1], Bernhard Loitsch[1], Daniel Rudolph[1], Stefanie Morkötter[1], Gianluca Grimaldi[1], Lukas Hanschke[1], Lucas Schweickert[1], Max Bichler[1], Gerhard Abstreiter[1,2], Jonathan Finley[1], and Gregor Koblmüller[1] — [1]Walter Schottky Institut and Physik Department, Technische Universität München, Garching, Germany — [2]Institute for Advanced Study, Technische Universität München, Garching, Germany

III-V semiconductor nanowires (NWs) are known to provide a large field for many applications in electronic and optoelectronic devices. In many of these NW device applications, the electronic properties of the NWs are mostly described by the 3D bulk-like properties of the NW core, in spite of the 1D-like structure of the NWs. Performance enhancements in such NW device applications are expected from exploiting 1D-quantum confinement effects. Here, we present the optical properties of GaAs-$Al_{0.3}Ga_{0.7}As$ core-shell NWs epitaxially grown on silicon with GaAs core diameters below 10 nm. Low-temperature micro-photoluminescence (PL) measurements reveal strongly blue-shifted PL energies (up to ∼100 meV) compared to the free exciton emission of GaAs. This indicates strong radial 1D-quantum confinement of the GaAs NW core. In addition, the strongly blue-shifted PL shows some sharp PL lines indicating that additional axial confinement effects of the excitons are present. Time-resolved PL experiments show clear bi-exponential decay transients that could be attributed to different recombination channels of these localized excitons.

HL 72.4 Thu 11:00 EW 203

Photoluminescence excitation measurements on ultrathin GaAs-AlGaAs core-shell nanowires — •Gianluca Grimaldi, Bernhard Loitsch, Daniel Rudolph, Stefanie Morkötter, Lukas Hanschke, Lucas Schweickert, Max Bichler, Gerhard Abstreiter, Jonathan Finley, and Gregor Koblmüller — Walter Schottky Institut, Technische Universität München, Garching, Germany

Thin semiconductor nanowires (NWs) can achieve quantum confinement of carriers in the radial direction, potentially enhancing performances of NW-based devices. Using a novel reverse-reaction growth scheme, GaAs-AlGaAs core-shell NWs with tunable core diameters down to below 10 nm can be epitaxially integrated on silicon [1].

Here we report on micro-photoluminescence spectroscopy (μ-PL) and photoluminescence excitation spectroscopy (PLE) on GaAs-AlGaAs core-shell NWs with ultrathin core diameters (7-20 nm). Along with the blueshift of PL, arising from radial confinement in the thin NW core, multiple sharp peaks are observed, with FWHM below 100 μeV. Power-dependent PL reveal saturation of these peaks for high excitation power, further suggesting presence of localized exciton states. PLE experiments show resonances, whose energy distance is smaller than what expected for excited states of the radial confinement, suggesting that additional confinement in the axial direction is present. The axial localization is attributed to the presence of wurtzite and zincblende stacking along the NWs.

Reference: [1] B. Loitsch, et al., in review (2014)

HL 72.5 Thu 11:15 EW 203

Optical characterization of high-periodicity InGaAs-InAlAs-based core-shell nanowire arrays — •Maximilian Speckbacher[1], Julian Treu[1], Thomas Stettner[1], Stefanie Morkötter[1], Markus Döblinger[2], Sonja Matich[1], Kai Saller[1], Max Bichler[1], Markus Christian Amann[1], Jonathan Finley[1], Gerhard Abstreiter[1,3], and Gregor Koblmüller[1] — [1]Walter Schottky Institut and Physik Department, TU München, Garching, Germany — [2]Department of Chemistry, Ludwig-Maximilians-Universität München, Munich, Germany — [3]TUM Institute for Advanced Study, Garching, Germany

$In_{1-x}Ga_xAs$ nanowires (NWs), site-selectively grown by molecular beam epitaxy (MBE) on Si(111) substrates and passivated insitu with an according lattice matched $In_{1-x}Al_xAs$ shell, were analyzed in depth using micro-photoluminescence (μ-PL). Varying both Ga- as well as Al-content allows for effective bandgap engineering, tuning the peak emission over a broad range across the important telecommunication regime. The core-shell NWs significantly enhance peak intensities compared to the unpassivated case with emission even up to room-temperature. This opens numerous opportunities for advanced NW-based heterostructures, such as integrated nanophotonic sources on Si (for hybrid III/V-Si photonics) and NW-based photovoltaics.

HL 72.6 Thu 11:30 EW 203

Angle dependent magnetoconductance oscillations and Hall measurements in GaAs/InAs Core/Shell Nanowires — •Patrick Zellekens[1,2], Fabian Haas[1,2], Nathalia Demarina[1,2], Torsten Rieger[1,2], Mihail Lepsa[1,2], Detlev Grützmacher[1,2], Hans Lüth[1,2], and Thomas Schäpers[1,2] — [1]Peter Grünberg In-

stitute (PGI-9 and PGI-2), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA – Fundamentals of Future Information Technologies

GaAs/InAs core/shell nanowires contain a cylindrical tube like conductor in the narrow bandgap InAs shell wrapping the wide bandgap GaAs core. These core/shell nanowires have been subject of flux dependent quantum transport measurements.

In this contribution, we present angle dependent magnetotransport measurements of GaAs/InAs core/shell nanowires with Hall contacts at various temperatures in a magnetic field applied at different tilt angles to the wire axis. Thereby it is possible to measure the crossover from flux periodic magnetoconductance oscillations ($B_{\parallel}$) to the regime of universal conductance fluctuations ($B_{\perp}$). A detailed analysis show clear indications of an anisotropic phase coherence length.

The same approach is also used to measure the Hall voltage in this nanowires for different temperatures and gate voltages to calculate the carrier concentration and mobility.

HL 73: Graphene: Structure (O with HL/TT)

Time: Thursday 10:30–13:00 Location: MA 041

HL 73.1 Thu 10:30 MA 041

Manganese Intercalation in Graphene/Ir(111): a structural study — •Stefan Böttcher[1], Hendrik Vita[1], Yuriy S. Dedkov[2], and Karsten Horn[1] — [1]Fritz-Haber Institute, Faradayweg 4-6, 14195 Berlin — [2]SPECS Surface Nano Analysis GmbH, Voltastrasse 5, 13355 Berlin

The graphene/substrate interaction is of interest for a many applications, and to understand and classify the interaction mechanism as such. For example, the 3d transition metals Fe, Co and Ni on the one hand, and Cu on the other suggest that a classification into strongly and weakly interacting systems may be possible, as judged by criteria such as the survival of the Dirac cone or the crystallographic structure of the graphene layer. Here we present a structural study, through LEED and STM, of manganese intercalation on graphene/Ir(111), a system that has so far not been studied. We follow the stages of the intercalation process, from the deposition of Mn on top through the formation of the intercalated phase. Manganese is found to be arranged pseudomorphically to the Ir(111) substrate underneath graphene. While several criteria for a weak interaction are fulfilled, the graphene/Mn/Ir(111) system also shows structural evidence for a strong interaction between the graphene and the Mn layer, e.g. a lower separation between graphene and the intercalated layer, a conclusion that is further supported by ARPES. Manganese intercalation may therefore be special because it fills the gap between the strongly and weakly interacting transition metals. In addition, at higher intercalation temperatures a new, possibly surface alloyed phase is observed.

HL 73.2 Thu 10:45 MA 041

Manganese Intercalation in Graphene/Ir(111): electronic structure — •Hendrik Vita[1], Stefan Böttcher[1], Yuriy Dedkov[2], and Karsten Horn[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]SPECS Surface Nano Analysis GmbH, Berlin, Germany

Transition metal surfaces are ideal templates for the growth of high quality graphene films. The system graphene/Ir(111) shows rather weak interaction between substrate and the graphene layer. It is well known that transition metals such as Ni and Co, intercalated under graphene/Ir(111), show a rather strong interaction with graphene, yielding massive modifications of the graphene π-band. The intercalation of Mn thin films underneath graphene seems interesting in this context, since Mn has a half filled 3d shell, and the graphene sheet may act as an inert, passivating cover. Here we investigate graphene/Mn/Ir(111) by deposition on top of graphene/Ir(111), and follow the intercalation process by annealing at moderate temperatures using XPS. Investigating the band structure by high resolution ARPES, the Dirac cone is preserved, and we observe a trigonal suppression of the replica Dirac cones, probably due to an enhanced corrugation of the graphene film. A totally different situation occurs if the intercalation process is performed at much higher temperatures. Drastic changes in the band structure emerge, with a shifted π-band to higher binding energies, and a chemical shift of the C1s core level. Additionally, a restructuring of the intercalated Mn thin film is observed by LEED.

HL 73.3 Thu 11:00 MA 041

Atomically Resolved Graphitic Surfaces in Air by Atomic Force Microscopy — •Daniel S. Wastl, Alfred J. Weymouth, and Franz J. Giessibl — University of Regensburg, Universitätsstrasse 31, 93053 Regensburg, Germany

Imaging at the atomic scale with atomic force microscopy in biocompatible environments is an ongoing challenge. We demonstrate here atomic resolution of graphite and hydrogen-intercalated graphene on SiC in air1. The main challenges arise from the overall surface cleanliness and the water layers which form on almost all surfaces2. To further investigate the influence of the water layers, we compare data taken with a hydrophilic bulk-silicon tip to a hydrophobic sapphire tip. While atomic resolution can be achieved with both tip materials at moderate interaction forces, the strong differences in force versus distance spectra can be related to the water layers on the tips and samples. Imaging at very low tip-sample interaction forces results in the observation of large terraces of a naturally-occurring stripe structure on the hydrogen intercalated graphene[1]. This structure has been previously reported on graphitic surfaces that are not covered with disordered adsorbates in ambient conditions (i.e. on graphite and bilayer graphene on SiC[3], but not on monolayer graphene on SiC). Both these observations indicate that hydrogen-intercalated graphene is close to an ideal graphene sample in ambient environments.

[1] Wastl, Weymouth, Giessibl, ACS Nano 8, 5233 (2014).
[2] Wastl Weymouth, Giessibl, Phys. Rev. B 87, 245415 (2013).
[3] Wastl et al., ACS Nano 7, 10032 (2013).

HL 73.4 Thu 11:15 MA 041

A route to free-standing graphene by removal of the Ni substrate by a gas phase reaction — •Ann-Kathrin Henss[1], Patrick Zeller[1], Michael Weinl[2], Matthias Schreck[2], and Joost Wintterlin[1] — [1]Ludwig-Maximilians-Universität, Munich, Germany — [2]Universität Augsburg, Augsburg, Germany

An essential step for the use of graphene in electronic devices is the removal of the underlying metal substrate after graphene growth. We have tested a new route to free-standing graphene grown on thin single crystalline Ni(111) films. The 150 nm thick metal films were epitaxially grown on a Si(111) wafer separated by a 120 to 150 nm thick yttria-stabilized zirconia (YSZ) buffer layer. Aligned monolayer graphene was grown by chemical vapor deposition using ethylene as precursor gas under ultra high vacuum conditions. The graphene quality was monitored by scanning tunneling microscopy and low energy electron diffraction. The subsequent removal of the nickel substrate was performed in a pure gas phase reaction. In the so called Mond process, a chemical transport reaction, nickel reacts with carbon monoxide to gaseous nickel tetracarbonyl at 350 K. By applying a temperature gradient in the reaction furnace the formed carbonyl complex is transported to areas with higher temperature leaving graphene on the isolating YSZ buffer layer of the substrate. X-ray photoelectron spectroscopy, scanning electron microscopy and Raman spectroscopy were used to study the samples after this process.

HL 73.5 Thu 11:30 MA 041

Freestanding lateral nanostructures of two-dimensional carbon materials — •Andreas Winter[1], Yasin Ekinci[2], Rainer Stosch[3], Thomas Weimann[3], Johannes Biskupek[4], Ute Kaiser[4], and Andrey Turchanin[1] — [1]Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany — [2]Laboratory for Micro- and Nanotechnology, Paul Scherrer Institut, 5232 Villigen, Switzerland — [3]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany — [4]Electron Microscopy Group of Materials Science, Ulm University, 89081 Ulm, Germany

Two-dimensional (2D) carbon materials like graphene, hexagonal boron nitride or carbon nanomembranes (CNMs) have recently attracted enormous interest due to their potential use in electronics, chemical and biological sensors, nanofilters, hybrid materials etc. Most

applications require a lithographic patterning of these 2D materials. Here we present various micro- and nanostructures of graphene and CNMs as well as their in-plane heterostructures fabricated via optical, e-beam and EUV interference lithography. The preparation of these structures on supporting substrates as well as large area freestanding nanomembranes with patterns varying from ca. 100 μm to 50 nm will be shown. Via electron irradiation, graphene and dielectric CNMs can be stitched together, forming electrically heterogeneous ultrathin 2D carbon sheets. We characterize their properties employing X-ray photoelectron and Raman spectroscopy, helium ion microscopy and high-resolution TEM.

HL 73.6 Thu 11:45 MA 041

Graphene Membranes as Electron Transparent Windows for Photoelectron Spectroscopy — •Jürgen Kraus[1], Robert Reichelt[1], Sebastian Günther[1], Luca Gregoratti[2], Matteo Amati[2], Maya Kiskinova[2], Alexander Yulaev[4], Ivan Vlassiouk[3], and Andrei Kolmakov[4] — [1]TU München Chemie Department, Lichtenbergstr. 4, D-85748 Garching — [2]Sincrotrone Trieste, Area Science Park, 34149 Trieste, Italy — [3]Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA — [4]Center for Nanoscale Science and Technology, NIST, Gaithersburg, MD 20899, USA

The high mechanical stability of graphene (g) allows the construction of ultrathin gas tight membranes. Transferred few layer thick g covering the orifice of an environmental cell could be used to seal a water droplet inside the cell from the surrounding vacuum of the ultra-high vacuum chamber into which the cell was introduced. The used membranes were transparent even for slow photoelectrons (PEs), so that the sealed water could be characterized by x-ray photoelectron spectroscopy (XPS). We also measured the electron attenuation length of monolayer g on Cu for PEs of 200-1000 eV kinetic energy. We were able to produce free standing monolayer g by locally electrochemically etching the Cu-substrate underneath the as-grown g. After deposition of gold on the membrane backside and acquiring Au 4f PEs from the opposite site, we proved that $< 1\%$ of a monolayer Au can be detected through the suspended g membrane. This pushes the applicability of our membrane based XPS technique towards surface characterization under ambient conditions.

HL 73.7 Thu 12:00 MA 041

Irradiation of Graphene-FETs with highly charged Ions — •Philipp Ernst[1], Roland Kozubek[1], Oliver Ochedowski[1], Jens Sonntag[2], Axel Lorke[2], and Marika Schleberger[1] — [1]Universität Duisburg-Essen, AG Schleberger, Duisburg, Germany — [2]Universität Duisburg-Essen, AG Lorke, Duisburg, Germany

We have studied the influence of ion bombardment on the properties of graphene field-effect transistor (FET) structures. We used highly charged ions (HCI) with different potential energies at roughly the same kinetic energy (charge state Xe^{32+} and Xe^{25+} with $E_{kin} = 220$ keV and $E_{kin} = 195$ keV). Electrical transport measurements, Raman spectroscopy, and atomic force microscopy were used to investigate the electrical and structural modifications of the graphene-FETs induced by the ion irradiation. The electrical analysis was performed *in-situ* in the ultra-high vacuum set up used for the irradiation. For all investigated fluences, the experiments show a reduction of the mobility, which scales with the potential energy of the ions. Remarkably, the influence of the impact of highly charged ions is already measurable at extremly low fluences < 15 ions/μm^2. As a consequence of the irradiation, a p-doping effect could be observed. Further experiments at lower kinetic energies (< 50 keV) are planned to clarify how the potential energy of the impinging HCIs will affect the observed irradiation effects in graphene.

HL 73.8 Thu 12:15 MA 041

Increasing the mobility of holes in graphene FETs by irradiation with swift heavy ions — •Tobias Foller, Philipp Ernst, Oliver Ochedowski, Roland Kozubek, Lukas Madauss, and Marika Schleberger — Fakultät für Physik and CeNIDE, Universität Duisburg-Essen, 47048 Duisburg, Germany

In this work graphene field-effect transistors (FETs) are modified by irradiation with swift heavy ions (SHI, Xe^{23+} with $E_{kin} = 91$ MeV). Graphene FETs are prepared by exfoliation of a HOPG crystal followed by deposition of metal contacts via Photolithography. They allow to investigate the mobility of charge carriers in graphene. Current measurements, Raman spectroscopy and atomic force microscopy have been used to investigate the electrical and structural modifications of graphene due to the ion irradiation. By irradiation with swift heavy ions under perpendicular incidence with small fluences (≈ 2500 ions/μm^2), we have succeeded in almost doubling the mobility of holes compared to the unirradiated sample.On the other hand irradiation under glancing incidence ($\leq 2°$) with fluences of 10 ions/μm^2 have revealed that, despite the rather small changes in the (I_D/I_G)-ratio in the Raman spectrum, the charge carrier mobility is significantly reduced.

HL 73.9 Thu 12:30 MA 041

Structure, strain distribution and energetics of basal-plane dislocations in bilayer graphene — •Konstantin Weber and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

A recent TEM study [1] demonstrated that substrate-grown graphene bilayers are typically not perfect in registry, but contain a high concentration of basal-plane dislocations. Using atomistic simulations based on the registry-dependent potential of Kolmogorov and Crespi [2] and the classical AIREBO potential we investigated the atomic structure and the properties of the 4 different types of dislocations with shortest possible Burgers vector in bilayer graphene, the thinnest imaginable crystal that can host such 1D defects. We find that each of the 4 different dislocations splits into two partial dislocations. The partials are equally spaced due to the absence of a stacking fault energy, a peculiar property of bilayer graphene. Furthermore, partials with a step component give rise to a pronounced buckling of the graphene bilayer. An analysis of the atomic structure, local strain distribution, disregistry and dislocation energy of the dislocations will be given and we will highlight how their properties differ from textbook examples of dislocations in 3D crystals.

[1] B.Butz, C. Dolle, F. Niekiel, K. Weber, D. Waldmann, H.B. Weber, B. Meyer, E. Spieker, *Nature* **505**, 533 (2014).
[2] A. Kolmogorov, V. Crespi, *Phys. Rev. B* **71**, 235415 (2005).

HL 73.10 Thu 12:45 MA 041

Plasma-enhanced chemical vapor deposition of graphene on metallic substrates — •Nicolas Wöhrl[1], Oliver Ochedowski[2], Steven Gottlieb[2], Stephan Schulz[1], and Volker Buck[2] — [1]Faculty of Chemistry and CENIDE, University Duisburg-Essen, 47057 Duisburg, Germany — [2]Faculty of Physics and CENIDE, University Duisburg Essen, 47057 Duisburg, Germany

In this work we present the synthesis of graphene on copper and nickel substrates by microwave Plasma-enhanced Chemical Vapor Deposition (PE-CVD) process. The special construction of the plasma source allows the deposition at a wide range of different process parameters giving a fast and inexpensive method to synthesize graphene. Additional advantages of the plasma deposition of graphene are lower substrate temperatures compared with thermal CVD processes. In contrast to the thermal CVD the gaseous precursors are already decomposed in the plasma and the plasma parameters are varied to investigate the influence on the nucleation and growth of graphene and on the defect density in the graphene layers. Optical emission spectroscopy is used to characterize the plasma properties while Raman spectroscopy and AFM measurements are used as nondestructive tools for the characterization of the synthesized graphene films. Especially Raman spectroscopy is used as a suitable tool to determine the number of graphene layers, the disorder and the defect density. We present a possible way to produce large area of monolayer graphene on metallic substrates with the prospect to make graphene available for industrial applications.

HL 74: Frontiers of electronic structure theory: 2D TMDC and excitonic effects

Time: Thursday 10:30–13:15 Location: MA 004

Invited Talk HL 74.1 Thu 10:30 MA 004

Interaction and Correlation Effects in Quasi Two-dimensional Materials — •Steven G. Louie — Physics Department, University of California at Berkeley, and Lawrence Berkeley National Lab, Berkeley, CA 94720 USA

Experimental and theoretical studies of atomically thin quasi two-dimensional materials and their nanostructures have revealed that these systems can exhibit highly unusual behaviors. Owing to their reduced dimensionality, these systems present opportunities for manifestation of concepts/phenomena that may not be so prominent or have not been seen in bulk materials. Symmetry and many-body interaction effects often play a critical role in shaping qualitatively and quantitatively their properties. In this talk, we present some theoretical studies on graphene as well as other quasi-2D systems such as monolayer and few-layer transition metal dichalcogenides (e.g., MoS2, MoSe2, WS2, and WSe2) and metal monochalcogenides (such as GaSe and FeSe). Several quantum phenomena are discussed, including novel and dominant exciton effects, tunable magnetism, electron supercollimation by disorder, unusual plasmon behaviors, and possible enhanced superconductivity in some of these systems. We investigate their physical origins and compare theoretical predictions with experimental data.

HL 74.2 Thu 11:00 MA 004

Screening of the Coulomb interaction in two-dimensional semiconductors: The case of transition metal dichalcogenides — •Ersoy Sasioglu, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute forAdvanced Simulation, Forschungszentrum Jülich and JARA, 52425Jülich, Germany

Experimentally determined large exciton binding energies and nonhydrogenic Rydberg series in monolayer transition metal (TM) dichalcogenides indicate a long-range behavior of the Coulomb interaction. By means of first-principles calculations in conjunction with the random-phase approximation [1,2] within the FLAPW method [3] we study screening of the Coulomb interaction in two-dimensional semiconducting TM dichalcogenides MX_2 (M=Cr, Mo, W; X=S, Se). We show that the screening in these systems deviates substantially from the bulk behavior, i.e., the short-range interaction is strongly screened, while the long-range interaction is anti-screened. This unconventional screening reduces the gradient of the Coulomb interaction giving rise to weak correlation effects, which explains the experimentally observed large exciton binding energies as well as the success of the one-particle density functional theory in the description of the electronic structure of these systems. This work has been supported in part by DFG-FOR-1346.

[1] C. Friedrich *et al.*, Phys. Rev. B. **81**, 125102 (2010).
[2] E. Şaşıoğlu *et al.*, Phys. Rev. B **83**, 121101(R) (2011).
[3] www.flapw.de

HL 74.3 Thu 11:15 MA 004

Ultra-fast transient absorption spectra of monolayer MoS2 by first principle — •Margherita Marsili[1], Deborah Prezzi[1], Davide Sangalli[2], and Andrea Marini[2] — [1]CNR Istituto di Nanoscienze S3, Modena, Italy — [2]CNR ISM, Montelibretti, Italy

We compute ultrafast transient absorption spectra of MoS2 monolayers by employing a novel approach which combines density-functional and non-equilibrium Green's function theories. This approach allows the description of pump-probe optical experiments where the system is excited by an ultrashort laser pulse, and the variation of the optical response is probed at different time delays, thus providing a wealth of information on the fundamental physics of the relaxation processes. The case of monolayer MoS2 is extremely challenging due to the interplay of excitonic, electron-phonon and spin-orbit coupling effects. We describe the excitation of the MoS2 electronic system and follow the subsequent dynamics using a fully non-collinear spin formulation of the theory, including excitonic effects. The results are compared with experimental pump-probe data.

HL 74.4 Thu 11:30 MA 004

Plasmon and exciton dispersion in two dimensions — •Pier Luigi Cudazzo — LSI Ecole Polytechnique and ETSF, Palaiseau, France

Understanding the electronic properties of 2D materials requires the investigation of their elementary excitations that dictate their optical and transport properties. Using state-of-the-art Green's function many body approach we present a first principle study of the collective excitations (namely excitons and plasmons) in 2D materials. In particular from the evaluation of the dielectric function we investigated the exciton dispersion in graphane and hBN and the plasmon dispersion in metallic TMDs[1-3]. From our results we provide an exact analytic form of the two-dimensional screened potential. In contrast to 3D systems where the macroscopic screening can be described by a static dielectric constant in 2D systems the macroscopic screening is non local (q-dependent) showing a logarithmic divergence for small distances and reaching the unscreened Coulomb potential for large distances[4].

[1] P. Cudazzo, et. al. New J. Phys. 15 125005 (2013). [2] P. Cudazzo, et. al. (in preparation) [3] P. Cudazzo, et. al. Phys. Rev. Lett. 104 226804 (2010). [4] P. Cudazzo, et. al. Phys. Rev. B 84 085406 (2011).

HL 74.5 Thu 11:45 MA 004

Origin of metallic edge states in transition-metal-dichalcogenide nanostructures — •Marco Gibertini and Nicola Marzari — Theory and Simulation of Materials (THEOS) and National Center for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, Switzerland

The existence of metallic edge states in transition-metal-dichalcogenide nanostructures has been reported both in the experimental and theoretical literature. Such nanostructures include for instance triangular islands and zigzag nanoribbons. Nonetheless, a thorough understanding of the mechanism giving rise to metallic states at the edge of such bulk insulating materials is still missing. Here we suggest a possible origin of such states and support our findings with first-principles density-functional-theory simulations. The key observation is that transition metal dichalcogenides like MoS_2 display a finite *formal* polarization that induces a charge reconstruction with the appearance of free carriers at the edges. We also suggest possible innovative applications in nanoelectronics and solar-energy devices.

HL 74.6 Thu 12:00 MA 004

Starting-point dependence in the Bethe-Salpeter equation: example of rutile TiO_2 — •Olga Turkina, Ute Werner, Dmitrii Nabok, and Claudia Draxl — Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Zum Großen Windkanal 6, D-12489 Berlin, Germany

Many-body perturbation theory, combining the GW approach and the Bethe-Salpeter equation (BSE), is a powerful tool for the description of one- and two-particle excitations. However, employing density functional theory as a starting point for these methods may lead to results that depend on the choice of the exchange-correlation (xc) functional. This starting-point dependence is well known for the G_0W_0 approximation. Such dependence is expected to occur also for BSE calculations, however, has not yet been investigated. With the example of rutile TiO_2, we show that this is, indeed, the case. We employ two different xc functionals: the generalized gradient approximation (PBE) and a hybrid functional (PBE0'), combining a fraction of 25% exact exchange with PBE. The electronic structure is calculated using the G_0W_0 approximation. The BSE is solved to obtain the optical absorption spectra. These are analyzed with regard to the influence of eigenvalues, wave functions, and screening as originating from different xc functionals.

HL 74.7 Thu 12:15 MA 004

Efficient exchange-correlation kernels for the description of excitonic effects in solids — •Santiago Rigamonti[1,4], Silvana Botti[2,4], Valérie Veniard[3,4], Claudia Draxl[1,4], Lucia Reining[3,4], and Francesco Sottile[3,4] — [1]Physics Department, Humboldt-Universität zu Berlin, Germany — [2]Friedrich-Schiller Universität Jena, Institut für Festkörpertheorie und -optik — [3]Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-DSM, F-91128 Palaiseau, France — [4]European Theoretical Spectroscopy Facility (ETSF)

One of the major challenges for time-dependent density-functional the-

ory is the accurate and efficient description of excitonic effects in solids, captured by the exchange-correlation (xc) kernel. In a recent empirical approach, the so-called "bootstrap" kernel has been proposed. Due to its high efficiency and some promising results [1] it appeared indeed interesting. In this work, we find a physically motivated derivation for it, opening the way to understand its weaknesses and to propose a new xc kernel. Our kernel is both simpler and more reliable, as confirmed by our numerical results [2]. We also propose a simple method to estimate exciton binding energies from the dielectric functions computed in the random-phase approximation alone. This method makes the approach accessible to a wide range of scientists.

[1] S. Sharma, J. K. Dewhurst, A. Sanna, and E. K. U. Gross, *Phys. Rev. Lett.* **107**, 186401 (2011).
[2] S. Rigamonti, S. Botti, V. Veniard, C. Draxl, L. Reining, and F. Sottile, *submitted*.

HL 74.8 Thu 12:30 MA 004

Excitonic effects in many-body calculations — •Matteo Gatti[1,2], Igor Reshetnyak[1], Giorgia Fugallo[1], Pierluigi Cudazzo[1], Francesco Sottile[1], and Lucia Reining[1] — [1]LSI, CNRS-Ecole Polytechnique and ETSF, Palaiseau, France — [2]Synchrotron Soleil, Gif-sur-Yvette, France

The Bethe-Salpeter equation (BSE) is the state-of-art approach to calculate the absorption spectra of a large variety of materials [1]. Here we show that that the BSE is a powerful and accurate method also for the calculation of the exciton dispersion [2-4] (i.e. the exciton energy as a function of the momentum q carried by the electron-hole pair), and of the off-diagonal elements of the dielectric function in reciprocal space $\epsilon_{G,G'}(q,\omega)$ [5]. On the one hand, this allows the ab initio simulation of spectra measured by Electron Energy-Loss Spectroscopy (EELS) and Inelastic X-ray Scattering (IXS), including its Coherent version (CIXS), well beyond the optical limit $q \to 0$. On the other hand, this opens the door to the calculation of spectral functions [6-8] using the cumulant expansion for the Green's function G with a screened Coulomb interaction W that includes excitonic effects beyond the random-phase approximation employed in the GW approximation.

[1] G. Onida, *et al.*, Rev. Mod. Phys. **74**, 601 (2002). [2] M. Gatti and F. Sottile, Phys. Rev. B **88**, 155113 (2013). [3] P. Cudazzo, *et al.*, Phys. Rev. B **88**, 195152 (2013). [4] G. Fugallo, *et al.*, unpublished. [5] I. Reshetnyak, *et al.*, unpublished. [6] M. Guzzo, *et al.*, Phys. Rev. Lett. **107**, 166401 (2011). [7] M. Gatti and M. Guzzo, Phys. Rev. B **87**, 155147 (2013). [8] M. Guzzo, *et al.*, Phys. Rev. B **89**, 085425 (2014).

HL 74.9 Thu 12:45 MA 004

Efficient parameter-free calculation of absorption spectra for insulators, semiconductors and metals from time-dependent current DFT — •Arjan Berger — LCPQ - IRSAMC, Université de Toulouse III - Paul Sabatier, CNRS, Toulouse, France and European Theoretical Spectroscopy Facility

In this work we show that with a simple dynamical kernel we can obtain good absorption spectra from time-dependent current-density functional theory (TDCDFT) for insulators, semiconductors and metals. Our approach is fully parameter free since no artificial broadening parameter is used to match calculated and measured spectra. The cost of a calculation is equal to an RPA calculation. Moreover, our TDCDFT approach scales better with system size than standard TDDFT implementations.

HL 74.10 Thu 13:00 MA 004

Optical excitations in MoS_2 within ab-initio many-body perturbation theory — •Matthias Drüppel, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

The transition metal dichalcogenides (TMDC), and MoS_2 as its most prominent member, open the door to a field of two dimensional atomically thin semiconductors which offer rich physics.

The state of the art theoretical description of electronic excitations in these materials starts with density-functional calculations (DFT), followed by the GW method in combination with a solution of the Bethe-Salpeter equation. The *converged* calculation (especially with respect to the size of the basis, i.e. number of plane waves, and k-meshs) of the last two steps has shown to be numerically extremely challenging.

We apply the efficient LDA+GdW [1] approach to the excited states which enables us to describe electronic excitations in MoS_2 at substantially lower numerical cost. In the LDA+GdW approximation the quasiparticle self-energy corrections to the LDA-DFT energies result from the difference between the correct screening (semiconducting) and hypothetical metallic screening.

This approach sets us in a position where more atoms per unit cells can be treated, e.g., for defects and for MoS_2 on substrates.

[1] M. Rohlfing, Phys. Rev. B. **82**, 205127 (2010)

HL 75: Transport: Quantum dots, quantum wires, point contacts 1 (TT with HL)

Time: Thursday 11:00–13:00 Location: A 053

HL 75.1 Thu 11:00 A 053

Interference of real and virtual transitions in quantum dot chains — •Fernando Gallego-Marcos, Rafael Sánchez, and Gloria Platero — Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Spain

We analyzed long-range transport through an ac driven triple quantum dot. Resonant transitions between separated and detuned dots are mediated by the exchange of n photons with the time-dependent field. An effective model is proposed in terms of higher-order transitions which involve the virtual only occupation of the intermediate dot [1]. The ac driving modulates the tunneling processes within the quantum dot system [2]. We investigate the interplay between real transitions through the centre dot and virtual long-range tunneling. We find configurations where the two paths interfere destructively and totally block the current. The effect of the driving phase will be emphasized.

[1] R. Sánchez, F. Gallego-Marcos, G. Platero,
Phys. Rev. B 89, 161402 (2014)
[2] F. Gallego-Marcos, R. Sánchez, G. Platero, arXiv:1408.4923

HL 75.2 Thu 11:15 A 053

Photon creation of a double quantum dot strongly coupled to the environment — •Michael Marthaler[1], Yasuhiro Utsumi[2], and Dmitri Golubev[3] — [1]Institut für Theoretische Festkörperphysik , Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany — [2]Department of Physics Engineering, Faculty of Engineering, Mie University, Japan — [3]O.V. Lounasmaa Laboratory, Aalto University School of Science, Finnland

We study a model which can describe a double quantum dot coupled to a transmission-line resonator. The charge eigenstates of the double dot couple strongly to the electromagnetic environment or phonons. We consider a situation where a transport voltage is applied and photons are created in the transmission-line resonator. Here we study the dependence of the average photon number in the resonator on the spectral function of the electromagnetic environment. We focus on three important cases, a strongly coupled environment with a small cut-off frequency, a structured environment peaked at a specific frequency and 1/f noise. We find that the electromagnetic environment can have a substantial impact on the photon creation. Resonance peaks are in general broadened and additional resonances can appear.

HL 75.3 Thu 11:30 A 053

Unconventional Superconductivity in Double Quantum Dots — Björn Sothmann[1], •Stephan Weiss[2], Michele Governale[3], and Jürgen König[2] — [1]Departement de Physique Theorique, Universite de Geneve, CH-1211 Geneve 4, Switzerland — [2]Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany — [3]School of Physical and Chemical Sciences, Victoria University of Wellington, New Zealand

The formation of electron pairs is a prerequisite of superconductivity. The fermionic nature of electrons yields four classes of superconducting correlations with definite symmetry in spin, space and time. Here, we suggest double quantum dots coupled to conventional s-wave superconductors in the presence of inhomogeneous magnetic fields as a model system exhibiting unconventional pairing [1]. We propose two detection schemes for unconventional superconductivity, based on ei-

ther Josephson or Andreev spectroscopy.

[1] B. Sothmann, S. Weiss, M. Governale, and J. König, Phys. Rev. B **90**, 220501(R) (2014).

HL 75.4 Thu 11:45 A 053

Shot noise of a triple quantum dot transistor: Blurred polygons and enhancement at blockade — •Andreas Trottmann, Michael Niklas, Andrea Donarini, and Milena Grifoni — Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

A single-electron transistor model with triangular triple quantum dot as central element is studied by means of a Bloch-Redfield-type method with counting fields. Such a device is known to exhibit Coulomb as well as interference blockade due to the presence of orbital degeneracies [1]. Computed Fano factors follow a blurred polygonal pattern as function of the voltages, tend to behave oppositely as against average current, and are enhanced in certain blockade regions in particular. Expressions in an interference blockade region elucidate a counteraction between real and virtual transitions, a blocking condition, and a loss of purity. These effects can be captured describing the orbitally degenerate states based on a pseudospin within a Bloch sphere. Gate and bias thresholds in the Fano factor pattern reflect disparate connectivities, especially a lifting of an interference blockade due to the reachability of a second orbitally degenerate level in the latter case. Blurring is caused by the voltages dependence of axes and frequencies controlling the precession of the pseudospin.

[1] A. Donarini, G. Begemann, and M. Grifoni, Phys. Rev. B 82, 125451 (2010).

HL 75.5 Thu 12:00 A 053

Circular-polarization-sensitive metamaterial based on triple quantum-dot molecules — •Panagiotis Kotetes[1], Pei-Qing Jin[2], Michael Marthaler[1], and Gerd Schön[1] — [1]Karlsruhe Institute of Technology — [2]Shanghai Maritime University

We propose a new type of chiral metamaterial based on an ensemble of artificial molecules formed by three identical quantum-dots in a triangular arrangement [1]. A static magnetic field oriented perpendicular to the plane breaks mirror symmetry, rendering the molecules sensitive to the circular polarization of light. By varying the orientation and magnitude of the magnetic field one can control the polarization and frequency of the emission spectrum. We identify a threshold frequency Ω, above which we find strong birefringence. In addition, Kerr rotation and circular-polarized lasing action can be implemented. We investigate the single-molecule lasing properties for different energy-level arrangements and demonstrate the possibility of circular polarization conversion. Finally, we analyze the effect of weak stray electric fields or deviations from the equilateral triangular geometry.

[1] P. Kotetes, P.-Q. Jin, M. Marthaler, and G. Schön, to appear in Phys. Rev. Lett. (arXiv:1406.6432).

HL 75.6 Thu 12:15 A 053

Electronic Transport through Cerium Nanocontacts — •Sebastian Kuntz[1], Oliver Berg[1], Christoph Sürgers[1], and Hilbert v. Löhneysen[1,2] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, D-76128 Karlsruhe — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie, D-76021 Karlsruhe

We report on conductance measurements of Ce nanocontacts in mechanically controlled break-junctions (MCBJ) made from polycrystalline wires. The wires were cut from two different Ce ingots. One ingot was taken as-prepared after cooling from the melt and one ingot was carefully annealed over $\sim$ one week. We investigate the effect of cooling rate and γ-β-α-phase transformation on the conductance G of the nanocontacts measured at low temperatures. From a number of measurements of $G(\Delta x)$ where Δx is the distance between the two electrodes, we obtain conductance histograms. We focus on the conductance G^* of the "last plateau" before, with increasing Δx, G drops to zero. For Ce, different G^* values between 0.6 and 1.7 G_0 ($G_0 = 2e^2/h$) are observed, while for other rare-earth metals like Gd and Dy the last plateau occurs at $G^* \simeq 0.6$ G_0 and $G^* \simeq 0.9$ G_0, respectively. A possible explanation for the different G^* values of Ce is the additional contribution from the $4f$ state to the conductance whose distance from the Fermi level depends on the phase at low temperatures (α or β) and, hence, on the cooling rate of the sample.

HL 75.7 Thu 12:30 A 053

coherent single charge transport in MBE-grown InSb nanowire — •ning kang[1], sen li[1], dingxun fan[1], yuqing huang[1], libing wang[1], philippe caroff[2], and hongqi xu[1,2] — [1]Key Laboratory for the Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, Beijing 100871, P. R. China. — [2]Solid State Physics, Lund University, Box 118, S-221 00 Lund, Sweden

InSb nanowire have unique properties, such as a narrow bandgap, strong spin-orbit interaction, large bulk mobility and a small effective mass. Here, we report fabrication and low-temperature electrical transport studies of InSb nanowires grown by MBE. Individual nanowire devices exhibit Coulomb blockade oscillations characteristic of single charge transport on length scales up to 700 nm. Detailed finite-bias transport measurements demonstrate coherent electron transport through discrete quantum levels. In the few electron regime, strong signatures of higher order inelastic cotunneling occur which can directly be assigned to excited states. With this spectroscopy we extract the main characteristics of a single InSb nanowire, namely, the Lande factor and the the magnitude of the spin-orbit interaction. We also present initial experimental studies of devices composed of superconductor in proximity to single InSb nanowire. We observed gate-tunable supercurrent flowing through the InSb nanowire and multiple Andreev reflection characteristics. Our results demonstrate that the InSb nanowires can provide an ideal platform to exploring phase coherence quantum transport and topological electronics in a solid state system.

HL 75.8 Thu 12:45 A 053

Heat current as a tool to study quantum dot decay rates — •Jens Schulenborg[1], Roman Saptsov[2,3], Janine Splettstoesser[1], and Maarten R. Wegewijs[2,3,4] — [1]Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, Göteborg, Sweden — [2]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany — [3]JARA - Future Information Technologies, Germany — [4]Institut für Theorie der Statistischen Physik, RWTH Aachen University, Germany

Over the past years, potential applications in nanoelectronics, metrology and quantum information sparked great interest in studying the *dynamics* of time-dependently driven quantum dots. Recently, we investigated the decay rates of an interacting single-level quantum dot, weakly tunnel coupled to an electronic reservoir and brought out of equilibrium by a step pulse[1,2]. In particular, the *fermion-parity rate*[1] was found to be an additional time scale, besides the spin- and charge decay rate, of which the value is fundamentally restricted[2].

This work shows that the *time-dependent heat current* emitted from the dot gives new insights into the physics described by the fermion-parity rate. Using a master equation for the dot coupled to an electrode, we extract the decay rates and determine how they influence the decay of charge- and heat current. We find that, while the fermion-parity rate does not at all enter the charge current, it is the dominant time scale for the *dissipation of interaction energy* carried by the heat current.

[1] L. D. Contreras-Pulido et al., Phys. Rev. B **85**, 075301 (2012).
[2] R. Saptsov et al., Phys. Rev. B **90**, 045407 (2014).

HL 76: Carbon nanotubes

Time: Thursday 11:30–13:00 Location: EW 015

HL 76.1 Thu 11:30 EW 015

Wafer-level fabrication and characterization of photosensitive CNT-FETs — •Laura Kasper[1,2], Thomas Blaudeck[1], Sascha Hermann[1,3], and Stefan E. Schulz[1,2,3] — [1]Technische Universität Chemnitz, Zentrum für Mikrotechnologien, 09107 Chemnitz — [2]Fraunhofer-Institut für Elektronische Nanosysteme (ENAS), 09126 Chemnitz, Germany — [3]DFG Cluster of Excellence "Center for Advancing Electronics Dresden" (cfaed), Carbon Path, 09107 Chemnitz, Germany

We report on the wafer-level fabrication and a quantitative analysis of the light detection properties of carbon-nanotube field-effect transistor (CNT-FET) arrays. We determine parameter ranges for the optical and electrical properties for achieving relevant photocurrents (> 100 pA) and responsivities (~ 1 uA/W). Aside of the dynamic range of the sensor devices, the noise-equivalent power varies clearly with the applied source-drain voltages. Local intensity scans of the sensor response (source-drain current as a function of the locus of incidence) along the transistor channel reveal the fundamental Schottky behavior of the device related to the CNT-metal contacts. The results are reported for two batches of CNT-FETs varying the number of semiconducting CNTs as transistor channel. Especially the illumination of FETs with high-density CNT transistor channels show a smoothing of their transfer characteristics. Illumination of single-CNT channels shows signs of power dissipation. The influence of a CNT sidewalls functionalization with metal nanoparticles acting as light-sensitive floating gates is discussed as well.

HL 76.2 Thu 11:45 EW 015

Optimizing Dispersion Preparation for the Wafer-Level Deposition of CNTs — •Toni Hille[1,2], Thomas Blaudeck[1], Sascha Hermann[1,3], and Stefan E. Schulz[1,2,3] — [1]Technische Universität Chemnitz, Zentrum für Mikrotechnologien, 09107 Chemnitz, Germany — [2]Fraunhofer-Institut für Elektronische Nanosysteme (ENAS), 09126 Chemnitz, Germany — [3]DFG Cluster of Excellence "Center for Advancing Electronics Dresden" (cfaed), Carbon Path, 09107 Chemnitz

In this work, we show systematic studies on the CNT dispersion preparation comprising homogenization, ultrasonication, and centrifugation and their optimal parameters for the wafer-level fabrication of CNT-FETs as building blocks of high-frequency and sensor components. With an in-situ monitoring of the optical absorption, a detailed analysis of the dispersion process for different surfactants (sodium lauryl sulfate, sodium deoxycholate, etc.), concentrations, and preperation conditions was possible. It turns out that the degree of debundeling can be tuned using an intermittent ultrasonication, varying the waiting times for the dispersion constituents to settle down between recurrent sonotrode pulses. The influence of temperature during centrifugation and storage of the dispersion is discussed as well.

HL 76.3 Thu 12:00 EW 015

A wafer-level test platform for statistical TEM analysis of the structural properties of integrated carbon nanotubes — •Martin Hartmann[1,2], Sascha Hermann[1,2], Darius Pohl[3], Bernd Relinghaus[3], and Stefan E. Schulz[1,2,4] — [1]Center for Microtechnologies (ZFM), TU Chemnitz,Chemnitz, Germany — [2]Center for Advancing Electronics Dresden (cfaed), TU Chemnitz, Chemnitz, Germany — [3]Leibniz Institute for Solid State and Materials Research (IFW), Dresden, Germany — [4]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany

A carbon nanotube-based field-effect transistor (CNT-FET) is a promising building block in many electronic and sensor applications. However, the actual performance of those devices has not reached predicted values yet. This can be related to the high sensitivity of the nanomaterial to its environment as well as its structural and compositional configuration. Thus better methods for the investigation of nanomaterials under application-close conditions are required. We demonstrate an in-depth analysis of the FET channel structure by high-resolution transmission electron microscopy (HRTEM). Therefore, a special test platform was developed that facilitates electrical and transmission studies of integrated nanomaterials like CNTs. In this approach, special emphasis was laid on a wafer-level technology used for high-throughput FET fabrication enabling statistical studies. The concept as well as first investigations on exposed CNT-FET channel regions are going to be presented giving insights into chiral and elementary composition.

HL 76.4 Thu 12:15 EW 015

Carbon nanotubes under strain: Electronic and Optical properties — •Christian Wagner[1], Jörg Schuster[2], Michael Schreiber[3], and Thomas Gessner[1,2] — [1]Center for Microtechnologies, TU Chemnitz, Germany — [2]Fraunhofer Institute ENAS, Chemnitz, Germany — [3]Institute of Physics, TU Chemnitz, Germany

Carbon nanotubes (CNTs) are becoming interesting for applications as they show some very unique properties upon strain: On load, their whole electronic band structure is shifting (according to their chiralities) and that makes them suitable for electronic and optical strain sensing at the nano scale.

We show the results of electronic structure calculations of strained CNTs (DFT and beyond) and the link to their electronic and optical properties. It can be shown that an empirical model can account for the CNT bands and their strain-dependent properties.

Based on the electronic structure, we derive transport properties of strained CNTs and their mixtures in a transistor configuration. For the modeling of the optical properties, we show optical spectra derived from electronic structure calculations. The optical spectra of unstrained CNTs are described by empirical models [1]. We aim to incorporate strain effects into these models by comparison to electronic structure calculations.

[1] K. Liu et al., Nat. Nanotech. 7, 325 (2012)

HL 76.5 Thu 12:30 EW 015

Carbon nanotube based field-effect transistors: comparison between atomistic quantum transport and numerical device simulation — •Florian Fuchs[1], Andreas Zienert[2], and Jörg Schuster[1] — [1]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany — [2]Center for Microtechnologies, Technische Universität Chemnitz, Chemnitz, Germany

We study carbon nanotube based field-effect transistors (CNTFETs) by means of two different approaches: numerical device simulation (NDS) based on the effective mass Schrödinger equation and atomistic quantum transport simulation based on the non-equilibrium Green's function formalism (NEGF). The required parameters for the NDS model are extracted from density functional theory data. An all-carbon CNTFET with n-doped source- and drain-electrodes in a gate-all-around geometry is investigated. The NDS predicts a band-to-band tunnel current once the valence band edge is shifted to the Fermi energy. This increases the off-current and leads to slightly ambipolar behavior. Using the NEGF on the other hand, localized states inside the channel can be observed because a potential well is created by the gate. As a result, the band-to-band tunnel current is suppressed and improved transistor properties are predicted by NEGF calculations. By varying the channel length, we demonstrate the potential of the studied CNTFET for future applications, which shows an on/off current ratio above 10^6 and a subthreshold swing below 80 mV/dec down to channel lengths of about 8 nm.

HL 76.6 Thu 12:45 EW 015

Ramanspektroskopie an gekreuzten Kohlenstoffnanoröhren — •Norman Susilo[1], Asmus Vierck[1], Florentina Gannott[2], Manuel Schweiger[2], Jana Zaumseil[2] und Janina Maultzsch[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin — [2]Lehrstuhl für Angewandte Physikalische Chemie, Physikalisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg

Eine der etabliertesten Methoden zur Untersuchung von Kohlenstoffnanoröhren (CNTs) ist die Ramanspektroskopie. Vielfach werden die Untersuchungen allerdings an Ensembles bzw. dünnen Bündeln von CNTs durchgeführt. Um den Einfluß von elektronischen und mechanischen Wechselwirkungen zwischen zwei CNTs besser zu verstehen, untersuchen wir definierte Kreuzungspunkte von CNTs.

Wir präsentieren eine statistische Analyse der Ramanspektren von sich in einem Winkel von 90° kreuzenden, individuellen, einwandigen CNTs. Wir diskutieren die Veränderungen der Ramanspektren an den Kreuzungspunkten bzgl. elektronischer und mechanischer Effekte. Es wird u.a. gezeigt, dass die Intensität der Defekt-induzierten D-Mode am Kreuzungspunkt der Kohlenstoffnanoröhren steigt.

HL 77: Low-dimensional systems: Topological order 1 (TT with HL)

Time: Thursday 11:30–13:00 Location: H 3010

HL 77.1 Thu 11:30 H 3010

Towards a complete characterization of 2d topological order using tensor networks and multipartite entanglement — •Roman Orus — Johannes-Gutenberg Universität, Mainz, Deutschland

Topological order in a 2d quantum matter can be determined by the topological contribution to the entanglement Renyi entropies. However, when close to a quantum phase transition, its calculation becomes cumbersome. In this talk I will show how topological phase transitions in 2d systems can be much better assessed by multipartite entanglement, as measured by the topological geometric entanglement of blocks. Specifically, I will present an efficient tensor network algorithm based on Projected Entangled Pair States (PEPS) to compute this quantity for a torus partitioned into cylinders, and then use this method to find sharp evidence of topological phase transitions in 2d systems with a string-tension perturbation. When compared to tensor network methods for Renyi entropies, this approach produces almost perfect accuracies close to criticality and, on top, is orders of magnitude faster. Moreover, I will show how the method also allows the identification of Minimally Entangled States (MES), thus providing a very efficient and accurate way of extracting the full topological information of a 2d quantum lattice model from the multipartite entanglement structure of its ground states.

HL 77.2 Thu 11:45 H 3010

Robustness of Symmetry Protected Topological Order in spin-2 quantum chains — •Augustine Kshetrimayum[1], Hong-Hao Tu[2], and Román Orús[1] — [1]Johannes Gutenberg University Mainz — [2]MPQ Munich

Topological order is a new kind of order that cannot be described using the Landau theory. It is associated to a non-local pattern of entanglement. When such non-local properties are protected by specific symmetries, it is known as Symmetry Protected Topological Order.

The existence of such a symmetry protected topologically ordered Intermediate Haldane phase for a spin-2 Heisenberg chain was suggested by Oshikawa in 1992. However, the evidence for its existence has remained quite elusive. More recently, it has been proven that such a phase exists in a family of generalized spin-2 quantum Heisenberg chains.

In this work, we study the robustness of this phase for generalized spin-2 quantum Heisenberg chains with uni-axial anisotropy, and in the thermodynamic limit. We find very robust symmetry-protected topologically ordered SO(5)-Haldane and Intermediate-Haldane phases, which we assess by a variety of methods including the entanglement spectrum of the system and the behavior of string-order parameters. Moreover, we study time-evolution properties of these phases. Our numerical results are based on using Matrix Product States (MPS) to represent the wave function, in combination with the infinite Time-Evolving Block Decimation (iTEBD) method.

HL 77.3 Thu 12:00 H 3010

Wire deconstructionism of two-dimensional topological phases — •Ronny Thomale[1], Titus Neupert[2], Claudio Chamon[3], and Christopher Mudry[4] — [1]Institut für Theoretische Physik, Universität Würzburg, Germany — [2]Princeton University, USA — [3]Boston University, USA — [4]PSI Zürich, Switzerland

A scheme is proposed to construct integer and fractional topological quantum states of fermions in two spatial dimensions. We devise models for such states by coupling wires of non-chiral Luttinger liquids of electrons, that are arranged in a periodic array. Which inter-wire couplings are allowed is dictated by symmetry and the compatibility criterion that they can simultaneously acquire a finite expectation value, opening a spectral gap between the ground state(s) and all excited states in the bulk. First, with these criteria at hand, we reproduce the tenfold classification table of integer topological insulators, where their stability against interactions becomes immediately transparent in the Luttinger liquid description. Second, we construct an example of a strongly interacting fermionic topological phase of matter with short-range entanglement that lies outside of the tenfold classification. Third, we expand the table to long-range entangled topological phases with intrinsic topological order and fractional excitations.

HL 77.4 Thu 12:15 H 3010

Symmetry Protected Phases in Geometrically Frustrated 1D Antiferromagnets — •Alexander Nietner, Emil J. Bergholtz, and Jens Eisert — Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin, Germany

Geometrically frustrated (GF) systems admit an exotic phenomenology, such as spin liquid states, which lack any local order parameter. To reach a better understanding of such behaviour we realize the spin one Heisenberg antiferromagnetic Δ-chain (HAD) as a simple GF system in a numerically feasible regime. Inspired by a projected entangled pairs picture, we relate this system to a double layered ferromagnetically coupled $s = 1/2$ HAD. We use the time dependent variational principle to compute the ground states of these systems and investigate their phase diagramme in the thermodynamic limit, analysing the entanglement spectra and the projective representations of the symmetry groups. Despite the simplicity of these systems, we find evidence of a topological phase transition for the latter one from the trivial phase in the weak ferromagnetic limit towards a symmetry protected nontrivial phase for a finite coupling strength. This is in good agreement with the fact that the corresponding $s = 1$ system is found to be in the topological Haldane phase.

HL 77.5 Thu 12:30 H 3010

Route to Topological Superconductivity via Magnetic Field Rotation — •Florian Loder, Arno P. Kampf, and Thilo Kopp — Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Germany

Apart from the very few spin-triplet superconductors with p-wave pairing symmetry, a candidate system for topological superconductivity is a conventional, two-dimensional s-wave superconductor in a magnetic field with a sufficiently strong Rashba spin-orbit coupling. Typically, the required magnetic field to convert the superconductor into a topologically non-trivial state is however by far larger than the upper critical field H_{c2}, which excludes its realization. Here we argue that this problem is overcome by rotating the magnetic field into the superconducting plane. We explore the topological transitions which occur upon changing the strength and the orientation of the magnetic field and show that an unusual superconducting state with finite-momentum pairing exists, which preserves its topological nature up to an in-plane field orientation. We discuss the realizability of this state at the superconducting interface between $LaAlO_3$ and $SrTiO_3$.

HL 77.6 Thu 12:45 H 3010

Topological phases of a chain of twist defects — •Abhishek Roy[1], Xiao Chen[2], and Jeffrey Teo[3] — [1]Institute of Theoretical Physics, University of Cologne, Koeln, Germany — [2]Department of Physics, University of Illinois at Urbana-Champaign, USA — [3]Department of Physics, University of Virgina, USA

A twist defect acts on a system of abelian anyons by permuting anyon labels in a manner that preserves their braiding properties.

We investigate a one dimensional chain of twist defects. The Hamiltonian consists of Wilson loop operators, each enclosing a pair of neighbouring defects. We explore both gapped and gapless phases. For the former, we use anyon pumping to classify the ground states. For the latter, we present mappings to known critical models.

We extend the above results from twofold defects (which are similar to Z_k parafermions) to threefold defects introduced by us earlier in an exactly solvable lattice model [1].

[1] J. C.Y. Teo, A. Roy, X. Chen. Phys. Rev. B 90, 115118

HL 78: Invited Talk Mariusz Ciorga

Time: Thursday 12:30–13:00 Location: ER 164

Invited Talk HL 78.1 Thu 12:30 ER 164

Electrical spin injection into high mobility 2DEG systems — Martin Oltscher, •Mariusz Ciorga, Josef Loher, Dieter Schuh, Dominique Bougeard, and Dieter Weiss — Institute for Experimental and Applied Physics, University of Regensburg

Effective spin injection into two-dimensional (2D) electron systems is a prerequisite for many new functionalities in future devices, with a Datta-Das spin field effect transistor [1] being a primary example. Whereas real progress in understanding of spin injection phenomena in bulk semiconductors has been achieved, electrical injection of spins into high mobility 2D systems remains a relatively open matter.

Here I present the results of our recent experiments [2] on electrical spin injection into high mobility 2D electron gas (2DEG) confined in an inverted AlGaAs/GaAs heterojunction, with ferromagnetic semiconductor (Ga,Mn)As employed as a spin polarizing material. We observed a clear nonlocal spin signal that could be tuned by a voltage applied across the injector. At maximum the signal largely exceeded the prediction of the standard drift-diffusion model. A strong correlation of this enhancement with the width of the contacts and with the electrons' mean free path led us to the conclusion that ballistic nature of the transport in the 2D region directly below the injector should be considered to fully describe the experimental outcome.

The work has been supported by Deutsche Forschungsgemeinschaft (DFG) through SFB689.

[1] S. Datta and B. Das, Appl. Phys. Lett. **56**, 665 (1990) [2] M. Oltscher *et al.*, Phys. Rev. Lett. **113**, 236602 (2014)

HL 79: Quantum information systems: Si vacancies and NV centers (with TT)

Time: Thursday 15:00–17:00 Location: ER 164

HL 79.1 Thu 15:00 ER 164

Spin Physics of vacancy-related defects in silicon carbide — •Michel Bockstedte[1,2] and Felix Schütz[1] — [1]Lst. Theor. Festkörperphysik, Friedrich-Alexander Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — [2]FB Materialwissenschaften & Physik, Universität Salzburg, 5020 Salzburg, Austria

SiC as a semi conductor fullfills all necessary requirements[1] for implenting qubits via defect electron spins, such as the silicon vacancy, the di-vacancy or a complex of a silicon vacancy and a nitrogen impurity. The spin-selective fluorescence in contrast to the prototypical NV-center in diamond operates in the spectral range favorable for telecom applications. Spin-manipulation of the intrinsic centers was demonstrated even at room temperature.[2,3] For the silicon vacany in SiC inter system crossings (ISCs) from high to yet unknown low spin states govern the spin-relaxation. By DFT and a DFT-based CI-hamiltonian we analyze the spin physics of the defect in 4H-SiC. Experimentally observed luminescence lines can be assigned to the inequivalent defect sites corobarating the experimental findings. Owing to the spin (S=3/2) and a stronger electron-phonon coupling in the excited state, ISCs destinct from the NV-center are predicted.

[1] J. R. Weber *et al.*, PNAS **107**, 8513 (2010).
[2] F. Koehl *et al.*, Nature**479**, 84 (2011).
[3] V. A. Soltamov *et al.*, Phys. Rev. Lett. **108** 226402 (2012)

HL 79.2 Thu 15:15 ER 164

SiC nano-crystalline NIR emitters based on optically excited and spin polarized defects — •F. Fuchs[1], A. Muzha[2], N. Tarakina[3,4], D. Simin[1], M. Trupke[5], P. Baranov[6], V. Dyakonov[1,3,7], A. Krueger[2,3], and G. Astakhov[1] — [1]Exp. Physics VI, University of Würzburg — [2]Institute of Organic Chemistry, University of Würzburg — [3]Wilhelm Conrad Röntgen RCCM, University of Würzburg — [4]Exp. Physics III, University of Würzburg — [5]Vienna Center for Quantum Science and Technology, TU Wien — [6]Ioffe Institute, St. Petersburg — [7]ZAE Bayern, Würzburg

The unification of luminescent markers for bioimaging and spin centers for quantum sensing [1] is challenging; especially when aiming for the ideal NIR window, stability and non-toxicity. Bulk silicon carbide (SiC) is a favored candidate despite its large band gap, which we could mitigate by the introduction of silicon vacancy defects—exhibiting NIR emission—via neutron irradiation. With a milling procedure, we fabricated SiC nano crystals ranging from 600nm down to 60nm in size, with a further fragmentation of the latter into clusters of high crystalline quality (size ca. 10 nm) separated by amorphous material. The luminescence of the vacancies persists in all size fractions, moreover, we detected room-temperature spin resonance [2]. This leads to new perspectives: defects in nano crystalline SiC as in-vivo luminescent markers and simultaneously as magnetic field or temperature sensors [3].

[1] Riedel et al.: Phys. Rev. Lett. 109, 22 (2012)
[2] Fuchs et al. arXiv: 1409.0756v1
[3] Kraus et al.: Sci. Rep. 4, 5303 (2014)

HL 79.3 Thu 15:30 ER 164

Coherent Spin Manipulation of Si-Vacancies in Silicon Carbide at Ambient Conditions — •Dmitrij Simin[1], Andreas Sperlich[1], Victor Soltamov[2], Pavel Baranov[2], Georgy Astakhov[1], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Wuerzburg, 97074 Wuerzburg — [2]Ioffe Physical-Technical Institute, 194021 St. Petersburg, Russia — [3]ZAE Bayern, 97074 Wuerzburg

For already over two decades, quantum information processing has been the hot topic in the field of information theory. To recognize and to employ the most suitable material and information carrier from the vast amount of possibilities is the declared goal of ongoing research activities all over the world. Among others, a promising candidate are Si-vacancies in Silicon Carbide [1], where spin control has been successfully conducted at ambient conditions [2, 3]. In our recent work we go one step further and present the successful time-resolved manipulation of the spin of the Si-Vacancies at ambient conditions using the pulsed-ODMR technique. We observed Rabi-oscillations in an ensemble of defects and determined spin-relaxation properties, demonstrating high potential of SiC for various quantum applications.

[1] D. Riedel et al., Phys. Rev. Lett. 109, 226402 (2012)
[2] H. Kraus et al., Nat. Phys. 10, 157-162 (2014)
[3] H. Kraus et al., Sci. Rep. 4, 5303 (2014)

HL 79.4 Thu 15:45 ER 164

Charge state control of nitrogen-vacancy centers in diamond — •Patrick Simon[1], Moritz V. Hauf[1], Ankit Rathi[1], Philipp Neumann[2], Helmut Fedder[2], Jörg Wrachtrup[2], Friedemann Reinhard[1,2], and Jose A. Garrido[1] — [1]Walter Schottky Institut, Physik-Department,Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany — [2]3. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

The nitrogen-vacancy (NV) defect in diamond is a promising candidate for quantum information processing or sensing purposes. In most applications reliable control of the charge state of the NV is of utmost importance.

In this work we demonstrate that the charge state of NV centers can be controlled using an in-plane gated diamond nanostructure based on selective surface termination. Applying a gate voltage changes the band bending at the hydrogen terminated diamond surface such that reversible charge state switching is enabled. We observed full control of NVs from a non-fluorescent state, potentially NV^+, across NV^0 to NV^-

HL 79.5 Thu 16:00 ER 164

Investigating the positively charged nitrogen-vacancy center in diamond as a long lived quantum memory — •Matthias Pfender[1], Nabeel Aslam[1], Christian Burk[1], Denis Antonov[1], Sebastian Zaiser[1], Helmut Fedder[1], Philipp Neumann[1], Patrick Simon[2], José A. Garrido[2], Martin Stutzmann[2], and Jörg Wrachtrup[1] — [1]3. Physikalisches Institut, Universität Stuttgart — [2]Walter Schottky Institut, Technische Universität München

The nitrogen-vacancy defect in diamond is one of the major candidates for a solid-state quantum processor. Its electron spin can be readout and initialized optically. Adjacent nuclear spins (e.g. ^{14}N, ^{15}N, ^{13}C) can be employed as inherently robust qubits [1], readout is facilitated via the electron spin in a QND measurement with T_1 lifetimes of several minutes. However, for strongly coupled nuclear spins, the coherence time is limited by the T_1 lifetime of the electron spin ($\approx$ 5ms). In Si:P, this obstacle could be overcome by ionizing the P donor to a spinless charge-state [2]. In this work, we employ in-plane gate structures to deterministically switch the charge state of near-surface NVs from NV^- over NV^0 to NV^+ [3], while investigating the electron spin properties using the nitrogen nuclear spin as a probe. Since the positive charge state has no unpaired electrons, the nuclear spin coherence time is prolonged beyond the 5ms imposed by the NV^- electron spin.

[1] Waldherr, G. et al., Nature 506, 204 (2014).
[2] Saeedi, K. et al., Science 342, 830 (2013).
[3] Hauf, M. V. et al., Nano Lett. 14, 2359 (2014).

HL 79.6 Thu 16:15 ER 164

A cavity-mediated quantum CPHASE gate between nitrogen-vacancy electronic spin qubits in diamond — •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 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. In combination with previously demonstrated single-qubit gates, CPHASE allows for arbitrary quantum computations. The coupling of the NV spin to the cavity mode is based upon Raman transitions via the NV excited states and can be controlled with the laser intensities and relative phase. We find characteristic laser frequencies at which a laser photon is only scattered into the cavity mode if the NV center spin is $|m_s = 0\rangle$, and not in the case $|m_s = -1\rangle$, or vice versa. The scattered photon can be reabsorbed by another selectively driven NV center and generate a conditional phase (CPHASE) gate. Gate times below 20 ns are within reach, several orders of magnitude shorter than typical NV spin coherence times. The separation between the two NV centers is only limited by the extension of the cavity.

[1] G. Burkard, D. D. Awschalom, arXiv: 1402.6351 (2014).

HL 79.7 Thu 16:30 ER 164

Long-range two-qubit gate between nuclear spins in diamond mediated via an optical cavity — •Adrian Auer and Guido Burkard — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

Nitrogen-vacancy (NV) centers in diamond represent a promising possibility for a solid-state based realization of a qubit due to their excellent electron- and nuclear-spin coherence properties. Single-qubit gates for the nitrogen nuclear spin have been implemented [1]. Here, we extend an earlier proposal [2] for cavity-mediated coupling between NV electron spins and develop a scheme to implement a universal two-qubit gate between ^{14}N or ^{15}N nuclear spins. By virtually exciting a single NV center with an external laser field, a photon can be scattered into a surrounding cavity; we show that this process depends on the spin state of the nitrogen nucleus. For the two-qubit gate, we consider two NV centers coupled to a common cavity mode and each being excited individually. Virtual cavity excitation can then mediate an effective interaction between the NV nuclear spin qubits, generating a controlled-Z gate. Operation times for the gate implementation are found to be below 100 nanoseconds, which is orders of magnitude faster than the decoherence time of nuclear spin qubits in diamond.

[1] S. Sangtawesin *et al.*, Phys. Rev. Lett. **113**, 020506 (2014).
[2] G. Burkard and D. D. Awschalom, arXiv:1402.6351.

HL 79.8 Thu 16:45 ER 164

Linear polarization properties of the NV^- center photoluminescence in diamond — •Dion Braukmann[1], Jörg Debus[1], Vladimir L. Korenev[2], Vitalii Yu. Ivanov[3], Dmitri R. Yakovlev[1], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44227 Dortmund, Germany — [2]Ioffe Physical-Technical Institute, Russian Academy of Science, 194021 St. Petersburg, Russia — [3]Institute of Physics, Polish Academy of Sciences, 02668 Warsaw, Poland

The negatively charged nitrogen-vacancy (NV^-) center in diamond has been studied in recent years on account of possible applications in quantum information processing, spin-electronics and, e.g., biophotonics. Particular focus has been drawn onto its optical properties. We report on polarization-dependent optical studies of NV^- centers in diamond subjected to high magnetic fields of up to 10 T. We observe asymmetric Zeeman splitting of the zero-phonon line photoluminescence, a strong optical alignment as well as Faraday rotation at room temperature. The linear polarization properties of the NV^- photoluminescence are studied as function of the diamond crystal orientation in the stationary and time-resolved regimes.

HL 80: Challenges in semiconductor theory

Time: Thursday 15:00–17:15 Location: EW 015

HL 80.1 Thu 15:00 EW 015

Full exact exchange and non-local correlation - a next step on the path to a physical Kohn-Sham density of states? — •Tobias Schmidt and Stephan Kümmel — University of Bayreuth, Germany

Density Functional Theory (DFT) provides an efficient and, in principle, exact framework to calculate the electronic structure of matter. In practice, DFT results strongly depend on the exchange correlation (xc) functional used. Hybrid functionals, i.e., combining a semi-local density functional with a fixed percentage of Fock exchange, have been in widespread use. However, there is no "perfect" hybrid: Hybrids with a low (ca. 20%) percentage of Fock exchange describe binding and structural properties well, but much higher amounts of Fock-exchange (ca. 50%) are needed if one aims at eigenvalues that well approximate the density of states.

In an attempt to overcome this gap, a local hybrid functional was designed. The constant mixing parameter of usual hybrids is replaced by a density functional. Thus, full Fock exchange is combined with non-local correlation. We discuss in how far this generalization leads to results that are similar or different from the usual global hybrids. We pay particular attention to the reduction of self-interaction errors, the long-range asymptotic behavior of the potential, and whether the Kohn-Sham density of states becomes more physical. First results on practically relevant, non-trivial systems with d-electrons, e.g., Palladium particles, will be presented.

HL 80.2 Thu 15:15 EW 015

Towards simple orbital-dependent density functionals for molecular dissociation — •Igor Ying Zhang[1], Patrik Rinke[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 12149 Berlin-Dahlem — [2]COMP/Department of Applied Physics, Aalto University School of Science, P.O. Box 11100, FI-00076 Aalto, Finland

Density functional theory (DFT) is one of the leading first-principles electronic-structure theories. However, molecular dissociation remains a challenge, because it requires a well-balanced description of the drastically different electronic structure at different bond lengths. One typical and well-documented case is the dissociation of both H_2^+ and H_2, for which all popular DFT functionals fail [1]. We start from the Bethe-Goldstone equation to propose a simple orbital-dependent correlation functional which generalizes the linear adiabatic connection approach. The resulting scheme is based on second-order perturbation theory (PT2), but includes the self-consistent coupling of electron-hole pairs, which ensures the correct H_2 dissociation limit and gives a finite correlation energy for systems with a (near)-degenerate energy gap. This coupling PT2-like (CPT2) approximation delivers a significant improvement over all existing functionals for both H_2 and H_2^+ dissociation. We will demonstrate the reason for this improvement analytically for H_2 in a minimal basis.[1] A. J. Cohen *et al.*, Chem. Rev. **112** 289 (2012). [2] F. Caruso *et al.*, Phys. Rev. Lett. **110** 146403 (2013).

HL 80.3 Thu 15:30 EW 015

Hybrid density-functional calculations of polarons in doped MgO. — •Sebastian Kokott, Sergey Levchenko, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Charge-carrier conductivity in oxides can influence their surface chemical properties [1]. However, the nature and properties of the charge carriers are not well understood. In this work, we investigate self-trapped polarons in MgO within an *ab initio* framework. Density-functional theory with the hybrid functional HSE06 is used for the atomic relaxtion and electronic structure calculations. The choice of the functional is validated by the analysis of the (de)localization bias according to the generalized Koopmans' condition [2] as a function of the fraction of Hartree-Fock exchange. We find a localized polaronic distortion of the MgO lattice which was not reported previously: two neighboring oxygen atoms forming an O_2^{2-} moiety with two trapped electronic holes. We do not find a self-trapped state for a single hole with the HSE06 functional. The formation energy of the polaron is about 1 eV, *i.e.*, thermally accessible at typical temperatures when *p*-doped MgO is used as a catalyst (800-1,000 K) [3]. We also explore polarons trapped at intrinsic and extrinsic point defects, in particular Mg vacancies and hydrogen intersitials. □ [1] Richter et al., Phys. Rev. Lett. **111**, 045502 (2013); [2] Lany and Zunger, Phys. Rev. B **80**, 085202, (2009); [3] Arndt et al., Catalysis Rev. **54** (4), 424-514 (2011).

HL 80.4 Thu 15:45 EW 015

Electronic structure and adsorption properties of Ni substitutional defects at MgO(001). — •Aliaksei Mazheika, Sergey V. Levchenko, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, DE

Ni-MgO solid solutions were demonstrated to be stable and active catalysts for CO_2 activation and conversion. However, despite numerous experimental investigations, the nature of the active sites, in particular at realistic conditions, remains unknown. As a first step towards understanding the nature of the sites, we calculate the electronic and atomic structure of Ni substitutional defects at the (100) surface of MgO, using the density-functional theory with the Heyd-Scuseria-Ernzerhof family of hybrid functionals HSE(α,ω) [1]. We determine the optimal fraction of the exact exchange α by comparing the positions of the defect levels and the valence-band maximum with respect to the vacuum level obtained with DFT and G_0W_0 where self-energy is evaluated with partial self-consistency of the eigenvalues. The obtained optimal value of $\alpha = 0.6$ also gives an agreement within 0.1 eV between the DFT and MP2 energies of CO adsorption at the Ni defect. The MP2 adsorption energy calculated for a small embedded cluster model was previously shown to be very close to the CCSD(T) adsorption energy [2]. An optimal compromise (within 0.05 eV) can be achieved between the accuracy of the defect level alignment and the CO adsorption energy for $\alpha = 0.5$.—[1] A.V. Krukau, O.A. Vydrov, A.F. Izmaylov, G. Scuseria. J. Chem. Phys., **125**, 224106 (2006); [2] I. Mehdaoui, T. Klüner. J. Phys. Chem. A, **111**, 13233 (2007).

HL 80.5 Thu 16:00 EW 015

Atomistic-continuum modeling of short laser pulse melting of Si targets — •Vladimir P. Lipp[1,2], Baerbel Rethfeld[2], Martin E. Garcia[1], and Dmitry S. Ivanov[1,2] — [1]University of Kassel, Kassel, Germany — [2]Technical University of Kaiserslautern, Kaiserslautern, Germany

We present an atomistic-continuum model to simulate ultrashort laser-induced melting processes in semiconductor solids on the example of silicon. The kinetics of transient non-equilibrium phase transition mechanisms is addressed with a Molecular Dynamics method at atomic level, whereas the laser light absorption, strong generated electron-phonon non-equilibrium, fast diffusion of and heat conduction due to photo-excited free carriers are accounted for in the continuum. We give a description of the model, which is then applied to study the mechanism of short laser pulse melting of free standing Si films. The effect of laser-induced pressure and temperature of the lattice on the melting kinetics is investigated. Two competing melting mechanisms, heterogeneous and homogeneous, were identified. Apart of classical heterogeneous melting mechanism, the nucleation of the liquid phase homogeneously inside the material significantly contributes to the melting process. The threshold fluence value, at which homogeneous nucleation of liquid starts contributing to the classical heterogeneous propagation of the solid-liquid interface, is found from the series of simulations at different laser input fluences. On the example of Si, the laser melting kinetics of semiconductors was found to be noticeably different from that of metals with fcc crystal structure.

HL 80.6 Thu 16:15 EW 015

A real-time DFT scheme for electronic transport — •Philipp Schaffhauser and Stephan Kümmel — Universität Bayreuth, Deutschland

We present an approach for calculating the charge transport through molecular systems that relies on solving the time-dependent Kohn-Sham equations in real-time and real-space. So far, propagation methods were mostly used for closed quantum systems and therefore did not allow for studying transport problems which involve a source and a drain. We resolve this problem by introducing absorbing and anti-absorbing boundary conditions. By comparing to established results we verify our computational scheme. Using the new formalism we examine how molecular distortions, and, e.g., breaks in the conjugation of organic systems, change the molecular conductivity.

HL 80.7 Thu 16:30 EW 015

Piezoelectricity in planar boron nitride via a geometric phase — •Matthias Droth[1] and Vitor Pereira[2] — [1]University of Konstanz, Germany — [2]Graphene Research Centre, National University of Singapore

Due to their low surface mass density, two-dimensional materials with a strong piezoelectric response are interesting for nanoelectromechanical systems with high susceptibility. In contrast to graphene, the two sublattices in two-dimensional hexagonal boron nitride (hBN) are occupied by different types of atoms, which allows for piezoelectricity. Recently, the piezoelectric tensor of extended hBN has been calculated via density functional theory (DFT). While an analytical description of piezoelectricity does exist for hBN nanotubes, this is, to our knowledge, not the case for two-dimensional hBN. We set up a Hamiltonian that involves the strain-induced pseudomagnetic field and derive the piezoelectric tensor using the modern theory of polarization. Our findings are in exact agreement with symmetry arguments and give an analytical explanation for the piezoelectric electron-phonon coupling in planar hBN. We also provide an estimation of the coupling strength and find a piezoelectric response similar to reported DFT results.

HL 80.8 Thu 16:45 EW 015

Anisotropic Electrostatic Friction of Organic Molecules on ZnO Surfaces — •Karol Palczynski and Joachim Dzubiella — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

We study the long-time self-diffusion of a single conjugated organic *para*-sexiphenyl (*p*-6P) molecule physisorbed on the inorganic ZnO $(10\bar{1}0)$ surface by means of all-atom molecular dynamics computer simulations. We find strongly anisotropic diffusion processes in which the diffusive motion along the polar [0001] direction of the surface can be many orders of magnitudes slower at relevant experimental temperatures than in the perpendicular direction. The observation can be rationalized by the underlying charge pattern of the electrostatically heterogeneous surface which imposes direction-dependent energy barriers to the motion of the molecule. Furthermore, the diffusive behavior is found to be normal and Arrhenius-like, governed by thermally activated energy barrier crossings. The detailed analysis of the underlying potential energy landscape shows, however, that in general the activation barriers cannot be estimated from idealized zero-temperature trajectories but must include the conformational and positional excursion of the molecule along its pathway. Furthermore, the corresponding (Helmholtz) free energy barriers are significantly smaller than the pure energetic barriers with implications on absolute rate prediction at experimentally relevant temperatures.

HL 80.9 Thu 17:00 EW 015

high resolution nuclear inelastic scattering of antimony trioxide — atefeh jafari[1,2,3], ronnie e. simon[1,2], abdelfattah Mahmoud[1], dimitrios bessas[3], volkr l. Deringer[4], ralf stoffel[4], •richard dronskowski[4], ilya sergeev[5], benedikt klobes[1], and raphael p. hermann[1,2] — [1]Jülich Centre for Neutron Science JCNS and Peter Grünberg Institute PGI, Forschungszentrum Jülich, Jülich, Germany — [2]Faculty of Sciences, University of Liège, Liège, Belgium — [3]European Synchrotron Radiation Facility, Grenoble, France — [4]Institute of Inorganic Chemistry, RWTH Aachen University Landoltweg 1, Aachen — [5]Deutsches Elektronen-Synchrotron, Hamburg, Germany

The lattices dynamics of the α and β phases of antimony trioxides (Sb2O3) have been carried out using Mössbauer spectroscopy, nuclear inelastic scattering (NIS) and density functional theory (DFT). The experimental results are in very good agreement with our DFT calculations.The acoustic cut-off frequency of α- Sb2O3 is approximately 78 cm-1 as determined from the density of phonon states, DPS. Complementary to other Raman or IR methods, NIS is a powerful technique which yields the element specific density of phonon states of Mössbauer isotopes. Moreover, due to the high resolution achieved with the backscattering sapphire monochromator, we could identify weak and partially superposed bands.

HL 81: Heterostructures and interfaces

Time: Thursday 15:00–18:15 Location: EW 201

HL 81.1 Thu 15:00 EW 201

Structural and Electronic Properties of Si-ZnO and Si-In_2O_3 Interfaces from First Principles — •Benjamin Höffling[1,2] and Friedhelm Bechstedt[1,2] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]European Theoretical Spectroscopy Facility (ETSF)

We develop a method for the construction of atomic models of heterostructural interfaces based on coincidence lattices, maximum bond saturation, and total energy minimization, which enables us to construct model geometries for the interface between diamond structure Si, *bcc*-In_2O_3 and wurtzite-ZnO. In particular we investigate the Si(001)-In_2O_3(001), the Si(001)-ZnO(10$\bar{1}$0) and the Si(001)-ZnO(20$\bar{2}$3) interface by means of density functional theory (DFT). We predict electronic properties of the interface using both DFT and modern quasiparticle theory based on semilocal exchange-correlation functionals and examine electronic band discontinuities as well as the details of the interface electronic structure. The influence strain and charge transfer on the electronic density of states is discussed.

The band offsets and, hence, the efficiency of Si-TCO based devices depend crucially on the charge transfer at the interface, i. e. on the nature of the chemical bonds at the junction.

HL 81.2 Thu 15:15 EW 201

Computer Simulation of Growth Kinetics of Compound Semiconductors — •Jan Oliver Oelerich and Sergei D. Baranovskii — Faculty of Physics and Material Sciences Center, Philipps-Universität Marburg

Growth of III/V semiconductor compounds on Si substrates is currently in the focus of experimental and theoretical research because of its promising applications in functionalization of semiconductors. While surface structures and properties of the grown materials are experimentally well accessible, little is known about the formation and structural characteristics of the interfaces between the Si substrate and the III/V semiconductor compound. To gain insight into the intermediate stages of epitaxial growth and the interface properties, we developed a Kinetic Monte Carlo (KMC) computer simulation package for the theoretical study of the kinetic characteristics of epitaxial growth. Two particular problems were addressed in the simulations. First, it was recently observed that growth of GaP on the Si-001 surface leads to significant intermixing of the two materials at their interface. In our simulation we were able to identify the driving forces of the intermixing and accurately reproduce the experimentally observed features. Second, melt-back etching of Ga droplets on the Si-001 surface was simulated. In a recent experimental study it was shown that deposition of Ga onto a Si substrate leads to formation of metallic Ga droplets, etching large, pyramidally shaped structures into the bulk Si. We can reproduce this behaviour in the simulation and thereby study intermediate stages of the etching during the Ga deposition.

HL 81.3 Thu 15:30 EW 201

Band alignment in lateral two-dimensional heterostructures — Stephan Vercauteren, Ortwin Leenaerts, Bob Schoeters, and •Bart Partoens — University of Antwerp, Department of Physics, Belgium

The properties of semiconductor interfaces is mainly determined by the alignment of their respective band structures. Various methodologies have been devised to obtain the band alignment for bulk semiconductors, ranging from the simple alignment of vacuum potentials to the explicit simulation of the heterostructure with first-principles methods. When the dimensionality of the semiconductors is reduced, several problems with these alignment methods arise. Especially in-plane heterostructures, which consist of laterally connected 2D crystals, are more difficult to treat. Naive reasoning suggests that the simple alignment of the vacuum levels above each material is sufficient to determine the band alignment, but this simple reasoning is incorrect. We demonstrate that the vacuum potential is generally different above different 2D materials and that this difference depends crucially on the thickness of the involved materials. Furthermore, care should be taken to obtain the band alignment through heterostructure modeling with first-principles methods. The boundary conditions have a strong impact on the band alignment which needs to be corrected for.

HL 81.4 Thu 15:45 EW 201

Stability and capping of magnetite ultra-thin films — •Karsten Fleischer, Ozhet Mauit, and Igor V. Shvets — School of physics, Trinity College Dublin, Ireland

Ultrathin films of Fe_3O_4 have been grown epitaxially on nearly lattice matched MgO(001). The stability of 4 nm thick films in ambient air and under annealing in an oxygen atmosphere at 570K has been studied. By magneto optical and Raman measurements, we can confirm the presence of the Fe_3O_4 phase and the formation of a maghemite top layer passivating the Fe_3O_4 thin film. In a second step, we are able to demonstrate that this top layer oxidation in ambient air can be prevented by a 2 nm thick magnesium ferrite passivation layer, while a thicker 20 nm MgO layer prevents oxidation even at elevated temperatures.

HL 81.5 Thu 16:00 EW 201

An XPS study on copper oxide based solar cells — •Benedikt Kramm, Philipp Hering, Philipp Schurig, Fabian Michel, Angelika Polity, and Bruno K. Meyer — 1. Physikalisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, 35392 Gießen

For semiconductor hetero junctions the energy band alignment is one of the crucial factors which deliver a judgment for a successful operating device. We fabricated hetero junctions based on p-type cuprous oxide with n-type $Al_xGa_{1-x}N$ (first type) and $Mg_xZn_{1-x}O$ (second type) as window layer. The $Al_xGa_{1-x}N$ film was grown epitaxial on sapphire substrates whereas the copper oxide was deposited on top by RF-magnetron sputtering. $Mg_xZn_{1-x}O$ was similar deposited on sapphire substrates by RF-magnetron sputtering and again finally Cu_2O was deposited. An advantage of $Mg_xZn_{1-x}O$ compared to $Al_xGa_{1-x}N$ is the low cost fabrication even on a large scale as well as the sustainability of the elements. But it is well known that $Mg_xZn_{1-x}O$ has its limits in conductivity with increasing Mg content. Nevertheless, it might be possible to align the conduction bands of $Mg_xZn_{1-x}O/Cu_2O$ hetero junctions and thus to force up the efficiency in power conversion. Using X-ray photoelectron spectroscopy (XPS), we figured out that the conduction band offsets are getting smaller with increasing Al content for the first type of hetero structures. A similar trend is observable for Mg in the second type. Here, we will present and compare the band offset results. Another focus is on the intermixing at the oxygen-nitrogen and oxygen-oxygen interfaces and how it affects the band alignment.

HL 81.6 Thu 16:15 EW 201

Depth dependence of the ionization energy of shallow hydrogen donor states in ZnO and CdS — •Thomas Prokscha[1], Hubertus Luetkens[1], Elvezio Morenzoni[1], Gerard Nieuwenhuys[1,2], Andreas Suter[1], Max Döbeli[3], Michael Horisberger[4], and Ekaterina Pomjakushina[4] — [1]LMU, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland — [2]Kamerlingh Onnes Laboratory, Leiden University, 2300 RA Leiden, The Netherlands — [3]Ion Beam Physics, ETH Zurich, CH-8093 Zurich, Switzerland — [4]LDM, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland

The ionization energy of shallow hydrogen-like muonium (Mu) donor

states in nominally undoped ZnO and CdS (0001) crystals has been measured in a near-surface region (10 - 180 nm depth) by using low-energy muons, and in the bulk using conventional muon spin rotation (μSR) [1]. The implantation depth of the muons is varied by tuning the implantation energy of the low-energy muons between 2.5 and 30 keV. The ionization energy of the shallow Mu donor is lowered by about 10 meV compared to its bulk value at a mean depth of 100 nm, and continuously decreasing on approaching the surface. At a depth of about 10 nm the ionization energy is reduced by 25 - 30 meV. The same reduction is observed at a Au/ZnO interface. We attribute this change to the presence of electric fields due to band bending at the surface/interface. Using a simple one-dimensional model the depth profile of the electric field can be determined.

[1] T. Prokscha et al., arXiv:1408.6972, accepted for publication in Physical Review B.

Coffee break

HL 81.7 Thu 16:45 EW 201

Strain-relaxation in GaAs / InGaAs core-shell nanowire heterostructures grown by MBE onto Si(111) — •Ali Al Hassan[1], Andreas Biermanns[1], Emmanouil Dimakis[2], Ryan B. Lewis[2], Lutz Geelhaar[2], and Ullrich Pietsch[1] — [1]Naturwissenschaftlich-Technische Fakultät der Universität Siegen, 57068 Siegen, Germany — [2]Paul-Drude- Institute für Festkörperelektronik, Hausvogteiplatz 3, 10117 Berlin, Germany

Core-shell semiconductor nanowires (NW) can be grown onto various substrates without inclusion of misfit dislocations due to the strain release towards the NW side planes. This approach offers the possibility to form radial hetero-structures (HS) between highly lattice-mismatched materials but the process of strain relaxation is not fully understood.

We investigate strain interaction and relaxation in GaAs/InxGa1-xAs/GaAs NWHS grown by MBE onto silicon (111). X-ray diffraction measurements along [111] show, independent from GaAs core and InGaAs shell thickness ratio (x_In= 25% in shell thickness of 17nm), only one out-of plane Bragg peak corresponding to a solid solution with the total In content composed in the NW (Vegards law). On the other hand, X-ray measurements along the (1-10) and (2-1-1) NW side plane show separate peaks for core and shell materials with a mismatch corresponding to an In content in the shell closer to the nominal value but different along the direction normal to NW side planes and normal to NW edges. The data are interpreted in terms of finite element calculations revealing the complexity of strain relaxation mechanism.

HL 81.8 Thu 17:00 EW 201

A molecular statics study of strain fields and defect stability in axial-heteroepitaxial nanopillars — •Thomas Riedl[1,2] and Jörg Lindner[1,2] — [1]University of Paderborn, Department of Physics, Warburger Straße 100, 33098 Paderborn, Germany — [2]Center for Optoelectronics and Photonics Paderborn (CeOPP), Warburger Straße 100, 33098 Paderborn, Germany

Semiconductor nanopillars containing a heteroepitaxial junction in the axial direction are attractive for electronic and optoelectronic applications, owing to the high elastic relaxation of misfit strains and the possibility to modify the electronic band structure by means of strain. Compared to planar substrates axial-heteroepitaxial nanopillars can accomodate larger misfits without formation of misfit-related defects. Previous studies predicting the stability of misfit dislocations in axial-heteroepitaxial nanopillars or nanowires used different variants of analytic continuum theory or the finite element method. In the present contribution we investigate the strain fields and the stability of misfit dislocations in zinc blende InAs/GaAs nanopillars by means of atomistic molecular statics simulation. Because of its applicability to various bonding configurations and availability of suitable parametrizations the Tersoff potential is employed. The stability of the coherent defect-free state and of the dislocated state is analyzed in terms of the pillar dimensions and the dislocation configuration, i.e. dislocation type and position for both [001] and [111] pillar axis directions. The results are compared with the predictions of continuum approaches and with experiments reported in the literature.

HL 81.9 Thu 17:15 EW 201

Time-resolved *in situ* spectroscopy during formation of single-domain GaP/Si(100) heterointerfaces — •Oliver Supplie[1,2], Matthias May[1,2], Andreas Nägelein[1], Gabi Steinbach[3], Oleksandr Romanyuk[4], Frank Grosse[5], Peter Kleinschmidt[1,2], Sebastian Brückner[1,2], and Thomas Hannappel[1,2] — [1]TU Ilmenau, FG Photovoltaik — [2]Helmholtz-Zentrum Berlin, Solar Fuels — [3]Helmholtz-Zentrum Dresden-Rossendorf — [4]Institute of Physics, Academy of Sciences of the Czech Republic — [5]Paul-Drude Institut, Berlin

Though III-V/Si(100) heterointerfaces are essential for future epitaxial high-performance devices, their atomic structure is a historic open question. We study the formation of the GaP/Si(100) heterointerface time-resolved with reflection anisotroppy spectroscopy during pulsed GaP nucleation on almost single-domain Si(100) surfaces [1] in CVD ambient. A terrace-related dielectric anisotropy evolves about 100 meV below the E_1 critical point energy of silicon and agrees well with a GaP/Si(100) interface dielectric anisotropy (IDA) calculated from thicker GaP epilayers on Si(100).[2] X-ray photoelectron spectroscopy reveals a chemically shifted contribution of the P and Si emission lines, which quantitatively correspond to about one monolayer and establish similarly quick as the IDA.[2] We attribute this contribution to Si–P bonds at the heterointerface,[2] which were suggested recently.[3]

[1] Brückner et al., *Phys. Rev. B* **86** : 195310, 2012.
[2] Supplie et al., *J. Phys. Chem. Lett.* submitted, 2014.
[3] Supplie et al., *Phys. Rev. B* **90** : 235301, 2014.

HL 81.10 Thu 17:30 EW 201

Structural investigations of graded buffer systems in the TEM — •Florian Aumeier, Josef Loher, Christian Neumann, Dominique Bougeard, Daniel Henzler, Johannes Wild, Felix Schwarzhuber, and Josef Zweck — Institute of Experimental and Applied Physics, Regensburg, Germany

We investigated quantum well (QW) structures in epitaxially grown GaAs and SiGe graded buffer systems with [001] as growth direction. In these systems the strain induced by the lattice constant mismatch is relaxed by intentional defects in a metamorphic buffer system. The aim was to analyze the crystal quality of the system, in particular the defect free growth of the QW itself. Our focus lies on the detection and characterization of crystal defects with transmission electron microscopy (TEM). Besides the normal Bright Field investigations we used the weak beam dark field (WBDF) method to characterize the different perfect and partial dislocations. Normally such systems are observed in the [110] direction. By looking also at the [100] direction it has been found, that defects, which are clearly visible in one direction are nearly invisible in the other. This may lead to a misinterpretation of the structural perfection, if one considers only one direction.

HL 81.11 Thu 17:45 EW 201

Towards enhancement mode AlInN/AlN/GaN FETs using p-GaN cap layers — •Jonas Hennig, Armin Dadgar, Hartmut Witte, Juergen Blaesing, and Andre Strittmatter — Otto-von-Guericke Universität Magdeburg, Fakultät für Naturwissenschaften, Universitätsplatz 2, 39104 Magdeburg

With their large electric breakdown-field GaN based field effect transistors are ideally suited for high power electronics for voltages above 600 V and currents up to hundreds of amperes. The abrupt spontaneous polarization change at the AlInN/GaN heterojunction produces large sheet carrier concentrations, higher than for conventional AlGaN/GaN heterojunctions which results in a highly conductive channel even without bias. For safety reasons, however, these devices are required to operate in normally-off mode. By introducing a magnesium doped GaN cap layer on top of the AlInN the resulting electric field may deplete the channel under the gate region from charge carriers at zero gate bias. We currently conduct studies on p-GaN/AlInN/AlN/GaN FET structures grown on Si (111) by MOVPE and will present first results on the impact on FET performance. The analyses are carried out by XRD, AFM, Hall-effect, and current-voltage measurements.

HL 81.12 Thu 18:00 EW 201

Thermal and optical defect spectroscopy in AlInN/AlN/GaN hetero-structures on Si(111) — •Aqdas Fariza, Hartmut Witte, Jonas Hennig, Jürgen Bläsing, Armin Dadgar, Andre Strittmatter, and Alois Krost — Institute of Experimental Physics, Otto von Guericke University Magdeburg, Magdeburg, Germany

AlInN/GaN based high electron mobility transistors (HEMTs) are ideally suited for high power applications because of high electron concentrations and mobility. Additionally, the growth of AlInN/GaN HEMTs on Si-substrates has many advantages to reduce device costs. But, the presence of defects and traps constitutes a major problem which leads

to leakage currents and other degradation effects. Some traps have been assigned to cause these phenomena but still there is lacking information for structures on Si substrates. Temperature dependent I-V- and C-V-characteristics were carried out as well as thermal and optical admittance spectroscopy and photo-induced current transient spectroscopy for trap characterization both in InAlN/AlN/GaN/Si(111) hetero-structures and in GaN/Si(111) buffer layers. In both sample types identical trap emissions between 60 meV and 350 meV were found. All methods demonstrate strong optical quenching effects and non-shifting peak positions when changing the emission rates caused by the presence of mid gap traps in GaN. In contrast, the InAlN layers yield a shallow thermally activated resistivity up to 40 meV.

HL 82: Invited Talk Dan Buca

Time: Thursday 15:00–15:30 Location: EW 202

Invited Talk HL 82.1 Thu 15:00 EW 202

Group IV GeSn alloys - a viable solution for Si-based light emitters — •Dan Buca, Stephan Wirths, Siegfried Mantl, and Detlev Grützmacher — Peter Grünberg Institut 9, Forschungszentrum Jülich, Jülich, Germany

Silicon photonics is the key to overcome current limits in bandwidth and energy consumption associated with metal interconnects of complementary metal-oxide-semiconductor (CMOS) chips. Despite of the progress in the development of optical components such as Si compatible waveguides, modulators or detectors, an integrated light source is still missing. Ge has gained a lot of attention as material for on-chip lasing due to its CMOS compatibility and its electronic band structure, where the indirect L-valley lies only approx. 140 meV below the direct Gamma-valley. Hence, several approaches are presently pursued to improve the emission efficiency such as high n-type doping, the application of tensile strain, or alloying Ge with Sn. Both latter approaches lower the Gamma-valley faster than the indirect valleys facilitating a transition to a direct band gap material. GeSn alloys offer a global gain material in contrast to strained structures that are commonly defined locally. Here, we present the synthesis of strain-relaxed GeSn layers with Sn-contents up to 14%. The analysis of temperature-dependent photoluminescence (PL) measurements provided direct evidence for the transition from indirect to fundamental direct bandgap GeSn alloys. Recently, we could confirm optical gain by optical pumping of waveguide structures fabricated on a thick Ge0.87Sn0.13 layer. Finally unambiguous lasing action is presented.

HL 83: Focus Session: Oxide semiconductors II (DS with HL)

Time: Thursday 15:00–19:00 Location: H 2032

Invited Talk HL 83.1 Thu 15:00 H 2032

Optical properties and band structure of transparent semiconducting oxides — •Rüdiger Goldhahn — Otto-von-Guericke-Universität Magedeburg, Institut für Experimentelle Physik

Semiconducting metal oxides such as cubic In_2O_3 and rutile SnO_2 have attracted much interest in recent years. High-quality bulk crystals and single-crystalline heteroepitaxial films, covering a wide range of electron concentrations, became available allowing the determination of intrinsic optical properties as well as related fundamental band-structure parameters. This talk summarizes recent achievements.

Spectroscopic ellipsometry from the infrared (IR) into the vacuum-ultraviolet (VUV) spectral region is applied for determining the components of the dielectric tensor. The analysis of the IR dielectric function yields the phonon frequencies and the coupled phonon-plasmon modes from which electron effective mass as a function of carrier density (non-parabolicity of the conduction band) is obtained. Many-body effects such as exciton screening, band-gap renormalization, and band filling have a strong impact on the behavior around the fundamental band gaps, a quantitative description of these properties will be presented. Finally, synchrotron-based studies in VUV provide the transition energies related to critical points of the band structure.

HL 83.2 Thu 15:30 H 2032

Optical and Magneto-Optical Investigation of Spinel Oxide Thin Films — •Vitaly Zviagin[1], Peter Richter[2], Christian Kranert[1], Tammo Böntgen[1], Michael Lorenz[1], Dietrich R.T. Zahn[2], Georgeta Salvan[2], Rüdiger Schmidt-Grund[1], and Marius Grundmann[1] — [1]Universtät Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, Germany — [2]Technische Universtät Chemnitz, Semiconductor Physics, Reichenheiner Str. 70, Germany

We present a (magneto-) optical and structural investigation of Co_3O_4, $ZnFe_2O_4$, $CoFe_2O_4$, $ZnCo_2O_4$ and Fe_3O_4 spinel oxides grown at different temperatures on MgO (100) and $MgAl_2O_4$ (100) substrates by pulsed laser deposition. The optical properties were determined by spectroscopic ellipsometry in the spectral range from 0.5 eV to 8.5 eV and at temperatures from 10 K to 300 K. The magneto-optical response was measured in the range from 1.5 ev to 5.5 eV at room temperature and with an applied magnetic field of 1.7 T. A parametric model for the dielectric function, consisting of Gaussian and Lorenzian functions located at the optical transition energies, as well as the off-diagonal elements of the dielectric tensor were obtained. The magneto-optical response depends markedly on the crystal quality thus indicating the occurrence of mixtures of normal and inverse spinel structures. The study of (magneto-) optical properties is accompanied by structural analysis of the thin films using Raman spectroscopy, atomic force microscopy, and X-ray diffraction.

HL 83.3 Thu 15:45 H 2032

Spectroscopic signatures of dinitrogen in Cu_2O:N thin films — •Julian Benz, Philipp Hering, Benedikt Kramm, Bruno K. Meyer, and Peter J. Klar — I. Physikalisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, 35392 Gießen

Cuprous oxide (Cu_2O) is an intrinsically p-type semiconductor with a band gap of 2.1 eV. By doping with nitrogen it is possible to increase the hole density significantly. Thin films of Cu_2O:N were prepared by reactive RF sputtering, providing N_2 gas as dopant in the plasma. Raman spectra of the N-doped samples exhibit additional signals in the region of 2200 cm^{-1} to 2300 cm^{-1} Raman shift, which scale with the nitrogen content. We assume that these signals can be assigned to the vibration of dinitrogen molecules bound at different sites inside the bulk and at the surface. To support our assumption, the influence of oxygen flow during growth, as well as growth and annealing temperature are investigated.

HL 83.4 Thu 16:00 H 2032

Structural properties and phonon modes of $(Al_xGa_{1-x})_2O_3$ — •Christian Kranert, Marcus Jenderka, Jörg Lenzner, Michael Lorenz, Holger von Wenckstern, Rüdiger Schmidt-Grund, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Semiconductor Physics Group, Leipzig, Germany

We present a combined X-ray diffraction and Raman scattering study on a 2-inch diameter thin film with a continuous composition spread (CCS) [1] in comparison to bulk-like ceramic samples. For the composition range for which the ceramic materials exclusively exhibit the β-modification, we obtained their individual lattice parameters as a function of the composition. These comply with Vegard's rule. We further investigated these samples by Raman spectroscopy. The obtained phonon energy dependencies on the composition in the β-phase are found to be linear as well.

The CCS approach for the thin films allows us to determine its properties for virtually any composition within the composition range of the sample. The comparison to the ceramic samples shows a reduced out-of-plane lattice parameter for the thin films. Despite that, the phonon energies show a good agreement to the bulk values.

The material β-Ga_2O_3 is of interest for deep UV optoelectronics.

Alloying with Al_2O_3 increases its band gap, which makes the alloy $(Al,Ga)_2O_3$ suitable for an application in Ga_2O_3-based heterostructures or as barrier material for Ga_2O_3 quantum wells.

[1] H. von Wenckstern et al., CrystEngComm **15**, 10020 (2013)

HL 83.5 Thu 16:15 H 2032

Angle dependent Raman investigations of the different phases of Sn_xO_y — •Christian T. Reindl, Martin Becker, Bruno K. Meyer, and Peter J. Klar — I. Physikalisches Institut, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

The two widely known tin oxide phases SnO_2 and SnO are easily distinguished by examining their Raman spectra. Such Raman spectra contain information about the crystal structure and orientation as well as its quality, impurities, etc. Ion beam sputtered samples of SnO_2 and SnO with well-defined orientations are investigated using rotational Raman spectroscopy, a technique where the sample is rotated in plane with respect to the incident laser polarization. The intensity of the scattered light is analyzed for different polarizations with respect to the incident light. The data obtained is used to confirm the assignments of Raman modes appearing in the spectra of SnO_2 and SnO and to determine the values of the corresponding Raman tensor elements. Samples grown in the regime between the formation of these two phases yield completely different Raman spectra implies the formation of a third tin oxide phase in this intermediate regime. We present first identification of the Raman modes of this additional Sn_xO_y phase. Furthermore, naturally grown crystals are investigated and compared to the samples grown by ion beam sputtering and chemical vapor deposition.

15 min. break.

Invited Talk HL 83.6 Thu 16:45 H 2032

Thermodynamic stability and electronic structure of TCO surfaces: A computational approach — •Karsten Albe, Peter Agoston, Manuel Diehm, and Arno Fey — TU Darmstadt, FB 11, Fachgebiet Materialmodellierung, Jovanka-Bontschits-Str. 2, 64287 Darmstadt

A detailed understanding of the surface properties of transparent electrodes is a prerequisite for optimizing optoelectronic devices. In this contribution the thermodynamic stability and electronic properties of several experimentally observed low-index surfaces of bcc indium oxide (In2O3) and tin oxide (SnO2) are discussed based on results obtained by electronic structure calculations within density-functional theory. The influence of hydrogen, organic surfacants, n-type dopants (Sn), as well as the in-plane lattice strain are studied and compared to results of STM-studies on single crystalline samples. The computed data are also contrasted with results from photoelectron spectrocscopy on magetron-sputtered layers.

HL 83.7 Thu 17:15 H 2032

Defect studies on In_2O_3 thin films grown by pulsed laser deposition — •Florian Schmidt, Manuel R. Lindel, Daniel Splith, Stefan Müller, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Abteilung Halbleiterphysik, Linnéstraße 5, 04103 Leipzig

In_2O_3 is a promising oxide semiconducting material for applications in transparent electronics. Highly tin-doped In_2O_3 for instance is already commercially exploited as transparent conducting electrode. However, less is known on the defect structure of the host material. The fabrication of rectifying Schottky contacts on In_2O_3 was reported recently [1] and opens up the possibility to apply space-charge spectroscopic methods, such as thermal admittanz spectroscopy (TAS) or deep-level transient spectroscopy (DLTS).

We investigated point defects in both undoped In_2O_3 and compensated In_2O_3:Mg thin films by means of TAS and DLTS. While a defect level with a thermal activation energy E_t of approximately 200 meV and an apparent capture cross-section σ_n of about 10^{-16} cm^2 was found both materials another deep defect with $E_t \approx 90$ meV and $\sigma_n \approx 5 \times 10^{-18}$ cm^2 was exclusively found in the Mg-doped sample.

[1] H. von Wenckstern *et al.*, APL Materials **2**, 046104 (2014).

HL 83.8 Thu 17:30 H 2032

Lattice dynamics of Copper-Oxide phases from ab initio calculations — •Marcel Giar, Thomas Sander, Markus Heinemann, Christian T. Reindl, Bianca Eifert, Peter J. Klar, and Christian Heiliger — I. Physikalisches Institut, Justus-Liebig-University, D-35392 Giessen, Germany

Lattice dynamic properties the three copper oxide phases Cu_2O, Cu_4O_3, and CuO are investigated employing DFT calculations using the VASP code. Phonon bandstructure and density of states for all three phases are derived from a supercell small displacement method. The splitting of the LO and TO modes at the Γ point is obtained by properly taking into account the non–analytical contributions to the dynamical matrix in the limit $\mathbf{q} \to 0$. We also examine Raman properties by calculating Raman susceptibilities and derived Raman spectra. Special attention is paid to the role of defects such as simple Cu vacancies (V_{Cu}) and Cu split vacancies (V_{Cu}^{Split}) in the Raman spectrum of Cu_2O.[1] Further, we present calculations on the low–frequency dielectric tensor from which also IR data can be derived.

[1] T. Sander, C. T. Reindl, M. Giar, B. Eifert, M. Heinemann, C. Heiliger, and P. J. Klar, Phys. Rev. B 90, 045203 (2014)

HL 83.9 Thu 17:45 H 2032

Determination of subgap states in oxides: a challenge for DFT functionals — Wolfgang Körner[1], •Daniel F. Urban[1], David Munoz Ramo[2], Paul D. Bristowe[2], and Christian Elsässer[1,3] — [1]Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany — [2]Department of Materials Science and Metallurgy, University of Cambridge, United Kingdom — [3]Institute for Applied Materials, Karlsruhe Institute of Technology

We present a density-functional-theory analysis of crystalline and amorphous Zn- and Sn-based oxide systems which focuses on the electronic defect-states within the band gap [1]. A comparison of these electronic levels reveals that the hybrid DFT exchange-correlation functionals PBE0, HSE06 or B3LYP agree with a self-interaction corrected local-density approximation (SIC-LDA) functional on occupied defect levels when similar treatments of the self-interaction are considered. However, for unoccupied levels the hybrid functionals and the SIC approach lead to very different predictions. We show that a prerequisite for the determination of the energetic position of subgap states in these oxides is that a functional needs to predict correctly the electronic band structure over a wide energy range and not just close to the band gap. We conclude that for accurate defect levels an adequate treatment of the self interaction problem is required especially in the presence of nearby metal-metal interactions.

[1] W. Körner, D. F. Urban, D. Munoz Ramo, P. D. Bristowe, C. Elsässer, Phys. Rev. B 90, 195142 (2014)

Invited Talk HL 83.10 Thu 18:00 H 2032

Synthesis and Stability of Indium (III) Oxide Polymorphs — •Aleksander Gurlo and Maged Bekheet — Fachgebiet Keramische Werkstoffe, Technische Universität Berlin, Fakultät III Prozesswissenschaften, Institut für Werkstoffwissenschaften und -technologien, Sekr. BA3, Hardenbergstraße 40, 10623 Berlin, Germany

In our presentation the synthesis, stability and properties of binary indium oxides will be addressed. Our recent works deal with the synthesis and characterization of the known and new polymorphs in indium-oxygen system. In this way (i) a new orthorhombic In2O3 polymorph has been synthesized under high-pressure high-temperature conditions and recovered to ambient pressure and temperature, (ii) the metastability of corundum-type In2O3 have been proved both theoretically and experimentally, (iii) new sol-gel methodologies to synthesize high pressure In2O3 polymorphs under ambient pressure conditions have been developed, (iv) the stabilisation of pseudo-cubic {012} morphology in corundum-type In2O3 over several length scales have been verified, (v) the mobility and carrier concentration of well-defined corundum- and bixbyite-type In2O3 nanocrystals have been measured at different temperatures and in different gas atmospheres, (vi) a synthetic methodology for hierarchically organized hollow spheres has been developed, (vii) the crystallization of bixbyite-type In2O3 has been proven using in-situ time-resolved synchrotron radiation, and (viii) the stabilization of high-pressure corundum-type In2O3 polymorph in nanocrystals have been explained.

HL 83.11 Thu 18:30 H 2032

Photocatalysis of Titania Thin Films Prepared by Sputtering versus Evaporation — Bodo Henkel[1], Thomas Neubert[2], Sebastian Zabel[1], •Thomas Strunskus[1], Michael Vergöhl[2], and Franz Faupel[1] — [1]Lehrstuhl für Materialverbunde, Institut für Materialwissenschaft, Christian Albrechts Universität zu Kiel — [2]Fraunhofer Institut für Oberflächen- und Schichttechnologie, Braun-

schweig

To achieve a deeper understanding about reasons for differing photocatalytic efficiencies of titania thin films made by different physical vapor deposition techniques, different grain and phase growth pathways of these titania thin films have been studied. Results are shown for two well established and widely used PVD methods, namely electron beam evaporation and reactive pulsed DC magnetron sputtering. In addition the effect of inducing oxygen vacancy defects by tempering in reducing atmospheres on their photocatalytic efficiency have been tested, as well as aging of these thin films. These titania thin films where characterized with respect to crystallinity, texture and phases (XRD and Raman), roughness and surface area (AFM), light transmission and band gap energy (UV-Vis), refractive index (Ellipsometry), film thickness (Profilometer, Ellipsometry, SEM cross section), grain growth and structure (AFM, SEM of surface and cross section) and photocatalytic efficiency (methylene blue degradation). Results show different nucleation and growth mechanisms for evaporated compared to sputtered titania thin films, which have severe influence on photocatalytic efficiency.

HL 83.12 Thu 18:45 H 2032

Interdependence of electroformation and hydrogen incorporation in titanium dioxide — Mara Strungaru[1], Mihai Cerchez[2], •Svenja Herbertz[2], Thomas Heinzel[2], Mhamed El Achhab[3], and Klaus Schierbaum[3] — [1]Faculty of Physics, Alexandru Ioan Cuza University, 700506, Iasi, Romania — [2]Solid State Physics Laboratory, Heinrich-Heine-Universität Düsseldorf — [3]Materials Science Laboratory, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf

Nanoporous titanium dioxide films are exposed to molecular hydrogen gas during electroformation. In addition to the usual reversible increase of the conductance of the films as hydrogen is offered, an irreversible decrease of the conductance is observed. The behavior is interpreted in terms of a phenomenological model where current carrying, oxygen-deficient filaments form inside the TiO_2 matrix in which hydrogen incorporation decreases the carrier density.

[1] M. Cerchez, H. Langer, M. E. Achhab, T. Heinzel, D. Ostermann, H. Lüder, and D. Ostermann, Appl. Phys. Lett. 103, 033522 (2013). [2] D. B. Strukov, G. S. Snider, D. R. Stewart, and R. S. Williams, Nature 453, 80 (2008). [3] T. Bjørheim, S. Stølen, and T. Norby, Phys. Chem. Chem. Phys. 12, 6817 (2010).

HL 84: Focus Session (CPP with HL): Hybrid photovoltaics and perovskites II

Time: Thursday 15:00–18:15 Location: C 130

Invited Talk HL 84.1 Thu 15:00 C 130

Photophysics of organic-inorganic hybrid lead iodide perovskite single crystals — •Maria Antonietta Loi — Zernike Institute for Advanced Materials, University of Groningen, The Netherlands

Hybrid organometal halide perovskites have been demonstrated to have outstanding performance as semiconductors for solar energy conversion. Further improvement of the efficiency and stability of these devices requires a deeper understanding of their intrinsic photophysical properties. Here we address the intrinsic material physics by investigating the structural and optical properties of high quality single crystals of Methyl Ammonium Lead Iodide from room temperature to 5K. X-ray diffraction reveals an extremely sharp transition at 163 K from a twinned tetragonal I4/mcm phase to a low-temperature phase characterized by complex twinning and possible frozen disorder. Above the transition temperature the photoluminescence is in agreement with a band-edge transition, explaining the outstanding performances of the solar cells. Whereas below the transition temperature, three different features arise, one of which is attributed to a singlet-free-exciton and the other two to bound-triplet excitons. The bound-triplet excitons are characterized by a decay dynamics of about 5μs and by a saturation phenomenon due to many-body interactions. This results in a description of the room temperature recombination as being due to spontaneous band-to-band radiative transitions and weak non-radiative Auger processes, whereas a diffusion-limited behaviour is expected for the low temperature range.

Invited Talk HL 84.2 Thu 15:30 C 130

Exciton stabilization in hybrid lead-halide perovskites: photophysical versus structural properties — •Annamaria Petrozza — Istituto Italiano di Tecnologya, Milan, Italy

Hybrid perovskites represent a new, disruptive technology in the field of optoelectronics. Hybrid halide perovskites, e.g. CH3NH3PbX3 [X = Cl, Br, or I], are usually deposited as polycrystalline thin-films with variable mesoscale morphology depending on the growth conditions. The obtained grain size ranges from tens to thousands of nm. Over the last two years the impressive improvement of photovoltaic performance has been driven by radical empirical evolution of the device architecture and processing methodologies. However, there is a considerable lack of understanding of material properties, both as pristine films and their embodiment in a device. Here we demonstrate, through a combination of femto-second transient absorption spectroscopy, structural analysis and multi-scale modeling as a function of crystal size and temperature, that the electron-hole interaction is sensitive to the microstructure of the material. We find that by control of the material processing during fabrication both free carrier and Wannier excitonic regimes are accessible. Thus, a definitive classification excitonic or free carrier semiconductor is not possible. The long-range order of the organic cation dipole field is disrupted by polycrystalline disorder introducing domain walls where dipole twinning breaks down. The variations in electrostatic potential found for smaller crystallites suppress exciton formation, while larger crystals of the same composition demonstrate an unambiguous excitonic state.

HL 84.3 Thu 16:00 C 130

Morphology-dependent ultrafast spectroscopy of lead-halide perovskite for electro-optical applications — •Simon Bretschneider, Melike Karakus, Valentin Kamm, Enrique Cánovas, and Frédéric Laquai — Max Planck Institut für Polymerforschung, Mainz

Lead-halide perovskite have emerged as a new class of materials for electro-optical, especially photovoltaic applications with power conversion efficiencies now up to 20% [1]. High-performance electro-optical devices rely on perovskite films without pinholes, flat surface and well-defined thickness. Due to the organic/inorganic nature of the lead-halide perovskite and the criticalness of a pure perovskite phase without impurities of the precursors, utilization of solution-processing is non-trivial.

The combination of time-resolved photoluminescence and transient absorption spectroscopy is a powerful tool, which allows for the investigation of generation and recombination of charge carriers in lead-halide perovskite films on a femto- to microsecond timescale and across a spectral range from Vis to NIR. In this work, we present pump-probe transient absorption measurements of solution-processed lead-halide perovskite films grown in ambient and dry nitrogen atmosphere using different post-processing annealing schemes. The findings of ultrafast spectroscopy suggest that the performance of lead-halide perovskite films for electro-optical applications relies more on homogeneous films than on specific crystal sizes.

[1]NREL Chart of record cell efficiencies (28.11.2014).

HL 84.4 Thu 16:15 C 130

Time-resolved confocal microscopy of hybrid metal halide perovskite thin films — •Kathrin Bader, Richard Ciesielski, Nadja Giesbrecht, Johann M. Feckl, Irene Grill, Fabian C. Hanusch, Thomas Bein, Pablo Docampo, Matthias Handloser, and Achim Hartschuh — Department Chemie and CeNS, LMU Munich, Germany

Organic-inorganic metal halide perovskite solar cells (PSCs) have seen an unprecedented development over the past 4 years due to their potential to fulfill most requirements for large scale production. Extremely fast progress in the field of perovskite absorbers has taken solar cell efficiencies from 10 % in 2012 [1] to over 19 % in 2014 [2]. A crucial parameter for the functioning of solar cells is a long charge carrier diffusion length that allows to effectively collect photogenerated charges. To determine this diffusion length several experimental methods have been reported that either provide indirect information

or use electrical contacts [3,4]. We used time-resolved laser scanning confocal microscopy to visualize the transport range and timescale of photo-excited species within the film. The experimentally observed transport length range up to several microns under high light intensity conditions. Our results help to explain the high short circuit currents that can be achieved in PSCs. Financial support by the DFG through the Nanosystems Initiative Munich (NIM) is gratefully acknowledged. [1] M. M. Lee et al., Science 338, 643 (2012) [2] H. Zhou et al., Science 345, 542 (2014) [3] S. D. Stranks et al., Science 342, 6156 (2013) [4] E. Edri et al., Nat. Commun. 5, 3461 (2014)

HL 84.5 Thu 16:30 C 130

Preparation and characterization of methylammonium lead halide perovskite solar cells in planar-type configuration — •Philipp Rieder[1], Matthias Fischer[1], Stefan Väth[1], Andreas Baumann[2], Kristofer Tvingstedt[1], and Vladimir Dyakonov[1,2] — [1]Experimentelle Physik 6, Julius-Maximilians-Universität Würzburg, 97074 Würzburg — [2]Bayerisches Zentrum für Angewandte Energieforschung, 97074 Würzburg

In recent years, the use of organometal halide compounds as the photoactive layer in solar cells has attracted a lot of attention, with power conversion efficiencies (PCE) reaching up to 20.1% already. The performance and properties of this material class are strongly dependent on the crystallinity of the layer, with the working principles still being unclear and part of ongoing research. By synthesizing our own methylammoniumiodide as the organic precursor, we are able to fabricate solution processed planar heterojunction perovskite solar cells with an active layer consisting of $CH_3NH_3PbI_3$ or $CH_3NH_3PbI_{3-x}Cl_x$. PCE values of the working devices exceeding 10% under solar illumination are achieved. The crystallinity and surface quality of the films are analyzed via scanning electron microscopy, atomic force microscopy and x-ray diffraction. The solar cells are characterized by means of current-voltage measurements, external quantum efficiency and photoluminescence.

HL 84.6 Thu 16:45 C 130

Spatially resolved photocurrent generation in organolead halide perovskite solar cells — Thomas J.K. Brenner, Andreas Paulke, Natalie Schön, Roberta Saponaro, and •Dieter Neher — Institute of Physics & Astronomy, University of Potsdam, Germany

Hybrid perovskite solar cells have shown to be efficient in various device structures, for example in planar, vapour deposited films, in and on mesostructured metal oxides and in solution-processed films of different crystallinity. Here, we study ITO/PEDOT:PSS/CH3NH3PbI3/PCBM/C60/BCP/Al devices with different perovskite crystallinity and identify regions of efficient photocurrent generation with submicrometer resolution. We establish a relationship between crystallinity and device performance and study the role of grain boundaries for photocurrent generation. We correlate our results to time delayed collection field (TDCF) measurements of charge generation to identify ways to further enhance photocurrent generation in this class of photovoltaic devices.

15 min. break.

HL 84.7 Thu 17:15 C 130

Unbalanced Charge Distribution Inside a Perovskite-Sensitized Solar Cell in Real Space — •Victor W. Bergmann[1], Stefan A.L. Weber[1], F. Javier Ramos[2], Mohammad Khaja Nazeeruddin[3], Michael Grätzel[3], Dan Li[1], Anna L. Domanski[1], Ingo Lieberwirth[1], Shahzada Ahmad[2], and Rüdiger Berger[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Abengoa Research, Seville, Spain — [3]Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Solar cells based on perovskite light absorbing materials reached power conversion efficiencies >20%. Today, the knowledge about the local charge generation processes inside these solar cells is limited. We prepared smooth cross sections by means of focused ion beam milling such that the full structure and functionality of the devices were preserved [1]. This way, the internal interfaces between the different materials in the cell are accessible for frequency modulation Kelvin Probe Force Microscopy (FM-KPFM). Upon illumination under short-circuit conditions, holes accumulate in front of the hole transport layer, which is proof of an unbalanced charge transport. This potential barrier reduces the charge transfer towards the electrode. Furthermore after light illumination, we measured remaining charges inside the active device area. These charges were attributed to traps in the material. In conclusion, the FM-KPFM method allows us not only to map the local contact potential variation but also to correlate it with the local structure of the functional layers.

[1] Bergmann et al. Nature Communications 5, 5001 (2014).

HL 84.8 Thu 17:30 C 130

Charge Transport in Dye-sensitized Solar Cells: What do J-transients really depend on? — •Frank Marlow, Abigail Hullermann, and Lisanne Messmer — MPI für Kohlenforschung, 45470 Mülheim an der Ruhr, Germany

J-transients (electrical current transients) following a laser excitation are considered as a powerful tool for the understanding of the action of dye-sensitized solar cells. In the last years, a sophisticated model for their understanding has been established which, however, turns out to be in contradiction with a number of experimental findings including the J-signal shape and the signal dependences on experimental parameters. It is especially remarkable that there are the always delays of the electrical signal after the laser excitation and that the possible diffusion times do not follow an Einstein diffusion relation which is a-priori assumed in many works.

HL 84.9 Thu 17:45 C 130

Spray deposition of titania films with introduction of crystalline nanoparticles for solid-state dye-sensitized solar cells — •Lin Song[1], Weijia Wang[1], Volker Körstgens[1], Daniel Moseguí González[1], Yuan Yao[1], Norma K. Minar[2], Dina Fattakhova-Rohlfing[2], Stephan V. Roth[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]LMU München, Department of Chemistry and Center for NanoScience, Butenandtstr.5-13 (E), 81377 Munich — [3]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany

Solid-state dye-sensitized solar cells (ssDSSCs), using solid-state hole transporting materials (HTM) as alternatives for dye generation and hole transport, have received immense attention because such photovoltaic devices avoid the leakage and corrosion problems in conventional DSSCs. In particular, ssDSSCs based on TiO2 and organic HTM are of great interest due to the combined advantages of both organic and inorganic components. We investigate this kind of solar cells fabricated using mesoporous titania films as electron transporting materials, a metal-free dye D149 as a light harvester, and P3HT as HTM. For optimizing the device performance, we introduce crystalline titania nanoparticles into the titania film in order to obtain a more effective titania photoanode. Moreover, spray coating is employed for the film deposition because it is simple, low cost, and usable for large-scale production. The morphology and crystallinity of titania films are investigated, showing a crucial influence on final device performance.

HL 84.10 Thu 18:00 C 130

ZnO coated TiO2 photoanodes with improved electron transfer for dye sensitized solar cells — •Bo Liu[1], Peter Lemmens[1], Andrey Bakin[2], Andreas Waag[2], Aidin Lak[3], Meinhard Schilling[3], Winfried Daum[4], and Samir Kumar Pal[5] — [1]IPKM, TU-BS, Braunschweig — [2]IHT, TU-BS, Braunschweig, Germany — [3]EMG, TU-BS, Braunschweig, Germany — [4]IEPT, TU Clausthal — [5]SNBC, Kolkata, India

ZnO coated TiO2 photoanodes for cost efficient dye sensitized solar cells are prepared using anodization of a metal electrode leading to an array of TiO2 nanotubes. Atomic layer deposition is used for the conformal covering by ZnO. Following hematoporphyrin sensitization the improved electron transfer is probed using time resolved fluorescence. Work supported by RTG-DFG 1953/1, Metrology for Complex Nanosystems and the Laboratory for Emerging Nanometrology, TU Braunschweig.

HL 85: Topological Insulators 2 (MA with HL/TT)

Time: Thursday 15:00–17:45 Location: EB 202

HL 85.1 Thu 15:00 EB 202

Topological surface states of Heusler-type topological insulators — •Shu-Chun Wu[1], Binghai Yan[1,2], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Max Planck Institute for Physics of the Complex Systems, Dresden, Germany

Some promising half-Heusler compounds, RPtBi (R = La, Lu, Y), are demonstrated experimentally to be superconductors and are predicted to be topological insulators. The topological feature of bulk is band inversion and the s orbital of Pt atom is the main clue. However, their topological surface states (TSSs) remain unclear. In this work, we use *ab initio* method to investigate the TSSs. In experiment, they are found at the Γ point inside the valence bands. Spin texture is also calculated to confirm the topologically nontrivial surface states. External strain can push the TSSs from the valence bands up into gap.

HL 85.2 Thu 15:15 EB 202

Topological surface states on NaBaBi with two opposite spin textures — •Yan Sun[1], Shu-Chun Wu[1], Claudia Felser[1], and Binghai Yan[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany. — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany.

By breaking the inversion symmetry of the 3D Dirac metal Na_3Bi, we realize topological insulator (TI) phases in a known compound NaBaBi using $ab-initio$ calculations. Two distinct TI phases emerge: one phase is due to the band inversion between $Bi-p$ and $Na-s$ bands, and the other phase (under pressure) is induced by the inverted $Bi-p$ and $Ba-d$ bands. Both phases exhibit Dirac-cone-type surface states, but opposite spin textures. In the upper cone, a left-hand spin texture exists for the s-p inverted phase (similar to a common TI, e.g. Bi_2Se_3) while a right-hand spin texture appears for the $p-d$ inverted phase. NaBaBi presents a prototype model for TIs that exhibit different spin textures in the same material.

HL 85.3 Thu 15:30 EB 202

Indirect exchange interaction through topological surface states in crystalline topological insulators of a SnTe class — •Nicolas Klier, Sam Shallcross, and Oleg Pankratov — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

As predicted theoretically [1,2] and confirmed experimentally [2,3] the interface of SnTe and vacuum (i.e. the material's surface) hosts topologically stable Dirac states. We investigate the properties of this state within a **k.p** model that includes a full account of the bulk band structure [4]. An essential advantage of an analytical band model [4] is that it allows to unequivocally trace the two key degrees of freedom that this system possesses: spin and pseudospin. The indirect exchange interaction between magnetic impurities is a perfect probe for the surface Dirac states, especially for their spin structure. We revealed explicitly the dependence of this interaction on the properties of the bulk band states, in particular on the spin orbit coupling strength and on the crystal field splitting parameters. Depending on these parameters, the interaction may be either of Ising type or of a novel anisotropic XY type with the spin direction aligned with the connection vector between the two impurities.

[1] B.A. Volkov, and O.A. Pankratov, *J*ETP Lett. **42**, 178, 1985.
[2] T.H. Hsieh *et al.*, *N*ature Comm. **3**, 982, 2012.
[3] Y. Tanaka *et al.*, *N*ature Phys. **8**, 800, 2012.
[4] B.A. Volkov, and O.A. Pankratov, *Z*h.Eksp. Theor. Fiz. **75**, 1362, 1978.

HL 85.4 Thu 15:45 EB 202

Edge states in topological magnon insulators — Alexander Mook[1], •Jürgen Henk[2], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle (Saale), Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany

For magnons, the Dzyaloshinskii-Moriya interaction accounts for spin-orbit interaction and causes a nontrivial topology that allows for topological magnon insulators. In this theoretical investigation [1] we present the bulk-boundary correspondence for magnonic kagome lattices by studying the edge magnons calculated by a Green function renormalization technique. Our analysis explains the sign of the transverse thermal conductivity of the magnon Hall effect in terms of topological edge modes and their propagation direction. The hybridization of topologically trivial with nontrivial edge modes enlarges the period in reciprocal space of the latter, which is explained by the topology of the involved modes.

[1] Phys. Rev. B **90** (2014) 024412.

HL 85.5 Thu 16:00 EB 202

Magnon waveguides from topological magnon insulators — •Alexander Mook[1], Jürgen Henk[2], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle

Topological magnon insulators exhibit a nontrivial topology due to the Dzyaloshinskii-Moriya interaction. They host topologically nontrivial edge magnons and, consequently, energy as well as spin currents along their edges [1,2].

Bringing two topological magnon insulators into contact results in topologically protected unidirectional interface magnons. As these interface modes decay toward both bulk regions, their currents are confined to a few nanometer wide strip around the interface. Owing to the topological nature of the edge states, the edge currents follow any geometry.

We address theoretically the formation of interface edge magnons and their currents. On top of this, we propose recipes to compose magnon waveguides with nano-scale confinement.

[1] L. Zhang et al., PRB **87**, 144101 (2013).
[2] A. Mook et al., PRB **90**, 024412 (2014).

HL 85.6 Thu 16:15 EB 202

Probing the Electronic Properties of Individual MnPc Molecules Coupled to Topological States — •Thomas Bathon[1], Paolo Sessi[1], Konstantin Kokh[2], Oleg Tereshchenko[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik 2, Universitaet Wuerzburg, Am Hubland, 97074 Wuerzburg, Germany — [2]Novosibirsk State University, 630090 Novosibirsk, Russia

Hybrid organic-inorganic interfaces have been widely reported to host emergent properties that go beyond those of their single constituents. Coupling molecules to the recently discovered topological insulators, which possess linearly dispersing and spin-momentum-locked Dirac fermions, may offer a promising platform towards new functionalities.

Here, we report a scanning tunneling microscopy and spectroscopy study of the prototypical interface between MnPc molecules and a Bi_2Te_3 surface. MnPc is found to bind stably to the substrate through its central Mn atom. The adsorption process is only accompanied by a minor charge transfer across the interface, resulting in a moderately n-doped Bi_2Te_3 surface. More remarkably, topological states remain completely unaffected by the presence of the molecules, as evidenced by the absence of scattering patterns around adsorption sites. Interestingly, we show that, while the HOMO and LUMO orbitals closely resemble those of MnPc in the gas phase, a new hybrid state emerges through interaction with the substrate.

HL 85.7 Thu 16:30 EB 202

first principle study of structural, electronic and magnetic properties of graphene nanoribbons deposited on the topological insulator Sb2Te3 — wei zhang[1,2], •farideh hajiheidari[1], yan li[1,3], manuel j. schmidt[1], and riccardo mazzarello[1,4] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, D-52074 Aachen, Germany — [2]Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany — [3]IEK-6, Forschungszentrum Jülich, D-52425 Jülich, Germany — [4]JARA-FIT and JARA-HPC, RWTH Aachen University, D-52074 Aachen, Germany

Magnetic perturbations are known to affect the surface properties of a topological insulator (TI) dramatically. According to mean-field calculations, zigzag graphene nanoribbons (zGNRs) possess spin-polarized edge states. Hence, zGNRs deposited on a TI could be a promising candidate for an experimental investigation of proximity effects between a magnetic system and a TI. In this work, we carry out a first-principles investigation based on density functional theory of zGNRs on the Sb2Te3 (001) surface. We use gradient-corrected density func-

tionals in combination with semi-empirical van der Waals corrections. Both H-free and H-terminated zGNRs are considered. In the case of H-free zGNRs, the strong interaction between the edge atoms and the TI surface is shown to lead to the bending of the zGNRs , however, the edge magnetism is preserved. Moreover, the magnetic anisotropy axis is perpendicular to the surface of the substrate. In the H-terminated case, on the other hand, the interaction is less significant and edge magnetism is fully preserved.

HL 85.8 Thu 16:45 EB 202

WSe_2 Synthesis, Characterization and Properties — •Catherine R Rajamathi, Binghai Yan, Marcus Schmidt, Kumari Gaurav Rana, Chandra Shekhar, Siham Ouardi, Guido Kreiner, and Claudia Felser — Max-Planck Institute for Chemical Physics of Solids, Dresden

Layered transition metal dichalcogenides (TMDs) are widely studied systems as they are chemically versatile and technologically enthralling. The facile tunability of their electronic structure by varying certain parameters - carrier type (n- or p-type), composition, structure or sample size expand their applications from catalysis to topological insulators. Single crystals were synthesized from its polycrystalline components using $SeCl_4$ as the transport agent. Mono- or few-layered tungsten selenide obtained by the scotch-tape technique discussed in this talk are direct-gap semiconductors. FET devices fabricated from a few-layered sample of WSe_2 show ambipolar transistor behavior. In addition, hybrid materials such as $WSe_{2-x}Te_x$ may be promising due to high magnetoresistance and surface states on WTe_2 single crystals.

HL 85.9 Thu 17:00 EB 202

Classification of spin liquids on the square lattice with strong spin-orbit coupling — •Johannes Reuther[1,2], Shu-Ping Lee[3], and Jason Alicea[3] — [1]Freie Universität Berlin — [2]Helmholtz-Zentrum Berlin für Materialien und Energie — [3]California Institute of Technology

The investigation of spin liquids is a fascinating field in condensed matter physics that is increasingly motivated by experiments. Exhaustive classifications of spin liquids have been carried out in several systems, particularly when full SU(2) spin-rotation symmetry is present. Systematic studies that explore strongly spin-orbit-coupled magnetic compounds (for which there are many experimental examples) are, however, relatively scarce. We report on a classification of Z_2 spin liquids on the square lattice when SU(2) spin symmetry is maximally lifted. Using projective symmetry group methods, we find that, surprisingly, the lifting of spin symmetry yields vastly more spin liquid states compared to SU(2)-invariant systems. A generic feature of the SU(2)-broken case is that the spinons naturally undergo $p + ip$ pairing; consequently, many of these Z_2 spin liquids feature a topologically nontrivial spinon band structure supporting gapless Majorana edge states. These boundary modes are often protected by a combination of time reversal and lattice symmetries and hence resemble recently proposed topological crystalline superconductors.

HL 85.10 Thu 17:15 EB 202

Fate of the 1/3 magnetization plateau in quantum triangular antiferromagnets with various anisotropies — •Fedor Simkovic[1], Natasha Perkins[2], and Andrey Chubukov[2] — [1]King's College, London, England — [2]University of Minnesota, Minneapolis, United States

The triangular Heisenberg lattice is investigated by means of semiclassical 1/S expansion. Although classically the up-up-down phase with 1/3 magnetisation exists only at one magnitude of the field, it is stabilised by quantum fluctuations and forms a magnetisation plateau around this point. We investigate into three types of anisotropies for the triangular lattice, and access the stability of the aforementioned phase towards the limits of decoupled chains, the square, honeycomb, Kagome, rhombille and scaled triangular lattices.

HL 85.11 Thu 17:30 EB 202

Matrix product operators: Local equivalences and topological order in 2D — •Oliver Buerschaper — Freie Universität Berlin

Projected entangled pair states (PEPS), which naturally generalize matrix product states (MPS) to higher dimensions, describe the low energy properties of local quantum Hamiltonians with an energy gap very well. For this reason they are increasingly used as a valuable tool in both analytical and numerical studies of strongly correlated 2D quantum systems. Some of the most interesting such systems exhibit topological order, i.e. patterns of long-range entanglement which cannot be detected by any local order parameter. At the same time, excitations in these systems typically exhibit fractional statistics and may be used, for instance, as a resource for topological quantum computation.

For both fundamental and practical reasons, it is thus of the utmost importance to understand and classify PEPS in 2D, especially those with topological order. Recently it was found that symmetries defined in terms of certain matrix product operators (MPO) provide a mechanism for the emergence of topological order in PEPS. Furthermore, the kind of topological order was seen to depend on the algebraic properties of the given MPO symmetry. Here we show that many, seemingly distinct MPO symmetries are, in fact, locally equivalent and characterize PEPS with the *same* kind of topological order. We discuss interesting ramifications for the classification of 2D quantum systems.

HL 86: Transport: Quantum dots, quantum wires, point contacts 2 (TT with HL)

Time: Thursday 15:00–18:30 Location: A 053

HL 86.1 Thu 15:00 A 053

Weak antilocalization and spin-orbit interaction in epitaxial nanowires — Brian Tarasinski[1], Ilse van Weperen[2], Debbie Eeltink[2], Vlad Pribiag[2], Erik Bakkers[2,3], Leo Kouwenhoven[2], and •Michael Wimmer[2] — [1]Leiden University, The Netherlands — [2]Delft University of Technology, The Netherlands — [3]Eindhoven University of Technology, The Netherlands

We develop a theory of weak antilocalization for three-dimensional nanowires that allows for a quantitative extraction of spin-orbit strength. To this end we perform numerical Monte Carlo simulations of classical trajectories that are used in the quasiclassical theory of weak antilocalization. In particular, we show that magnetoconductance in three-dimensional nanowires is very different compared to wires in two-dimensional electron gases

Focusing on the case of Rashba spin-orbit interaction, we then use this theory to extract the Rashba spin-orbit strength from weak antilocalization measurements in epitaxially grown InSb nanowires. We find a spin-orbit energy on the order of 0.25-1 meV.

HL 86.2 Thu 15:15 A 053

Tunable weak anti-localization in InAs nanowire device — •Libin Wang[1], Jingkun Guo[1], Sen Li[1], Ning Kang[1], Dong Pan[2], Jianhua Zhao[2], and Hongqi Xu[1] — [1]Key Laboratory for the Physics and Chemistry of Nanodevices and Department of Electronics, Peking University, Beijing 100871, China — [2]Institute of Semiconductors, Chinese Academy of Sciences, Beijing 100083, China

III-V semiconductor nanowire had attracted much attention as a possible building block for future electronic systems because of its high performance and possibility of gate voltage manipulation of electron spins. InAs nanowires are particularly attractive due to its strong spin-orbit interaction. We report the fabrication and magnetotransport measurement of individual InAs nanowires with diameter of 40 nm on a SiO_2/Si substrate with a globe back gate. The observed magnetoresistance at low temperature can be used to estimate the characteristic phase coherence length and the spin-orbit scattering length. We observe a crossover between weak anti-localization and weak localization with the change of temperature and applied electric field. Our results give information on the fundamental spin relaxation and quantum coherence effect of InAs nanowire.

HL 86.3 Thu 15:30 A 053

Full-counting statistics of Landau-Zener interference in quantum dot arrays — •Michael Niklas[1], Robert Hussein[2], and Sigmund Kohler[2] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Instituto de Ciencia de

Materiales de Madrid, CSIC, 28049 Madrid, Spain

We investigate current cumulants for the transport in coupled quantum dots driven by a time-periodic field that sweeps the system repeatedly through an avoided crossing and, thus, acts like a beam splitter. Consequently, as a function of the detuning and the driving amplitude, the cumulants exhibit Landau-Zener-Stückelberg-Majorana (LZSM) interference patterns similar to those observed for the current in driven double quantum dots [1]. These patterns indicate regions with sub- and super-Poissonian noise level. As a flexible method that allows us to study driving fields with arbitrary shape, we developed a propagation scheme for the iterative computation of current cumulants. We demonstrate that it is applicable also for larger systems such as quantum dot arrays or dimer chains.

[1] F. Forster et al., Phys. Rev. Lett. **112**, 116803 (2014).

HL 86.4 Thu 15:45 A 053

Fractionalized double quantum wires — •Tobias Meng[1,2] and Eran Sela[3] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland — [3]Raymond and Beverly Sackler School of Physics and Astronomy, Tel-Aviv University, Tel Aviv, 69978, Israel

We discuss how electron-electron interactions can lead to novel phenomena in double quantum wire systems. Explicitly, we find that double wires with time reversal symmetry and strong electron-electron interactions can exhibit fractional conductances and cross-conductances in their normal state. They also allow to pump the fraction of a spin in their superconducting state. These effects are an extension of fractional helical Luttinger liquid physics, and can be understood as the one-dimensional cousins of bilayer fractional quantum Hall effects.

HL 86.5 Thu 16:00 A 053

Non-equilibrium Renormalization Group for Kondo Qdots in a Microwave Photon Field — •Andisheh Khedri[1,2,3], Ammar Nejati[1], and Johann Kroha[1] — [1]Universität Bonn — [2]RWTH Aachen — [3]FZ Jülich

Recent experiments on Kondo quantum dots in a static magnetic field and a microwave photon field show a resonant enhancement of the zero-bias differential conductance at a photon energy which scales with the applied magnetic field, but which is substantially larger than the bare Zeeman energy of the dot levels [1]. This behavior cannot be explained by direct, photoinduced spin-flip excitations of the dot. It points to a strong renormalization of the Zeeman energy (Landé factor) in the presence of the microwave field. We propose that the observed resonant conductance is caused by photo-assisted Kondo spin-flip scattering of the lead electrons, i.e., by electronic lead–dot transitions, assisted by coherent photon absorption and/or emission. We develop the non-equilibrium perturbative renormalization group (RG) theory [2] for this problem. The renormalization of the various coupling functions for spin vertices without photon processes as well as involving photon absorption, emission and scattering is anaylzed as well as the Qdot level shifts. We find a subtle interplay between Kondo scattering and coherent photoassisted processes, restoring the logarithmic RG flow and leading to strong renormalization of the Landé factor.

[1] B. Hemingway, S. Herbert, M. Melloch, A. Kogan, PRB **90**, 125151 (2014)
[2] A. Rosch, J. Paaske, J. Kroha, P. Wölfle, PRL **90**, 076804 (2003).

HL 86.6 Thu 16:15 A 053

Competing energy scales in the renormalization group flow of quantum dot setups with periodically varying parameters — •Katharina Eissing[1,2], Dante Marvin Kennes[1,2], and Volker Meden[1,2] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University, 52074 Aachen, Germany — [2]JARA Fundamentals of Future Information Technology, 52056 Aachen, Germany

The functional renormalization group (fRG) has proven to be a versatile tool to investigate correlated, low-dimensional systems in and out of equilibrium. It was recently extended to study quantum dot setups with explicitly time dependent Hamiltonians [Phys. Rev. B 85, 085113 (2012)]. In systems in which one or more of the dot or lead parameters are varied periodically in time a periodic steady state is reached after all transients have died out. However, due to the limited simulation time the physics of this state can only be described, if we take advantage of the periodicity by combining the Floquet theorem and set up a functional RG with Green functions written in the Floquet basis. For the interacting resonant level model which in equilibrium and if driven by a time constant bias voltage is characterized by power-law scaling of observables in the relevant energy scales (e.g. temperature T or bias voltage V_b, respectively) with interaction dependent exponents this allows to investigate if and how the driving frequency Ω acts as a cutoff of the underlying renormalization group flow. The competition of this scale with the emergent low-energy scale T_K (Kondo scale) is investigated. I discuss how this competition is reflected in the observables characterizing the stationary transport through the dot.

15 min. break.

Invited Talk HL 86.7 Thu 16:45 A 053

Microscopic Origin of the 0.7-Anomaly in Quantum Point Contacts: Correlations in 1D — Florin Bauer[1], Jan Heyder[1], Dawid Borowsky[1], D. Taubert[1], D. Schuh[2], B. Bruognolo[1], Werner Wegscheider[3], Jan von Delft[1], and •Stefan Ludwig[1] — [1]Fakultät für Physik, LMU München — [2]Institut für Angew. Physik, Universität Regensburg — [3]ETH Zurich, Switzerland

Quantum point contacts (QPCs), the ultimate building blocks of quantum electronic circuits, are 1D constrictions in a 2D electron system (2DES). When a QPC is pinched off, its conductance famously decreases in integer steps of the conductance quantum, $G_Q = 2e^2/h$. An unexpected kink of the pinch-off curve near $0.7G_Q$ with an intriguing dependence on temperature, magnetic field and source-drain voltage, the 0.7-anomaly, has been subject of debates for the last two decades [1]. In this talk I will show that the divergence of the 1D density of states (DOS) at low energies, a prerequisite of the quantized conductance, is also the origin of the 0.7-anomaly. It naturally arises from strong correlations fostered by an enhanced DOS. They cause an anomalous increase of the spin susceptibility and back-scattering. Our microscopic model is built on a combination of systematic measurements of a highly tunable QPC and detailed numerical calculations [2]. We discuss commonalities and differences to previous more phenomenological attempts to explain the 0.7-anomaly, namely the model of spontaneous spin polarization and the Kondo model [1].

[1] A. Micolich, J. Phys.: Condens. Matter **23**, 443201 (2011)
[2] F. Bauer et al., Nature **501**, 73 (2013)

HL 86.8 Thu 17:15 A 053

Spin dynamics in a quantum point contact showing the 0.7-anomaly — •Dennis Schimmel[1,2], Florian Bauer[1,2], Jan Heyder[1,2], and Jan von Delft[1,2] — [1]Ludwig-Maximilians-Universitaet Muenchen — [2]Arnold Sommerfeld Center for Theoretical Physics

The 0.7-anomaly in the first conductance step of a quantum point contact is believed to arise from an interplay of geometry, spin dynamics and interaction effects. Various scenarios have been proposed to explain it, each evoking a different concept, including spontaneous spin polarization, or a quasi-localized state, or ferromagnetic spin fluctuations, or a van Hove ridge (a geometry-induced maximum in the density of states). Though these scenarios differ substantially regarding numerous details, they all imply anomalous dynamics for the spins in the vicinity of the QPC. Our model consists of a one-dimensional system with a parabolic barrier. Interactions are restricted to a central region around the barrier and short-range. The leads are solved exactly and the central region is then treated using the functional renormalization group within a coupled ladder approximation scheme. Within this setup, we have performed a detailed study of the spin dynamics in the central region by calculating the dynamical spin-spin correlation function $\chi(x,x',\omega) = \int_0^\infty \langle S_z(x,t)S_z(x',0)\rangle e^{i\omega t}$. We will discuss its behavior as function of frequency, interaction strength and gate voltage and comment on the implications of these results for each of the above-mentioned scenarios.

HL 86.9 Thu 17:30 A 053

Nonequilibrium transport through Anderson impurities: A comparative study based on continuous-time quantum Monte Carlo simulations and hierarchical quantum master equations — •Rainer Härtle[1], Guy Cohen[2], David R. Reichman[2], and Andrew J. Millis[3] — [1]Institut für theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany — [2]Department of Chemistry, Columbia University, New York, USA — [3]Department of Physics, Columbia University, New York, USA

The hierarchical quantum master equation approach [1,2] is a promising new method for describing quantum impurity systems under nonequilibrium conditions. It employs a hybridization expansion with

an advanced truncation scheme [2] to determine the time evolution of the impurity's density matrix from a product initial state. The method is a systematic expansion for which convergence can be demonstrated so that numerically exact results can in principle be obtained. To elucidate the rigor of this procedure, we study the nonequilibrium dynamics of an Anderson impurity and benchmark the results with respect to continuous time quantum Monte Carlo methods [3]. The comparison shows excellent agreement as long as the temperature is above the Kondo scale. A discussion of the computational burden and of the scaling of numerical errors with truncation level is given. New results are presented for long-time dynamics arising in the presence of a magnetic field and/or an asymmetric coupling to leads.

[1] J. Jin et al., JCP 128, 234703 (2008).
[2] R. Härtle et al., PRB 88, 235426 (2013).
[3] G. Cohen et al., PRB 87, 195108 (2013).

HL 86.10 Thu 17:45 A 053

From thermal equilibrium to nonequilibrium quench dynamics: A conserving approximation for the interacting resonant-level — •Yuval Vinkler-Aviv[1,3], Avraham Schiller[3], and Frithjof B. Anders[2] — [1]Dahlem Center for Complex Quantum Systems and Fachberiech Physik, Freie Universität Berlin, 14195 Berlin, Germany — [2]Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund, Germany — [3]Racah Institute of Physics, The Hebrew University, Jerusalem 91904, Israel

We develop a low-order conserving approximation for the interacting resonant-level model (IRLM), and apply it to (i) thermal equilibrium, (ii) nonequilibrium steady state, and (iii) nonequilibrium quench dynamics. The thermal equilibrium is used to carefully gauge the quality of the approximation by comparing the results with established methods such as renormalisation group approaches and establishes a good agreement for small interaction strengths. A closed expression for the nonequilibrium steady-state current is derived and analytically and numerically evaluated. We find a negative differential conductance at large voltages, and the exponent of the power-law suppression of the steady-state current is calculated analytically at zero-temperature. The response of the system to quenches is investigated for a single-lead as well as for two-lead setup at finite voltage bias, and results are presented for the time-dependent current for different bias and contact interaction strength.

[1] Phys. Rev. B **90**, 155110 (2014).

HL 86.11 Thu 18:00 A 053

Bound states in the continuum: Chiral lattices and van Hove singularities — •Jordi Mur-Petit and Rafael A. Molina — Inst. Estructura de la Materia, IEM-CSIC, Madrid, Spain

We present two distinct mechanisms for the formation of bound states in the continuum in lattices with van Hove singularities and/or chiral symmetry connected to leads. Bound states in the continuum (BICs) are square-integrable solutions of the time-independent Schrödinger equation with eigenenergies above the potential threshold. We derive some algebraic rules for the number of such states depending on the dimensionality and rank of the system Hamiltonian including the coupling to the leads. Next, we study the transport properties of relevant physical examples in square, honeycomb and triangular lattices, and propose different experiments to probe the presence of these BICs and related Fano resonances. Our results should find applications in a variety of set-ups, from semiconductor nanostructures to microwave resonator arrays, to cold atoms in optical lattices.

[1] V. Fernández-Hurtado, J. Mur-Petit, J.J. García-Ripoll, and R.A. Molina, New J. Phys. 16, 035005 (2014).
[2] J. Mur-Petit and R.A. Molina: Phys. Rev. B 90, 035434 (2014).

HL 86.12 Thu 18:15 A 053

Charge fluctuation effects in superconductor-quantum dot hybrid systems — •Sebastian Pfaller, Andrea Donarini, and Milena Grifoni — Institut I - Theoretische Physik Universität Regensburg

In a recent experiment [1] quasi particle transport through a carbon nanotube quantum dot coupled to superconducting (SC) leads was investigated both experimentally and theoretically. While most of the features could be explained by a perturbative theory up to lowest order in quasi particles tunnelling, other features like the broadening of the differential conductance peaks were not captured.

In order to account for these effects, we include charge fluctuation processes of quasi particles by extending the dressed second order theory of Kern *et al.* [2] to the case of SC leads. This yields an intrinsic broadening of the quantum dots energy levels, and, consequently, a renormalization of the sharp peaks coming from the BCS density of states. Moreover, new transport channels are obtained. They appear as peaks at zero and finite bias in the dI/dV-stability diagrams.

[1] M. Gaass, S. Pfaller, T. Geiger *et al.*, Phys. Rev. B **89**, 241405 (2014).
[2] J. Kern, and M. Grifoni, Eur. Phys. J. B **86**, 384 (2013).

HL 87: Low-dimensional systems: Topological order 2 (TT with DS/HL/MA/O)

Time: Thursday 15:00–18:30 Location: H 3010

HL 87.1 Thu 15:00 H 3010

Topological entropy in the classical toric code model — •Johannes Helmes and Simon Trebst — Institut für Theoretische Physik, Universität zu Köln, Germany

For interacting quantum many-body systems the study of entanglement entropies is well established to analyze the fundamental nature of their ground states. In particular, the O(1) correction to the prevalent boundary-law can be used to identify topological order. However, not only in quantum systems, but also in classical systems we can track topological contributions to the classical entropy by employing an analogous approach.

We report results for the classical toric code model in a magnetic field which has a topologically protected zero field degeneracy. We show, how the classical entropy tracks the break-down of the classical topological order upon increasing the external field or temperature. In more technical terms, we apply the replica technique to calculate Renyi entropies from classical Monte Carlo simulations using a newly developed update scheme for efficient loop-gas sampling.

HL 87.2 Thu 15:15 H 3010

Symmetry fractionalization in SU(2n) antiferromagnetic Heisenberg chains — •Andreas Weichselbaum[1] and Thomas Quella[2] — [1]Ludwig Maximilians University, Munich, Germany — [2]University of Cologne, Germany

We explore generalizations of the Affleck-Kennedy-Lieb-Tasaki (AKLT, 1987) model for spin-1 antiferromagnetic Heisenberg chains to higher-rank SU(2n) symmetries. In particular we show that by proper tuning of higher order spin interactions there also exist exact low-dimensional matrix-product ground states with fractionalized edge states. These states are adiabatically connected to the ground state of the plain SU(2n) Heisenberg model. The parameter space is explored using state of the art density matrix renormalization group (DMRG), explicitly utilizing SU(N) symmetry up to N=6 based on the QSpace tensor library.

HL 87.3 Thu 15:30 H 3010

Protection of topological phases by quantum deformed symmetries — •Thomas Quella — Universität zu Köln, Institut für Theoretische Physik, Köln, Germany

We show that topological phases of quantum spin systems may enjoy protection even in the absence of ordinary group symmetries. The relevant mechanism is explained in full detail for the example of 1D spin chains with quantum group (q-deformed) symmetry $SO_q(3)$. We also sketch the generalization to quantum deformations of other continuous Lie groups such as those associated with $SU(N)$ or $SO(N)$. Our results provide a complete classification of quantum group symmetry protected topological phases for real values of q.

HL 87.4 Thu 15:45 H 3010

Topological phase transition in the quench dynamics of a Fermi gas — •Pei Wang — Department of Physics, Zhejiang University of Technology, Hangzhou 310023, China and Institute for Theoretical Physics, University of Goettingen, German

We study the quench dynamics of a one-dimensional ultracold Fermi gas with synthetic spin-orbit coupling. At equilibrium, the ground state of the system can undergo a topological phase transition and become a topological superfluid with Majorana edge states. As the interaction is quenched near the topological phase boundary, we identify an interesting dynamical phase transition of the quenched state in the long-time limit, characterized by an abrupt change of the pairing gap at a critical quenched interaction strength. We further demonstrate the topological nature of this dynamical phase transition from edge-state analysis of the quenched states. Our findings provide interesting clues for the understanding of topological phase transitions in dynamical processes, and can be useful for the dynamical detection of Majorana edge states in corresponding systems.

HL 87.5 Thu 16:00 H 3010

Diagnosing the statistics of excitations from the dynamical structure factor — •Siddhardh Morampudi[1], Ari Turner[2], and Frank Pollmann[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [2]Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, Maryland

We show that the statistics of excitations in quantum spin liquids yield characteristic features in the dynamical structure factor. Quantum spin liquids are exotic phases of matter which fall beyond the traditional paradigm of symmetry breaking. Originally proposed by Anderson with regard to high temperature superconductivity, they are now widely believed to arise in frustrated spin systems such as the antiferromagnetic Heisenberg model on the kagome lattice. Recently, various theoretical methods to characterize spin liquids have been introduced, especially with regard to numerical simulations. In this work, we obtain results connecting the statistics of the excitations to features of the dynamical structure factor which can be obtained from neutron scattering. We furthermore demonstrate how the results can be used to distinguish different types of gapped spin liquids.

HL 87.6 Thu 16:15 H 3010

Dissipative Chern Insulators — •Jan Carl Budich[1,2], Peter Zoller[1,2], and Sebastian Diehl[3] — [1]Institute for Theoretical Physics, University of Innsbruck, 6020 Innsbruck, Austria — [2]Institute for Quantum Optics and Quantum Information, Austrian Academy of Sciences, 6020 Innsbruck, Austria — [3]Institute of Theoretical Physics, TU Dresden, D-01062 Dresden, Germany

Engineered dissipation can be employed to prepare interesting quantum many body states in a non-equilibrium fashion. The basic idea is to obtain the state of interest as the unique steady state of a quantum master equation, irrespective of the initial state. Due to a fundamental interference of topology and locality, the dissipative preparation of gapped topological phases with a non-vanishing Chern number has so far remained elusive. Here, we study the open quantum system dynamics of fermions on a two-dimensional lattice in the framework of a Lindblad master equation. In particular, we discover a novel mechanism to dissipatively prepare a topological steady state with non-zero Chern number by means of short-range system bath interaction. Quite remarkably, this gives rise to a stable topological phase in a non-equilibrium phase diagram. We demonstrate how our theoretical construction can be implemented in a microscopic model that is experimentally feasible with cold atoms in optical lattices.

HL 87.7 Thu 16:30 H 3010

Absence of an interaction driven Chern insulating phase on the honeycomb lattice — •Johannes Motruk, Adolfo G. Grushin, and Frank Pollmann — Max-Planck-Institut für Physik komplexer Systeme, Dresden, Deutschland

Mean field calculations in the literature have suggested the existence of an interaction-induced Chern insulator (CI) phase in a tight-binding model of spinless fermions on a honeycomb lattice with nearest- and next-nearest-neighbor interactions. The CI phase is an example of a state that breaks time-reversal symmetry spontaneously and possesses a quantized Hall conductance. However, it has been proven elusive in exact diagonalization (ED) studies of this system. Since ED is limited to small system sizes, the fate of this phase in the thermodynamic limit still remains unclear. Using the infinite density matrix renormalization group (iDMRG) algorithm we reach system sizes exceeding those accessible in ED calculations while keeping track of quantum fluctuations neglected in mean field studies. We map out the phase diagram as a function of both nearest- and next-nearest-neighbor interaction strengths for an infinite cylinder geometry and find different charge-ordered phases but no sign of the interaction driven Chern insulator phase.

15 min. break.

HL 87.8 Thu 17:00 H 3010

Quasiparticle interference patterns from different impurities on the surface of pyrochlore iridates: signatures of the Weyl phase — •Fabian Lambert[1], Andreas Schnyder[2], Roderich Moessner[3], and Ilya Eremin[1] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — [3]Max Planck Institute for the Physics of Complex Systems, D-01187 Dresden, Germany

Weyl semi-metals exhibit topologically protected surface Fermi arcs, which pairwise connect projections of bulk band touchings in the surface Brillouin zone. The nontrival spin and orbital character of these topological surface states can be tested experimentally using quasiparticle interference (QPI) measurements. Here, we compute the QPI patterns for a Hubbard Hamiltonian on a pyrochlore lattice. For weak impurity potentials, the QPI patterns can be computed within the First Born approximation. To account for the antiferromangetic spin configuration of $R_2Ir_2O_7$, we treat the Hubbard interaction at the mean-field level. In the antiferromagnetic state the quadratic band touching of the model is split into eight linear band touchings, each of which carries a non-trivial Chern number, thereby realizing a Weyl phase with broken time- reversal symmetry. Using exact diagonalization, we compute the surface spectrum and quasiparticle interference patterns of this Weyl phase for various surface impurities. We show that the spin and orbital texture of the surface states can be inferred from the absence of certain backscattering processes and from the symmetries of the QPI features.

HL 87.9 Thu 17:15 H 3010

Interacting surface states of three-dimensional topological insulators — •Titus Neupert[1], Stephan Rachel[2], Ronny Thomale[3], and Martin Greiter[3] — [1]Princeton Center for Theoretical Science, Princeton University, Princeton, New Jersey 08544, USA — [2]Institute for Theoretical Physics, Technische Universitaet Dresden, 01171 Dresden, Germany — [3]Institute for Theoretical Physics, University of Wuerzburg, Am Hubland, D-97074 Wuerzburg, Germany

We numerically investigate the surface states of a strong topological insulator in the presence of strong electron-electron interactions. We choose a spherical topological insulator geometry to make the surface amenable to a finite size analysis. The single-particle problem maps to that of Landau orbitals on the sphere with a magnetic monopole at the center that has unit strength and opposite sign for electrons with opposite spin. Assuming density-density contact interactions, we find superconducting and anomalous (quantum) Hall phases for attractive and repulsive interactions, respectively, as well as chiral fermion and chiral Majorana fermion boundary modes between different phases. Our setup is preeminently adapted to the search for topologically ordered surface terminations that could be microscopically stabilized by tailored surface interaction profiles.

HL 87.10 Thu 17:30 H 3010

Resonant scattering in the topological Dirac semimetal Cd_3As_2 — Vladimir Gnezdilov[1,2], Azat Sharafeev[1], •Peter Lemmens[1], Raman Sankar[3], and Fangcheng Chou[3] — [1]IPKM, TU-BS, Braunschweig — [2]ILTPE NAS, Ukraine — [3]CCMS, National Taiwan Univ., Taipei, Taiwan

In the symmetry-broken topological Dirac semimetal with strong spin-orbit coupling, Cd_3As_2, a pronounced temperature evolution of quasielastic electronic Raman scattering and resonant effects are observed. These effects are then compared to observations in topological insulators, as Bi_2Se_3.

Work supported by RTG-DFG 1953/1, Metrology for Complex Nanosystems and the Laboratory for Emerging Nanometrology Braunschweig, TU Braunschweig.

HL 87.11 Thu 17:45 H 3010

Angle-resolved Photoemission Investigation of SmB_6 — •Peter Hlawenka[1], Oliver Rader[1], Konrad Siemensmeyer[1], Eugen Weschke[1], Andrei Varykhalov[1], Natalya Shitsevalova[2], Slavomir Gabani[3], Karol Flachbart[3], and Emile Rienks[1] — [1]Helmholtz-Zentrum Berlin — [2]Institute for Problems of Material Science, Kiev — [3]IEP, Slovak Academy of Science, Kosice

Recently the mixed valence compound SmB_6 has drawn great attention. Theoretically predicted surface states, which should result from a hybridisation of localised f-bands with conduction electrons and a band inversion, would make SmB_6 the first realisation of a so called topological Kondo insulator [1-2]. Conductivity and transport measurements, as well as spin-resolved photoemission spectroscopy seem to fortify the scenario of a topological nature of the conductive surface [3-5]. We investigate the surface electronic structure of SmB_6 by means of high resolution angle-resolved photoemission spectroscopy measurements below 1 K. We will present new insights into the surface states that determine the low temperature conductivity of this material.

[1] Dzero et al., PRL 104, 106408 (2010).
[2] Lu et al., PRL 110, 096401 (2013).
[3] Wolgast, PRB 88, 180405 (2013).
[4] Kim, Sci. Rep. 3, 3150 (3013).
[5] Xu et al., Nat. Com. 5, 4566 (2014).

HL 87.12 Thu 18:00 H 3010

Calculation of topological properties of strongly correlated electrons without inversion symmetry using Wannier charge centres. — •Robert Triebl and Markus Aichhorn — Institute of Theoretical Physics and Computational Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria

We study the topological properties of a role model for interacting Z_2 topological insulators, namely the Kane-Mele-Hubbard model including a staggered sublattice potential controlled by a parameter λ_ν, which breaks inversion symmetry. The applicability of a naïve mean field approach was analysed by comparing to a variational cluster approach, employing a two-site dynamical impurity approximation (DIA). The obtained Greens function determines the topological Hamiltonian, which maps the interacting system to an effective free-particle model with the same topological properties. Since inversion symmetry is lost, we calculate the Z_2 invariant for both Mean Field and topological Hamiltonian using Wannier charge centers. We conclude that a two-site DIA in combination with Wannier charge centers is an easy-to-implement and stable method to determine topological invariants for interacting systems. Comparing with mean field results we find that the direction of magnetisation is crucial for topological properties and hence an inherent mean field magnetisation may lead to incorrect results.

HL 87.13 Thu 18:15 H 3010

An analytical study of the entanglement spectrum of graphene bilayers — •Sonja Predin and John Sliemann — Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

We present an analytical study of the entanglement spectrum of graphene bilayers. The entanglement spectrum has been proposed as a ground state property that exhibits characteristic energy excitations[1]. Futhermore, it was claimed that gapless systems possess the same number of Dirac cones as their entanglement spectrum [2]. In addition, it was suggested that the entanglement spectrum is a promising tool to characterize topological phases. In this work we will show that the energy spectrum of an gapless system and its entanglement spectrum can have a different topology. In particular, we will show that Lifshitz transitions change the topology of the energy spectrum of graphene bilayers in a different way than the topology of entanglement spectrum. The topology of the energy spectrum of graphene bilayers for small energies is changed by Lifshitz transitions by changing the connectivity by the appearance of the three additional Dirac cones around every Dirac point [3]. The entanglement spectrum, on the other hand, is changed by deforming a Dirac cone into a neck charaterized by vanishing eigenvalues of the entanglement Hamiltonian.

[1] H. Li and F. D. M. Haldane,
Phys. Rev. Lett. 101, 010504 (2008)
[2] A. M. Turner, et al., Phys. Rev. B, 82, 241102R (2010)
[3] J. Cserti, et al., Phys. Rev. Lett. 99, 066802 (2007)

HL 88: GHz Dielectrics - Materials for mobile communication II (DF with DY/HL/MM)

Organizer: Martin Letz (Schott AG Mainz)

Time: Thursday 15:00–17:00 Location: EB 407

Topical Talk HL 88.1 Thu 15:00 EB 407

Temperature stable low loss ceramics for resonators and filters — •Ian Reaney — Materials Science and Engineering, University of Sheffield, Sheffield, UK

Micro wave (MW) dielectric ceramics are required to be temperature stable and have a low dielectric loss to prevent heating of the sample when operated at or near resonance. They are used in many applications but specifically in this contribution the use of MW dielectric ceramics as resonators, filters and antennas is considered. The relevant technologies for these application are reviewed along with their selective materials parameters. The underpinning crystal chemistry that leads to optimisation of properties is also reviewed and some new materials and novel processing routes to improve device performance are discussed.

HL 88.2 Thu 15:30 EB 407

Titanate-based paraelectric glass-ceramics for applications in GHz electronics — •Hubertus Braun[1,2,3], Martin Letz[2], Martun Hovhannisyan[2], and Hans-Joachim Elmers[1] — [1]Johannes-Gutenberg Universität Mainz — [2]SCHOTT AG, Mainz — [3]Graduate School Materials Science in Mainz

In the current work, titanate-based glass-ceramics ($TiO_2 > 45$ mol %) in the La_2O_3-TiO_2-SiO_2-B_2O_3 system are developed ($\varepsilon_r \approx$ 20-30, Qf $\approx$ 10.000 GHz, $|\tau_f| < 10$ ppm/K) which show promising properties as microwave materials and offer numerous advantages in comparison to conventional sintered ceramics. Glass-ceramics which are obtained via a true glassy phase are comparatively new in this field and will be presented as suitable alternative. Glass-ceramics are produced in a two step process: At first, a basic glass is casted in a conventional glass production process. Then the glass undergoes a temperature treatment with a defined temperature profile to initiate a controlled partial crystallization of desired paraelectric phases inside the glassy matrix. Obtaining materials via a homogeneous glassy phase enables intrinsically pore-free materials with comparatively superior surface properties. The effect of solid solution type doping on the dielectric properties and glass stability is investigated. The effect of solid solution type doping on the A(La) and B(Ti) site of the crystalline phases with ions of similar ionic radius is investigated concerning their influence on the dielectric properties and glass stability. Further the materials are analyzed concerning suitability for dielectric loaded antenna applications.

HL 88.3 Thu 15:50 EB 407

Microwave electric properties of thin-film $Ba_xSr_{1-x}TiO_3$ varactors with highly-conducting epitaxial $SrMoO_3$ oxide electrodes — •Arzhang Mani[1], Aldin Radetinac[1], Mohammad Nikfalazar[2], Sergiy Melnyk[2], Philipp Komissinskiy[1], Yuliang Zheng[2], Rolf Jakoby[2], and Lambert Alff[1] — [1]Institute of Materials Science, Technische Universität Darmstadt, 64287 Darmstadt, Deutschland — [2]Institut für Mikrowellentechnik und Photonik, Technische Universität Darmstadt, 64283 Darmstadt, Deutschland

We present high-frequency properties of MIM thin-film varactors with dielectric $Ba_xSr_{1-x}TiO_3$ (x = 0.4, 0.5, 0.6). Single crystalline $Ba_xSr_{1-x}TiO_3$ layers were grown epitaxially on highly-conducting oxide $SrMoO_3$ electrodes with room-temperature resistivity of 30 $\mu\Omega\cdot$cm. Au/Pt top electrodes were deposited by magnetron sputtering on top of the $Ba_xSr_{1-x}TiO_3$ / $SrMoO_3$ heterostructures and patterned with photolithography and lift-off. Influence of Ba content (x), thickness of $Ba_xSr_{1-x}TiO_3$ layer, and size of the top electrodes on performance of the varactors were investigated in the frequency range of 100 MHz to 10 GHz. Capacitance of 15 pF, quality factor of 15, and tunability of 40% at 0.3 MV/cm were obtained at 100 MHz. The obtained results suggest a high potential of the oxide perovskite electrode material $SrMoO_3$ [1] for fabrication of highly tunable varactors in microwave applications.

[1] A. Radetinac *et al.*, Appl. Phys. Lett. **105**, 114108 (2014).

HL 88.4 Thu 16:10 EB 407

Continuously tuneable, high performance phase shifters based on liquid crystal for applications in phased array antennas — •Matthias Jost, Christian Weickhmann, and Rolf Jakoby — Institute of Microwave Engineering and Photonics, Technische Universität Darmstadt, Merckstr. 25, 64283 Darmstadt, Germany

During the last decade, calamitic-nematic liquid crystals (LCs), well-known from the LC-display technology (LCD), have become increasingly popular in the field of microwave engineering. Due to their unique property of exhibiting local anisotropy, they offer the possibility of realising passive, continuously tuneable devices, such as phase shifters, tuneable filters, polarisers or matching networks. LC can be oriented continuously between the two extreme states (parallel or perpendicular to an applied RF field), either by applying a magneto-static or an electro-static field. Depending on the orientation of the LC, its permittivity and dielectric loss changes. This work presents the recent progress of our research in the topic of hollow waveguide based LC phase shifters for application in phased array antennas. This kind of phase shifter is suitable for high performance applications due to its high figure of merit (FoM), defined by the ratio of the maximum differential phase shift over the highest insertion loss in all tuning states. Full wave simulation results as well as measurement results of realised phase shifters will be shown and a perspective of a phased array antenna for satellite communication will be given.

Topical Talk HL 88.5 Thu 16:30 EB 407

Low loss flexible and stretchable dielectrics for microwave applications — •Mailadil Sebastian — Department of Electrical Engineering, University of Oulu, 90014 Oulu

Flexible, bendable and stretchable dielectrics which can cover even curved surfaces are important for applications in electronic control systems, consumer electronics, heart pacemakers, body worn antenna etc. The requirements for a material to be used as a flexible dielectric waveguide are mechanical flexibility, high relative permittivity, low dielectric loss, high thermal conductivity, low coefficient of thermal expansion (CTE) etc. It is very difficult to identify a single material which possesses all these properties simultaneously. There are a number of ceramic materials with high relative permittivity and low dielectric loss but are brittle in nature. Butyl and silicone rubbers have low loss with good mechanical flexibility and stretchability but they have low relative permittivity and high CTE. Therefore, the practical applications of a rubber or a ceramic alone is limited. By integrating the flexibility, stretchability and low processing temperature of a rubber with high relative permittivity and low loss of ceramics, a composite may be formed, which can deliver improved performances. In this talk the effect of addition of several ceramics such as SiO_2, Al_2O_3, TiO_2, $Ba(Mg_{1/3},Ta_{2/3})O_3$, $Ba(Zn_{1/3},Ta_{2/3})O_3$, $BaTiO_3$, $Ba_{0.7}Sr_{0.3}TiO_3$, $SrTiO_3$, AlN, $Sr_2Ce_2Ti_5O_{15}$ in butyl and silicone rubbers on the microwave dielectric properties, thermal conductivity, thermal expansion, moisture absorption, mechanical properties etc will be discussed.

HL 89: Graphene: Electronic structure (O with HL/TT)

Time: Thursday 15:00–18:15 Location: MA 041

HL 89.1 Thu 15:00 MA 041

Tuning the electronic structure of artificial graphene with potential modulation — •Pilkwang Kim and Cheol-Hwan Park — Department of Physics, Seoul National University, Seoul 151-747, Korea

Among the many different directions of research for tuning the electronic properties of massless Dirac fermions residing in materials like graphene, one of the promising candidates is the artificial graphene system where a conventional two-dimensional electron gas is modulated by external periodic potential, as first predicted theoretically [1,2]. Recently, experimentalists have confirmed the existence of massless Dirac fermions originating from metallic surface states [3,4]. In this presentation, we discuss our theoretical study on the possibility of tuning the electronic properties of massless Dirac fermions residing in 2DEG by exploiting the external potential degree of freedom. This work was supported by Korean NRF funded by MSIP (Grant No. NRF-2013R1A1A1076141).

[1] C.-H. Park and S. G. Louie, Nano Lett. 9, 1793 (2009).

[2] M. Gibertini, A. Singha, V. Pellegrini, M. Polini, G. Vignale, A. Pinczuk, L. Pfeiffer, and K. West, Phys. Rev. B 79, 241406 (2009).

[3] K. K. Gomes, W. Mar, W. Ko, F. Guinea, and H. C. Manoharan, Nature 483, 306 (2013).

[4] S. Wang, L. Z. Tan, W. Wang, S. G. Louie, and N. Lin, Phys. Rev. Lett. 113, 196803 (2014).

HL 89.2 Thu 15:15 MA 041

Using collective electrostatic effects to tune the electronic structure of graphene — •Gernot J. Kraberger[1], David A. Egger[1,2], and Egbert Zojer[1] — [1]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria — [2]Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth 76100, Israel

Graphene has unique structural and electronic properties, which have attracted huge research interest since its isolation. As a prerequisite of using this material in devices, it is necessary to modify its properties in a controlled way that it fits the needs of the application. This work uses density functional theory calculations to investigate a new approach to change the electronic structure of graphene: using the collective field of a highly ordered arrangement of dipoles to shift the potential in specific regions of graphene (i.e., exploiting so-called collective electrostatic effects). First we discuss a "proof-of-concept" model system: Along a line in graphene, pairs of neighboring carbon atoms are replaced by a boron and a nitrogen atom. Each of the resulting BN-pairs exhibits a dipole moment, which means that a one-dimensional chain of dipoles is formed. This chain impacts the electrostatic potential in its surroundings such that the electronic states in graphene are locally shifted relative to the Fermi level. With two oppositely oriented lines of dipoles it is then even possible to localize states in well-defined stripes. Finally, we explore to what extent similar effects can be generated by assembling rows of quadrupolar molecules on top of the graphene sheet instead of modifying the graphene layer itself.

HL 89.3 Thu 15:30 MA 041

Graphene on weakly interacting metals: Dirac states vs. surface states — •Wouter Jolie, Fabian Craes, and Carsten Busse — II. Physikalisches Institut, Universität zu Köln, Germany

The epitaxial growth of graphene and other two-dimensional materials on metal surfaces has become a well-established procedure and is extensively used for studies of the electronic properties of two-dimensional materials using surface science methods. However, the substrate itself can have a significant contribution to these properties. We demonstrate this on three different systems: graphene on a thick silver film on Ir(111), graphene on one monolayer of silver on Ir(111), and graphene on Ir(111). We explore the interplay between the states of the substrate (in form of nearly free surface states) and the states of the two-dimensional material on top (in form of graphenes' Dirac fermions) with scanning tunneling spectroscopy, a technique sensitive to the local density of states of the surface. We show that, when present, the surface state represents the dominant contribution in form of Friedel oscillations and confined states on graphene quantum dots. We compare these findings with a system with suppressed surface states where a clear feature of graphene is found in the density of states.

HL 89.4 Thu 15:45 MA 041

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

Graphene nanostructures represent an exciting topic for research, as a strong spatial confinement together with the edge structure impose new electronic properties, making them promising candidates for future nanoscale electronic units. Here, we investigate by means of low-temperature scanning tunnelling microscopy and spectroscopy oblong quasi-freestanding epitaxial graphene nanoflakes prepared on Ag(111) and Au(111) by intercalation with virtually no edge bonding [1]. We implement quasiparticle interference (QPI) mapping to analyze stand-

ing wave patterns arising from elastic scattering processes within a single nanoflake. The Fourier analysis of the obtained QPI maps shows that in addition to ringlike structures due to the *intervalley* and *intravalley* scattering observed for large graphene sheets, additional scattering features are visible, which can be related to the transverse modes in a nanoflake [2]. Our experimental results are supported by tight-binding calculations of realistic flakes, which very well reproduce the experimentally observed fingerprints of confinement in the Fourier transform of the standing wave patterns.

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

HL 89.5 Thu 16:00 MA 041

Graphene-supported metal clusters: A two photon photoemission study — Kira Jochmann and •Thorsten Bernhardt — Institut für Oberflächenchemie und Katalyse, Universität Ulm, 89069 Ulm

During the last decade considerable attention was drawn to the growth of graphene on metal single crystal surfaces, where it provides an ideal template for the ordered growth of regular metal cluster arrays. Building on various investigations about the detailed growth of these cluster super-lattices, we make use of the possibility to easily grow nanostructures with equally spaced and mono-disperse clusters for fundamental research in laser selective photochemistry. Our new experimental setup enables time-resolved measurements due to a femtosecond laser system on the one hand and surface analysis via scanning tunnelling microscopy on the other hand. In first light interaction measurements time-resolved two-photon photoemission spectroscopy (2PPES) was applied to gain an insight into the unoccupied electronic structure of the Ir(111)/graphene/Ir cluster system at different graphene and cluster coverages. In subsequent experiments the combination of femtosecond laser pump-probe mass spectrometry with resonance enhanced multi-photon ionization and STM will be employed to reveal photo-dissociation dynamics of different adsorbate molecules with spatio-temporal resolution.

HL 89.6 Thu 16:15 MA 041

From ribbons to constrictions: STM lithography on ballistic sidewall graphene nanoribbons — •Jens Baringhaus[1], Mikkel Settnes[2], and Christoph Tegenkamp[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, 30167 Hannover, Germany — [2]Technical University of Denmark, DTU Nanotech, Center for Nanostructured Graphene (CNG), 2800 Kgs. Lyngby, Denmark

The selective graphene growth on the sidewalls of SiC mesa structures produces well-ordered graphene nanoribbons (GNR) with exceptional transport properties. Using a 4-tip STM, a probe spacing and temperature independent conductance of e^2/h is found, indicating single channel ballistic transport even at room temperature [1]. The robustness of the ballistic channel makes these GNR ideal templates for morphological alterations. For this purpose, one of the STM tips is used for local lithography. Careful control over the feedback parameters and the bias voltage allows to either fully cut the ribbon or to create narrow, a few nm wide constrictions. Every STM lithography step is monitored directly by local transport. After a full cut, the transport characteristics of the sidewall GNR are completely destroyed. In contrast, in narrow constrictions the ballistic channel is preserved, but only present at bias voltages exceeding 10 mV. Additionally, localized currents manifest as resonances in the IV curves at bias voltages of about 8 mV. Using a standard tight binding and recursive Green's function approach, the resonances are found to be robust against temperature as well as different types of disorder, e.g. Anderson or edge disorder.

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

HL 89.7 Thu 16:30 MA 041

Chiral Enhanced Phonon Spectroscopy of Graphene — •Fabian D. Natterer[1], Yue Zhao[1,2], Jonathan Wyrick[1], Wen-Ying Ruan[3], Yang-Hao Chan[4], Mei-Yin Chou[3,4], Nikolai B. Zhitenev[1], and Joseph A. Stroscio[1] — [1]Center for Nanoscale Science and Technology, NIST, Gaithersburg, USA — [2]University of Maryland, College Park, USA — [3]Georgia Institute of Technology, Atlanta, USA — [4]Academia Sinica, Taipei, Taiwan

In graphene, many phenomena are driven by the interaction with phonons, such as the relaxation of hot carriers or the mediation of many-body interactions. The proper characterization of phonons can therefore shed important insights into graphene based devices. Such devices were characterized by inelastic electron tunneling spectroscopy (IETS) but weak signals and other spectral features obscured a clear distinction between phonons and miscellaneous excitations. In this talk, I show that we are able to map large parts of the graphene phonon density of states by using a back gated graphene device, where the charge carrier density can be varied in magnitude and sign. Our averaging technique combines individual IETS data, obtained over the entire charge carrier range, with the benefit of improving the signal for inelastic excitations. Surprisingly, we observe that the graphene phonon intensity is enhanced when the charge carrier type is switched, indicating that this amplification occurs whenever the inelastic transition allows a change in the graphene chirality. The chiral enhancement follows a linear trend with energy and reaches almost an order of magnitude for the highest mode.

HL 89.8 Thu 16:45 MA 041

Luminescence of Graphene in the Visible Spectral Range after Short-Pulse Excitation in the Near Infrared — •Martin Rothe, Günter Kewes, Nikolai Severin, Jürgen P. Rabe, and Oliver Benson — Department of Physics and IRIS Adlershof, Humboldt-Universität zu Berlin, D-12489 Berlin, Germany

Graphene is well known for its unique electronic and optical properties. The study and manipulation of its nonlinear optical response at energies in the range of visible light is of interest for the understanding of its charge carrier dynamics in this energy regime [1]. We find a broad luminescence of graphene and graphene multilayers in the entire visible spectral range after excitation with fs laser pulses in the near infrared. The spectrum that starts even above twice the excitation energy indicates multi-photon absorption or efficient electron scattering processes. This method of luminescence excitation is not only well suited for imaging with high contrast but can also gain insight into fundamental electron relaxation and collective excitation processes [2].

[1] Liu, et al., Phys Rev B: 82, 081408 (2010)
[2] Lange, et al., arXiv:1404.6518 (2014)

HL 89.9 Thu 17:00 MA 041

Electroluminescence from carbon-based nanostructures — •Ji Hoon Ryoo and Cheol-Hwan Park — Department of Physics, Seoul National University, Seoul 151-747, Korea

Light emission from carbon nanostructures upon current flowing reflects their novel electronic structures and is important for applications purposes. Peculiar emission versus photon energy profiles in the electroluminescence from carbon nanostructures have been attributed to inter-band electronic transitions [1], electron-phonon interactions [2] and interference effects [3]. In this presentation, we discuss the origin of multi-peak intensity versus energy feature in the electroluminescence from graphene based on recent experimental results, and look into how the electronic structure of graphene affects its electroluminescence. This work was supported by Korean NRF funded by MSIP (Grant No. NRF-2013R1A1A1076141). Computational resources have been provided by Aspiring Researcher Program through Seoul National University (SNU) in 2014.

[1] D. Mann, Y. K. Kato, A. Kinkhabwala, E. Pop, J. Cao, X. Wang, L. Zhang, Q. Wang, J. Guo, H. Dai, Nature Nanotech. 2, 33-38 (2007).
[2] S. Essig, C. W. Marquardt, A. Vijayaraghavan, M. Ganzhorn, S. Dehm, . Henrich, F. Ou, A. A. Green, C. Sciascia, F. Bonaccorso, K.-P. Bohnen, H. v. Löhneysen, M. M. Kappes, P. M. Ajayan, M. C. Hersam, A. C. Ferrari, R. Krupke, Nano Lett. 10, 1589-1594 (2010).
[3] M. Engel, M. Steiner, A. Lombardo, A. C. Ferrari, H. v. Löhneysen, P. Avouris, R. Krupke, Nature Comm. 3, 906 (2012).

HL 89.10 Thu 17:15 MA 041

Structure and electronic states of the zig-zag graphene/h-BN interface — •Robert Drost[1], Andreas Uppstu[2], Kezilebieke Shawulienu[1], Fabian Schulz[1], Sampsa K. Hämäläinen[1], Mikko Ervasti[2], Ari Harju[2], and Peter Liljeroth[1] — [1]Department of Applied Physics, Aalto University School of Science, Finland — [2]COMP Centre of Excellence and Helsinki Institute of Physics, Department of Applied Physics, Aalto University School of Science, Finland

Some of the most exciting properties of graphene (G) are only realised in atomically precise nanostructures. The zig-zag (ZZ) edges of this two-dimensional crystal host localised states that have been proposed to be used in spin- and valleytronic applications: Using the spin degree of freedom of the electron or the valley degree of freedom of the honeycomb crystal structure to transmit and process information. While well studied theoretically, experimental realisations remain challenging. We passivate the ZZ edge of epitaxial G with hexagonal

boron-nitride (BN), a 2D insulator isostructural to G, to preserve the edge state in the band gap of the insulator. We investigate the growth of atomically perfect G/BN heterostructures on Ir(111) and Ni(111) substrates and discuss the effect of varying substrate interaction. The intrinsic properties of the G/BN interface may be revealed by intercalation with gold. Using low-temperature STM, we demonstrate the existence of a localised electronic state on the ZZ oriented G/BN interfaces. Tight binding and DFT calculations show that the interface retains many important properties of the graphene edge state.

HL 89.11 Thu 17:30 MA 041

Embedding graphene quantum dots into hexagonal boron nitride — Ferdinand Farwick zum Hagen[1], Caio Silva[1], Christoph Schlueter[2], Nicolae Atodiresei[3], Wouter Jolie[1], Daniela Dombrowski[1], Antonio J. Martinez-Galera[1], Domenik Zimmermann[1], Ulrike Schröder[1], Vasile Caciuc[3], Thomas Michely[1], Stefan Blügel[3], Tien-Lin Lee[2], and •Carsten Busse[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Diamond Light Source, Didcot, UK — [3]Peter Grünberg Institute, Forschungszentrum Jülich, Germany

Graphene (gr) nanostructures can be stabilized by embedding them into an insulating matrix. Hexagonal boron nitride (hBN) is especially suited as it is isostructural to graphene, and dangling C bonds can be satisfied by B and N. In this study, we used sequential epitaxial growth of gr and hBN on Ir(111) to embed graphene quantum dots (GQDs).
First, we investigate pristine hBN/Ir(111) with special attention to the hBN-substrate interaction which is characterized by the local varying layer height as determined with x-ray standing waves (XSW), complemented by density functional theory (DFT) calculations. Distinct differences with respect to gr/Ir(111) are found: A stronger corrugation within the moiré and an enhanced chemical interaction in the strongly bound parts of the supercell. Second, the edge atoms of GQDs on Ir(111) are investigated and an enhanced C-substrate interaction is found. Third, the chemical and structural changes at these edges upon embedding in hBN are probed. The in-plane structure is analyzed using scanning tunneling microscopy (STM).

HL 89.12 Thu 17:45 MA 041

Single 3*d* transition metal atoms on multi-layer graphene systems: electronic configurations, bonding mechanism and role of the substrate — Violetta Sessi[6], Sebastian Stepanow[1,2], Alexander N. Rudenko[3], Sören Krotzky[1], Klaus Kern[1], Fanny Hiebel[4], Pierre Mallet[4], Jean-Yves Veuillen[4], Ondřej Šipr[5], •Jan Honolka[1,5], and Nick B. Brookes[6] — [1]Max-Planck Institut für Festkörperforschung, Stuttgart, Germany — [2]Department of Materials, ETH Zürich, Switzerland — [3]Radboud University Nijmegen, Inst. for Molecules and Materials, Netherlands — [4]Institut Néel, CNRS-UJF, Grenoble, France — [5]Inst. of Physics, ASCR, Prague, Czech Republic — [6]ESRF, Grenoble, France

We present our recent study on electronic configurations of Fe, Co, Ni and Cu adatoms on graphene and graphite by x-ray magnetic circular dichroism and charge transfer multiplet theory [1]. A delicate interplay between long-range interactions and local chemical bonding is found to influence the adatom equilibrium distance and magnetic moment. The results for Fe and Co are consistent with purely physisorbed species having, however, different 3*d*-shell occupations on graphene and graphite (d^{n+1} and d^n, respectively). On the other hand, for the late 3*d* metals Ni and Cu a trend towards chemisorption is found, which strongly quenches the magnetic moment on both substrates.

[1] V. Sessi et al., New J. of Physics 16, 062001 (2014) [Fast Track Communication]

HL 89.13 Thu 18:00 MA 041

Ab initio **calculation of XNLD in reflection of graphene** — •Dominik Legut[1], Peter M. Oppeneer[2], Christine Jansing[3], Marc F. Tesch[3,4], Markus Gilbert[3], Andreas Gaupp[3], Hans-Christoph Mertins[3], Andrey Sokolov[4], Suk-Ho Choi[5], Hud Wahab[6], Heiko Timmers[6], and R.G. Elliman[7] — [1]IT4Innovations Centre, VSB-TU Ostrava, Ostrava, Czech Republic — [2]Department of Physics and Astronomy, Uppsala, Sweden — [3]FH Münster, Steinfurt, Germany — [4]HZB, Berlin, Germany — [5]Department of Applied Physics, Kyung Hee University, Korea — [6]University of New South Wales Canberra, Canberra BC, Australia — [7]Department of Elect. Mat. Eng., Australian National University, Canberra, Australia

The reflection spectroscopy and in particular angular dependence of the x-ray natural linear dichroism (XNLD) were calculated on free standing monolayered graphene. The anisotropic XNLD was computed in the single electron picture within the framework of the DFT. The excitations stemming from carbon K-edge are considered. The spectral shape of the XNLD is compared with recorded data. The dependence of the reflection spectroscopy, here XNLD, based on the change of the electronic structure of bi-layer and tri-layered graphene is predicted.

HL 90: Phase change / resistive switching (DS with HL)

Time: Thursday 15:00–18:45 Location: H 0111

HL 90.1 Thu 15:00 H 0111

Nanosecond laser-induced phase transitions in pulsed laser deposition-deposited GeTe films — •Xinxing Sun, Erik Thelander, Jürgen W. Gerlach, and Bernd Rauschenbach — Leibniz Institute of Surface Modification, Permoserstr. 15, D-04318, Leipzig, Germany

Phase changes in chalcogenide-based alloys have been widely studied in terms of the application in optical data storage and the same class of phase change materials is a promising candidate for further applications in non-volatile memories. In this study, phase transformations between the amorphous and crystalline state in GeTe thin films grown by pulsed laser deposition (PLD) are investigated. The phase transformations are induced by irradiation with nanosecond laser pulses at 248 nm and pulse duration of 20 ns. The structural and optical properties of the GeTe films were studied by x-ray diffraction and optical reflectivity measurements as a function of the number of irradiation pulses between 0 and 30 pulses and of the laser fluence up to 195 mJ/cm2. A reversible phase transition is found by using pulse numbers more than 5 pulses at a fluence above the threshold fluence for crystallization (between 11 and 14 mJ/cm2) and single pulse at a fluence of between 162 and 182 mJ/cm2 for amorphization. The influence of film thickness (6-300 nm) and irradiation with pulse repetition frequency (1-400 Hz) on the crystallization behavior of GeTe films is also discussed. A high optical contrast between the amorphous and crystalline state is achieved, proving that PLD-deposited GeTe films have excellent potential for application in phase change storage.

HL 90.2 Thu 15:15 H 0111

Growth of Germanium Telluride Thin Films on Passivated Silicon Surfaces by Molecular Beam Epitaxy — •Rui Ning Wang[1], Jos Boschker[1], Raffaella Calarco[1], Jamo Momand[2], and Bart Kooi[2] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]University of Groningen, Zernike Institute for Advanced Materials, Groningen, The Netherlands

As a phase change material, and as a ferroelectric semiconductor, germanium telluride is worth investigating both from the fundamental and technological point of view. And especially for fundamental research, the ability to produce GeTe thin films of great crystalline quality is of prime importance.

Epitaxial growth of GeTe on Si(111)-(7x7) by molecular beam epitaxy was first demonstrated by Giussani et al. [1] and it has been recently shown that the crystalline quality of such GeTe thin films can be significantly improved by growing on a passivated Si(111)-$(\sqrt{3}\times\sqrt{3})$R30°-Sb surface [manuscript accepted in J. Phys. Chem. C 19/11/2014].

To better understand the role of the surface passivation in the epitaxy of GeTe, growth on the hydrogen passivated Si(111)-(1x1)-H surface was investigated as well. In this presentation, the growth of GeTe on these different silicon surfaces is reported and compared between each other.

[1] A. Giussani et al., Phys. Status Solidi B, vol. 249, no. 10, pp. 1939-1944, Oct. 2012.

HL 90.3 Thu 15:30 H 0111

Epitaxial and textured Ge-Sb-Te phase-change thin films investigated by Cs-corrected STEM — •Ulrich Ross, Andriy

Lotnyk, Erik Thelander, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung e.V. Permoserstr. 15 D-04318 Leipzig

Chalcogenide phase change compounds are under intense scrutiny for emerging data storage and fast switching electronic memory applications. The unique properties of this class of materials are based on the distinct change in electrical conduction and optical reflectivity upon transition between crystalline and amorphous states. Much interest has been focused on compounds from the stoichiometric tie-line $(GeTe)_x$-$(Sb_2Te_3)_{1-x}$ in the Ge-Sb-Te intermetallic system. For the development of phase change memory in particular, oriented, epitaxial and layered thin films have been reported to display significantly enhanced switching properties.

We have performed a detailed high-resolution scanning transmission electron microscopy (STEM) investigation of fast grown $Ge_2Sb_2Te_5$ thin films on native amorphous silicon oxide as well as oriented $BaF_2(111)$ and Si(111) substrates, produced by pulsed laser deposition. Formation of the crystalline phases was induced by deposition at elevated temperatures as well as post-deposition heat treatment. An analytical probe aberration-corrected FEI Titan^3 G2 60-300 S/TEM was used in order to correlate treatment conditions and local structure at the atomic scale. The interplay between grain texture, lattice disorder and local composition variations will be discussed.

HL 90.4 Thu 15:45 H 0111

Optical and structural dynamics of the photoinduced phase transition of GST — •Lutz Waldecker[1], Timothy Miller[2], Roman Bertoni[1], Simon Wall[2], and Ralph Ernstorfer[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]ICFO - Institut de Ciències Fotòniques, Castelldefels (Barcelona), Spain

The phase change material $Ge_2Sb_2Te_5$ (GST) exhibits large changes in its optical and electronic properties across the structural phase transition between its amorphous and crystalline states. We use single-shot optical and diffraction measurements to follow the system*s dynamics after initiating the phase transition with a femtosecond laser pulse. We observe large changes in the dielectric function instantaneously after photoexcitation, when the lattice still shows long-range order. Energy transfer from electrons to the lattice heats leads to melting on a few picosecond timescale and the amorphization is achieved by thermal processes on longer timescales.

HL 90.5 Thu 16:00 H 0111

Static and dynamic THz spectroscopy of epitaxially grown GeTe-Sb_2Te_3 alloys — •Valeria Bragaglia[1], Karsten Holldack[2], and Raffaella Calarco[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany

In the last few years, the number of investigations on the dynamics of photo induced effects in GeTe-Sb_2Te_3 alloys increased. Full optical measurements were mostly employed in order to get information on both, the electronic and structural response upon excitation. The films investigated are typically grown by sputtering and result in a polycrystalline structure [1].

In our study we focus on epitaxially grown GST which presents a high degree of structural quality. Static measurements where performed in transmittance and reflectance configuration on crystalline and amorphous GST employing Fourier transform Infrared spectroscopy (THz) which allows to access the spectral range of 20-700 cm^{-1}. Epitaxial crystalline GST shows both free carrier and phonon absorption contributions. In particular, employing a multilayer structure model, we conclude that a Drude model convolved with several Lorentzian contributions arising from soft phonon modes simulate well the experimental data. Ultrafast dynamic measurements of amorphous and crystalline GST under laser excitation are ongoing employing 800 nm fs-laser pump and ps-THz probe in the same spectral range in order to investigate time resolved electronic response upon excitation.

[1] M.J. Shu et al., Appl. Phys. Lett. 102, 201903 (2013).

HL 90.6 Thu 16:15 H 0111

Memristive Hebbian Plasticity: Device requirements for the emulation of Hebbian plasticity based on memristive devices — •Martin Ziegler[1], Mirko Hansen[1], Marina Ignatov[1], Thorsten Bartsch[2], and Hermann Kohlstedt[1] — [1]Nanoelektronik, Technische Fakultät, Christian-Albrechts-Universität zu Kiel — [2]Klinik für Neurologie, Universitätsklinikum Schleswig-Holstein, Christian-Albrechts-Universität zu Kiel

Essential requirements of individual memristive devices for the emulation of Hebbian plasticity in neuromorphic circuits are defined and discussed. Memristive devices based on ionic and exclusively electronic mechanisms are explored. The ionic devices consist of the layer sequence metal/isolator/metal and represent today's most popular devices. The electronic device is a MemFlash-cell. The MemFlash-cell is based on a conventional floating gate transistor with a diode configuration wiring scheme exhibiting a memristive (pinched) I-V characteristic. The electric characteristics of both types of devices are experimentally and theoretically explored with a focus on artificial synaptic plasticity mechanisms. A phenomenological plasticity model suitable for memristive devices is presented, based on advanced novel learning rules, which provide Hebbian plasticity in accordance to the Bienenstock-Cooper-Munro(BCM) rule.

HL 90.7 Thu 16:30 H 0111

Memristive Tunnel Junctions — •Mirko Hansen[1], Martin Ziegler[1], Thomas Mussenbrock[2], Sven Dirkmann[2], and Hermann Kohlstedt[1] — [1]AG Nanoelektronik, Technische Fakultät, Christian-Albrechts-Universität zu Kiel, Germany — [2]Lehrstuhl für Theoretische Elektrotechnik, Fakultät für Elektrotechnik und Informationstechnik, Ruhr-Universität Bochum, Germany

We present results on a device which consists of a tunnel barrier and a thin niobium oxide layer in between two metal electrodes.

By using the well established niobium/aluminium technology to fabricate aluminium oxide tunnel junctions with a smooth interface, we are able to fabricate very thin (<3 nm) and highly resistive niobium oxides layers. The homogeneous change in resistance (Roff/ Ron > 100) and RxA vs. A plots suggest an area-dependent and non-filamentary switching mechanism, which is explained by taking the interface effects at the tunnel barrier and the top electrode into account.

The memristive tunnel junctions were optimized for the use in neuromorphic circuits and were fabricated on 4" wafers using standard optical lithography, (reactive) DC sputtering and wet etching.

HL 90.8 Thu 16:45 H 0111

Emulation of neuronal functionality by using a VO_2-based oscillator circuit — •Marina Ignatov, Martin Ziegler, Mirko Hansen, Adrian Petraru, and Hermann Kohlstedt — Nanoelektronik, Technische Fakultät, Christian-Albrechts-Universität zu Kiel, Germany

A negative-differential oscillator circuit based on a vanadium dioxide (VO_2) device is presented. The oscillator circuit allows to emulate basic neuronal functionalities, including spike coding. The obtained results are compared to common spiking neuron models. Additionally, a theoretical analysis of the oscillator circuit is used to gain insight into the functionality of the circuit and to give advice for the device development and the implementation of the circuit. In this respect, important requirements for the strongly correlated electron material VO_2 are presented and discussed in detail. Further, possible modifications of the oscillator circuit model for a better agreement with neuronal spikes are presented.

15 min. break.

HL 90.9 Thu 17:15 H 0111

Effect of oxygen engineering and doping on resistive switching in HfO_2 based RRAM devices grown by MBE — •S.U. Sharath[1], Jose Kurian[1], Erwin Hildebrandt[1], Philipp Komissinskiy[1], Thomas Bertaud[2], Christian Walczyk[2], Pauline Calka[2], Thomas Schroeder[2], and Lambert Alff[1] — [1]Materialwissenschaft, Technische Universität Darmstadt, Germany — [2]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

Thin films of titanium nitride (TiN, electrode) and hafnium oxide (HfO_2) were grown using molecular beam epitaxy (MBE). Oxygen engineering using strongly oxygen deficient growth parameters and trivalent doping of HfO_2 thin films has been utilized to stabilize oxygen vacancy concentrations far beyond the thermodynamical equilibrium. Thin films of hafnium oxide grown at 320 °C on TiN crystallize in a monoclinic symmetry (m-HfO_2) at higher oxidation conditions, whereas the oxygen deficient hafnium oxide films showed oxygen vacancy stabilized tetragonal like phase of hafnium oxide (t-HfO_{2-x}) which was verified by X-ray diffraction [1]. A large concentration of oxygen vacancies lead to a defect band at the Fermi-level as observed by X-ray photoelectron spectroscopy (XPS). The electrical switching measurements show that the forming voltage is reduced for oxygen

deficient films paving the way for low power devices in future. In oxygen deficient HfO_{2-x} thin films grown on TiN/Si(001), the thickness dependence of the forming voltage is strongly suppressed [2].

[1] S. U. Sharath et al., Appl. Phys. Lett., 104, 063502 (2014).
[2] S. U. Sharath et al., Appl. Phys. Lett., 105, 073505 (2014).

HL 90.10 Thu 17:30 H 0111

BiFeO3-based resistive switching cells with flexible rectifying contact — •Tiangui You[1], Nan Du[1], Stefan Slesazeck[2], Thomas Mikolajick[2,3], Guodong Li[4], Danilo Bürger[1], Ilona Skorupa[1], Hartmut Stöcker[5], Barbara Abendroth[5], Andreas Beyer[6], Kerstin Volz[6], Oliver G. Schmidt[1,4], and Heidemarie Schmidt[1] — [1]TU Chemnitz — [2]NaMLab gGmbH Dresden — [3]TU Dresden — [4]IFW Dresden — [5]TU Bergakademie Freiberg — [6]Philipps-Universität Marburg

Nonvolatile resistive switching in BiFeO3 (BFO) has attracted increasing attention. However, the underlying resistive switching mechanism is still controversial which restricts its application in nonvolatile memory[1] and logics[2]. Here we develop a model on modifiable Schottky barrier height and elucidate the physical origin underlying resistive switching in Au-BFO-Pt/Ti resistive switching cells containing mobile oxygen vacancies.[3] Increased switching speed is possible by applying a large amplitude writing pulse as the migration of mobile oxygen vacancies is tunable by both the amplitude and length of the writing pulse. The local resistive switching has been investigated by conductive atomic force microscopy and exhibits the capability of down-scaling the resistive switching cell to the grain size.

[1] Y. Shuai, et al., J. Appl. Phys. 2011, 109, 124117
[2] T. You, et al., Adv. Funct. Mater. 2014, 24, 3357
[3] T. You, et al., ACS Appl. Mater. Interfaces 2014, 6, 19758

HL 90.11 Thu 17:45 H 0111

Reversible Changes Induced by Liquid Electrolyte Gating in the WO_3 Electronic Structure — •Carlos E. ViolBarbosa[1], Julie Karel[1], Simone G. Altendorf[2], Janos Kiss[1], Yuki Utsumi[1], Mahesh G. Samant[2], Liu Hao Tjeng[1], Claudia Felser[1], and Stuart S. P. Parkin[2] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany 01187 — [2]IBM Almaden Research Center, San Jose, California, USA 95120

Tungsten trioxide (WO_3) is a d0 transition metal oxide that has attracted broad interest due its optical and electrical properties. WO_{3-x} has a rich phase diagram. Many of the studies in this material make use of modifications in the carrier concentration by chemical doping or creation of oxygen deficiencies. In this work, we utilize ionic liquid electrolyte gating in a electric-double-layer transistor device to induce a metallic state in WO_3 films, a process we will show is reversible.

The modifications in the electronic structure (core levels and valance band) resulting from the gating are probed by hard X-ray photoelectron spectroscopy. Electrolyte gating leads to a significant population of W 5d states in the conduction band and an enormous change in the W 4f core levels. Ab initio density functional theory are used to help describe the origin of these modifications in the electronic structure.

HL 90.12 Thu 18:00 H 0111

Resistive switching of polycrystalline, multiferroic $YMnO_3$ thin films — •Agnieszka Bogusz[1,2], Sławomir Prucnal[1], Daniel Blaschke[1], Ilona Skorupa[1], Danilo Bürger[2], Oliver G. Schmidt[2,3], and Heidemarie Schmidt[2] — [1]Institute Of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf — [2]Department of Materials for Nanoelectronics, Chemnitz University of Technology — [3]Institute for Integrative Nanosciences, IFW-Dresden

Resistive switching (RS) phenomena have been widely investigated in the field of materials science, physics, and electrical engineering in the past decade. Recently, multiferroics have been considered as promising candidates for memristive switches. Specific properties of multiferroics might bring additional and/or new functionalities into the memristive switches. This work investigates the RS properties of multiferroic $YMnO_3$ thin films reported as a unipolar resistive switch [1]. $YMnO_3$ was grown at 400°C on $Pt/Ti/SiO_2/Si$ substrates by pulsed laser deposition (PLD) and crystallized by flash lamp annealing (FLA). Film thickness and the concentration of point defects were controlled during the PLD process. Transport and RS properties of $Au/YMnO_3/Pt/Ti/SiO_2$ structures were determined by two-point probe measurements in a top-bottom configuration. Results imply that the filamentary, unipolar RS in $YMnO_3$ originates from the electroredox reactions induced by the Joule heating. [1] A. Bogusz et al.,AIP Advances 4, 107135 (2014)

HL 90.13 Thu 18:15 H 0111

Kinetic Monte-Carlo simulations of resistive switching in silver doped titanium dioxide thin films — Sven Dirkmann[1], Jan Trieschmann[1], Mirko Hansen[2], Martin Ziegler[2], Hermann Kohlstedt[2], and •Thomas Mussenbrock[2] — [1]Ruhr-Universität Bochum, Lehrstuhl für Theoretische Elektrotechnik, 44780 Bochum — [2]Christian-Albrechts Universität zu Kiel, AG Nanoelektronik, 24143 Kiel

Low power consumption, low frabrication costs, fast write and read cycles, and scalability into the nanometer range make resistive switching devices attractive for future non-volatile memory applications and neuromorphic circuits. The majority of devices rely on nano-ionic mechanisms – one of which is electrochemical metallization, where the change in resistance is due to the formation and re-formation of conducting filaments. This contribution is devoted to demonstrate and discuss the formation and re-formation of Ag filaments in an $Ag/TiO_2/Pt$ sandwich-like thin film system at experimental time-scales by means of kinetic Monte-Carlo simulations. It is shown that filamentary electrochemical metalization devices provide distinct and reliable "on" and "off" states, but their dynamic range is limited.

HL 90.14 Thu 18:30 H 0111

Tailoring the electrical properties of a TiO_2 layer by ion-beam irradiation for memristive applications — •Daniel Blaschke[1], Agnieszka Bogusz[1], René Hübner[1], Franziska Nierobisch[1], Vikas Rana[3], Andrea Scholz[1], Sibylle Gemming[1,2], and Peter Zahn[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf — [2]Chair of Scale-bridging Materials Modeling, Physics Departement, TU Chemnitz — [3]Peter Grünberg Institut, Forschungszentrum Jülich

Reactively sputtered TiO_2 thin films on $Pt/Ti/SiO_2/Si$ substrates were irradiated with low energy Ar^+ ions of different energies to create surface or bulk modifications in the material. Furthermore, the fluence was varied to optimize the level of the modifications, which are e.g. amorphization, surface smoothing, and preferential sputtering of oxygen. These effects were detected by TEM, AFM and supported by TRIDYN simulations, respectively. The impact of these changes on the electrical properties of the TiO_2 layers was monitored by I-V and C-V measurements in top-bottom geometry with Pt, as well as Ti/Pt top contacts. The results indicate a transition from a Schottky-like behavior of the Pt/TiO_2 interface to an ohmic one with increasing fluence, which is very similar to the behavior of a Ti/TiO_2 interface. Furthermore, the capacity of the complete MIM stack increases with fluence, which points to a reduced effective thickness of the dielectric TiO_2 layer after irradiation.

The project is funded by the Initiative and Networking Fund of the Helmholtz Association (Virtual Institute Memriox, VH-VI-422).

HL 91: Frontiers of electronic structure theory: Many-body effects, methods

Time: Thursday 15:00–18:30 Location: MA 004

Invited Talk HL 91.1 Thu 15:00 MA 004

Natural orbital functional theory with higher-order occupation probabilities — •Ralph Gebauer[1], Roberto Car[2], and Morrel Cohen[2,3] — [1]International Centre for Theoretical Physics (ICTP), Trieste, Italy — [2]Department of Chemistry, Princeton University, Princeton, USA — [3]Department of Physics and Astronomy, Rutgers University, USA

We introduce a novel energy functional for ground-state electronic-structure calculations. Its fundamental variables are the natural spin-orbitals of the implied singlet many-body wave function and their joint occupation probabilities. The functional derives from a sequence of controlled approximations to the two-particle density matrix. Algebraic scaling of computational cost with electron number is obtainable in general, and Hartree-Fock scaling in the seniority-zero version of the theory. Results obtained with the latter version for saturated small molecular systems are compared with those of highly-accurate quantum-chemical computations. The numerical results are variational, capturing most of the correlation energy from equilibrium to dissociation. Their accuracy is considerably greater than that obtainable with current density-functional theory approximations and with current functionals of the one-particle density matrix only.

HL 91.2 Thu 15:30 MA 004

Electronic Properties of Surfaces and Interfaces with Self-Consistent Interatomic van der Waals Density Functional — •Nicola Ferri[1], Robert A. Distasio Jr.[2], Alberto Ambrosetti[1], Roberto Car[2], Matthias Scheffler[1], and Alexandre Tkatchenko[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Princeton University, USA

Ubiquitous long-range van der Waals (vdW) interactions play a fundamental role in the structure and stability of a wide range of systems. Within the DFT framework, the vdW energy represents a crucial, but tiny part (0.001%) of the total energy, hence its influence on the electronic density, $n(\mathbf{r})$, and derived electronic properties is typically assumed to be rather small. Here, we address this question via a fully self-consistent (SC) implementation of the interatomic Tkatchenko-Scheffler vdW functional [1] and its extension to surfaces [2]. For several transition metal surfaces, self-consistency increases their dipole moments and induces non-trivial electron density rearrangements. As a consequence, we observed changes of up to 0.3 eV in the surface work-functions, with vdW self-consistency improving the agreement with experiments. Similar behavior is observed for molecules adsorbed on metals, where vdW contributions influence both Pauli push-back and charge transfer, the two phenomena that determine interface work-functions. [1] A. Tkatchenko and M. Scheffler, PRL (2009). [2] V. G. Ruiz, W. Liu, E. Zojer, M. Scheffler, and A. Tkatchenko, PRL (2012).

HL 91.3 Thu 15:45 MA 004

Exact functionals for a lattice model — •Tanja Dimitrov[1], Heiko Appel[1,3], and Angel Rubio[1,2,3] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Nano-bio Spectroscopy Group/ETSF Scientific Development Centre, Universidad del Pais Vasco UPV/EHU, San Sebastian — [3]MPI for the Structure and Dynamics of Matter, Hamburg

Standard local exchange-correlation and semi-local functionals in ground-state density functional theory are known for their shortcomings in describing correct charge transfer, dissociation energies of molecular ions, and barriers of chemical reactions [1,2]. To understand the failures of approximate functionals, to gain insight into the behavior of the exact functional, and to devise new approximations, we investigate the exact solution of the many-body Schrödinger equation in Fock space for a lattice model with a softened Coulomb interaction term. Using quadratic optimization with quadratic constraints, or alternatively exact diagonalization, we explicitely construct the *exact* density-to-potential and density-to-wave-function map. We discuss the behavior of functionals in the low-density limit.

[1] A. J. Cohen et al. Science **321**, 792 (2008).
[2] P. Mori-Sanchez et al., Phys. Rev. Lett. **100**, 146401 (2008).

HL 91.4 Thu 16:00 MA 004

Many-body dispersion meets non-local density functionals: A unified approach for van der Waals correlations — •Jan Hermann, Matthias Scheffler, and Alexandre Tkatchenko — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

It is an ongoing challenge to develop an efficient method for van der Waals (vdW) non-local correlation within DFT which would be both accurate and broadly applicable. Current approaches can be loosely divided into the fragment-based ones, two-point density functionals and methods based on the density-density response function. The fragment-based models utilize parameters not derivable from the electron density. Two-point approaches are explicit density functionals, but difficult to generalize to include many-body correlations.

Here, we show that these seemingly contrasting approaches can be unified within a single framework based on the adiabatic-connection formalism in the random-phase approximation. We use a local response-function model from the VV09 functional [1] together with the many-body dispersion approach to create an atom-based model with no external parameters. We introduce a consistent correlation-functional-based coupling of the short- and long-range correlation energy. We show that this unification provides new insights into the different approaches, naturally deals with the partitioning of ionic and delocalized states and paves path towards self-consistent description of many-body vdW correlations.

[1] O. A. Vydrov, T. Van Voorhis, Phys. Rev. Lett. 103, 063004

HL 91.5 Thu 16:15 MA 004

Reduced Density-Matrix Functional Theory: correlation and spectroscopy — Stefano Di Sabatino[1], Jan A. Berger[2], Lucia Reining[3], and •Pina Romaniello[1] — [1]Laboratoire de Physique Théorique, CNRS, IRSAMC, Université Toulouse III - Paul Sabatier, Toulouse, France and ETSF — [2]Laboratoire de Chimie et Physique Quantiques, IRSAMC, Université Toulouse III - Paul Sabatier, CNRS, Toulouse, France and ETSF — [3]Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-DSM, Palaiseau, France and ETSF

We study the performance of approximations to electron correlation in reduced density-matrix functional theory (RDMFT) and of approximations to the observables calculated within this theory [1]. We use the exactly solvable Hubbard molecule as test case. In particular we focus on the atomic limit and we explore how degeneracies and spin-symmetry breaking are treated in RDMFT. We find that, within the used approximations, RDMFT is not able to describe the signature of strong correlation in the spin-singlet ground state, whereas it give the exact result for the spin-symmetry broken case. [1] S. Di Sabatino, J.A. Berger, L. Reining, and P. Romaniello, submitted

HL 91.6 Thu 16:30 MA 004

Does *GW* obey the straight-line condition? — Matthias Dauth[1,3], Fabio Caruso[2], Stephan Kuemmel[1], and •Patrick Rinke[3] — [1]University of Bayreuth, Germany — [2]University of Oxford, England — [3]Aalto University, Helsinki, Finland

Many-body theory in the *GW* approach has become the method of choice for calculating charged excitations in solids. Recently, it is also increasingly being applied to molecules, but fundamental questions regarding its accuracy remain. One such fundamental theorem requires that the total energy changes linearly with gradual (i.e. fractional) ionisation of the molecule. In this work we investigate, if *GW* is piecewise linear or if it exhibits a derivation of the straight line error (DSLE). Since the derivative of the total energy with respect to the electron number gives the ionisation energy, we quantify the DSLE by taking the difference between the energy of the highest occupied state of the neutral and the lowest unoccupied state of the singly ionised molecule (which would be equal in the DSLE-free case). We find for a subset of molecules from the quantum chemical G2 benchmark set, that the DSLE in self-consistent *GW* amounts to 1.1 eV on average. This DSLE can be mitigated in perturbative G_0W_0 by varying the starting point. We use density-functional theory as starting point and vary the amount of exact exchange α in the Perdew-Burke-Ernzerhof hybrid functional (PBEh). G_0W_0 becomes DSLE-free for $\alpha \approx 0.4$. The average deviation from the experimental IPs is then very close to that of self-consistent *GW* and amounts to ∼0.25 eV.

HL 91.7 Thu 16:45 MA 004

Green's Function embedding for Advanced Electronic Structure Methods based on Dynamical Mean-Field Theory — •Wael Chibani[1], Xinguo Ren[2], Matthias Scheffler[1], and

Patrick Rinke[3] — [1]*Fritz-Haber-Institute of the Max-Planck-Society, Berlin, Germany* — [2]*Key Laboratory of Quantum Information, USTC, Hefei, China* — [3]*Aalto University, Helsinki, Finland*

We introduce an embedding scheme for periodic systems that facilitates a self-consistent treatment of the physically important part of a system with electronic structure methods, that are computationally too expensive for periodic systems. We use dynamical mean-field theory [1] (DMFT) to couple to the rest of the system, which is treated with less demanding approaches such as Kohn-Sham density functional theory. In contrast to the original DMFT formulation for correlated model Hamiltonians, we consider here the unit cell as local embedded cluster in an *ab initio* way, that includes all electronic degrees of freedom. The performance of our scheme is demonstrated by treating the embedded region with hybrid and GW self-energies (scGW) for simple bulk systems. The total energy and the density of states converge rapidly with respect to the computational parameters and approach their bulk limit with increasing cluster size. For non self-consistent GW calculations we observe Plasmon satellites for Si – in good agreement with periodic G_0W_0 calculations [2] – that vanish at self-consistency. Our scGW gap of $\sim$ 0.9 eV for a two atom unit cell agrees well with previous G_0W_0 calculations and experiment. [1] A.Georges *et al.*, Rev.Mod.Phys.(2006), [2] M.Guzzo *et al.*, PRL(2011)

HL 91.8 Thu 17:00 MA 004

Improved Ground State Electronic Structure and Optical Dielectric Constants With a Semi-Local Exchange Functional — •Vojtěch Vlček[1], Gerd Steinle-Neumann[1], Linn Leppert[1], Rickard Armiento[2], and Stephan Kümmel[1] — [1]University of Bayreuth, Germany — [2]Linköping University, Sweden

For a set of solids, we explore a recently developed generalized gradient exchange functional (AK13) that has two characteristic features: its enhancement factor diverges for large reduced density gradients s as $s \ln(s)$ and its potential changes discontinuously at integer electron numbers. We apply the functional to semiconductors, Mott insulators, and ionic crystals and compare results for band structure and dielectric constants with a standard GGA. The AK13 functional provides a better description of the KS orbitals and we observe a qualitative improvement both in the bandgaps and in the optical dielectric constants, especially for the small gap semiconductors we explore (Ge, α-Sn, and CdO)

HL 91.9 Thu 17:15 MA 004

Accurate, efficient localized resolution of identity of the Coulomb operator across the periodic table — •Arvid Ihrig[1], Jürgen Wieferink[1], Igor Ying Zhang[1], Patrick Rinke[1,2], Volker Blum[1,3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Aalto University, Helsinki, Finland — [3]Duke University, Durham, USA

A key component of advanced electronic structure methods is the explicit evaluation of the Coulomb operator. The corresponding four-center integrals can be solved with a "resolution of identity" (RI) approach for numeric atom-centered orbitals, as they are used in, e.g., FHI-aims [1]. In RI, basis function products are expanded in an auxiliary basis. The complete auxiliary basis is used for "RI-V", the most accurate and most commonly used RI. We developed a localized RI ("RI-LVL"), which expands the products only in the subset of those auxiliary functions centered on the same atoms as the basis functions. This approach yields a superior scaling with system size, both in terms of computational time and memory requirements. At the same time it also retains the accuracy of the RI-V, as we have shown for HF, MP2, PBE0 and RPA calculations. The systems we investigated include weakly interacting molecular dimers (S22 test set) as well as TiO_2, Cu, and Au clusters. In all test cases we found that RI-LVL reproduces RI-V very accurately. Even for RPA-calculations of gold with very large basis sets the deviation to RI-V is only $\sim$1.5 meV per atom. [1] V. Blum *et al.*, Comput. Phys. Commun. **180**, 2175 (2009).

HL 91.10 Thu 17:30 MA 004

Explicitly correlated self consistent field theory — •Christian Lasar and Thorsten Klüner — Carl von Ossitzky Universität, Oldenburg, Germany

There is a variety of methods available which aim to describe molecules and molecular reactions with chemical accuracy. The two main classes of these methods are density functional theory (DFT) and electron correlation approaches. DFT achieves great accuracy for many molecules and is applicable to quite large molecules. Unfortunately, DFT is not systematically improvable since the exact form of the exchange correlation functional remains unknown. Correlation methods do not suffer from this lack of systematic improvement. Unfortunately, they often require too much computational resources for large molecules. Additionally, they show a very slow convergence with the size of the basis set. Explicitly correlated methods are known to be able to solve this convergence problem. In these methods, the wavefunction is augmented with a function f_{ij} which explicitly depends on two electronic coordinates. Combining the advantages of low computational resources and the ability for systematic improvement, one ends up in the following ansatz for the wavefunction $\Psi = (1 + \sum_{ij} f_{ij})\Phi$, where Φ is one slater determinant. With this ansatz the long determinant expansion is avoided. Additionally, there will be a fast convergence with the basis set size. We currently investigate the derivation of the working equations and their implementation for different functions f_{ij}. Some results for small molecules have already been obtained and will be presented in this contribution.

HL 91.11 Thu 17:45 MA 004

Comparison of two self-consistent GW schemes — •Peter Koval[1], Dietrich Foerster[2], and Daniel Sanchez-Portal[1,3] — [1]Donostia International Physics Center, San Sebastián, Spain — [2]Laboratoire Ondes et Matiére d'Aquitaine, Bordeaux, France — [3]Material Physics Center, San Sebastián, Spain

GW approximation (GWA) as a competitor of DFT provides a better description of electronic structure in several respects. However, a GW calculation is more expensive than similar DFT calculation. This fact contributed to a wide usage of simpler calculations based on GWA (SEX, COSEX, plasmon-pole approximations etc.) This manyfold of approximations hampers a non-biased evaluation of merits of GWA to describe the electronic correlations. We produced a rigorous GW implementation where the only approximation is the use of localized orbitals [1]. The usage of spectral functions allowed us to realize two self-consistent GW schemes: scGW [2] and qsGW [3] in one code [4]. Furthermore, we used all-electron Gaussian basis sets that allows for a coherent comparison with quantum chemistry methods. We use coupled-cluster methods CCSD and CCSD(T) as reference and compare ionization potentials of 15 molecules. The calculations show trends in scGW and qsGW and give hints on possible sources of discrepancies/directions towards improving GWA. [1] D. Foerster, P. Koval, D. Sánchez-Portal, *J. Chem. Phys.* **135**, 074105 (2011); [2] L. Hedin, *J. Phys. Cond. Mat.* **11**, R489 (1999); [3] S. V. Faleev, M. van Schilfgaarde, T. Kotani, *Phys. Rev. Lett.* **93**, 126406 (2004); [2] P. Koval, D. Foerster, D. Sánchez-Portal, *Phys. Rev.* B **89**, 155417 (2014).

HL 91.12 Thu 18:00 MA 004

Quasiparticle Self-Consistent GW for Molecules — •Ferdnand Kaplan[1,2,3], Michiel van Setten[1,2,5], Florian Weigend[1,3], and Ferdinand Evers[1,2,3,4] — [1]Institute of Nanotechnology (INT) — [2]Institute for Theoretical Condensed Matter Physics (TKM) — [3]Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany — [4]Universität Regensburg, D-93040 Regensburg, Germany — [5]Université catholique de Louvain, B-1348 Louvain-la-Neuve, Belgium

One of the most used approaches for the computational study of nanoscale systems and molecules is the density functional theory (DFT). However, DFT calculations of single particle excitation spectra, e.g. ionization potentials, often suffer from method-inherent difficulties. To systematically improve the estimation of quasi-particle energies for molecular system, we have implemented the GW method. The approach represents a perturbative expansion of the many-body Green's function with respect to the screened Coulomb interaction, W.

On G_0W_0 level the GW-self energy is calculated with the Kohn-Sham Green's function of the underlying DFT. Hence, one finds a strong dependence of the excitation energies on the reference system, i.e. DFT functionals. To overcome this problem, we implemented a self-consistent cycle which takes into account the deviations of the quasiparicle(qp)-wavefunctions from their Kohn-Sham parents.

We find that this procedure converges to a fixed point solution which is independent of the reference system. For the testset of molecules anlyzed by us so far, the results for ionization-energy and electron-affinity improve upon G_0W_0, when comparing to experimental data.

HL 91.13 Thu 18:15 MA 004

Pure state N-representability conditions: Should they be taken into account in Reduced density matrix functional theory? — •Iris Theophilou[1], Nektarios Lathiotakis[2,3], and

Nicole Helbig[1] — [1]Peter Grünberg Institut (PGI-1), Forschungszentrum Jülich, Jülich, Gernany — [2]Theoretical and Physical Chemistry Institute (TPCI), National Hellenic Research Foundation , Athens, Greece — [3]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

In Reduced Density Matrix Functional Theory (RDMFT) the natural occupation numbers are minimized under the ensemble N-representability conditions, i.e they are restricted to be between zero and one and sum to the number of electrons. Recently, the pure state N-representability problem for the one-body reduced density matrix has been solved [M. Altunbulak and A. Klyachko, Commun. Math. Phys. 282, 287 (2008)]. In this talk we discuss to which extend these pure state conditions are satisfied without being enforced in 3 electron systems using some standard RDMFT functionals. Our aim is to impose those pure state conditions that are not automatically satisfied and check whether this improves RDMFT results.

HL 92: VCSELs, optical interconnects and Si photonics

Time: Thursday 15:45–17:45 Location: EW 202

HL 92.1 Thu 15:45 EW 202

Towards an all-Silicon Nanolaser — Sebastian Schmitt[1,2], •George Sarau[1], and Silke Christiansen[1,2] — [1]Max Planck Institut für die Physik des Lichts Erlangen — [2]Helmholtz Zentrum für Materialien und Energie, Berlin

While optical circuit elements based on silicon (Si) photonics are already well established and almost have reached market maturity, fully integrated Si based optoelectronic devices for optical data processing and sensing would require a small near-infrared (NIR) light source, because at lower wavelength the Si host medium is absorbing. So far, Si bonded III-V hybrid or semiconductor nanostructure lasers have generated the most remarkable results, nevertheless the hybrid integration of III-V semiconductors is unlikely to become technologically relevant.Highly integrated and low cost devices would require a CMOS compatible fabrication and therefore a small Si monolithic laser operating at room temperature remains a desirable goal. By applying a novel type of optical cavity, we show that Purcell enhancement of spontaneous emission in Si can generate NIR light beyond the lasing threshold at room temperature.

HL 92.2 Thu 16:00 EW 202

Record-large 23 GHz modulation bandwidth at 85°C of energy-efficient 980 nm VCSELs for optical interconnects — •Philip Moser[1], Gunter Larisch[1], Maya Volwahsen[1], James Lott[1], and Dieter Bimberg[1,2] — [1]Institut für Festkörperphysik und Zentrum für Nanophotonik, Technische Universität Berlin, Berlin, Deutschland — [2]King Abdulaziz University, Jeddah, Saudi Arabia

Energy-efficient oxide-confined vertical-cavity surface-emitting lasers (VCSELs) emitting at 980 nm, particularly well suited for very short reach (< 2m) and ultra short-reach (< 2 mm) optical interconnects, are presented. At 85°C a record-large 23 GHz modulation bandwidth f3dB is achieved with a 5 *m oxide-aperture diameter VCSEL. At 25°C the maximum f3dB is 24.7 GHz. At lower currents before the saturation of f3dB our VCSELs are faster and more energy-efficient at 85°C than at 25°C, making them especially well suited for future optical interconnect technologies with terabit performance, high bandwidth density and low power dissipation.

HL 92.3 Thu 16:15 EW 202

Quantum well-pumped red AlGaInP VECSEL — Fabian Sauter[1], •Stefan Baumgärtner[1], Hermann Kahle[1], Cherry May Mateo[2], Roman Bek[1], Uwe Brauch[2], Michael Jetter[1], and Peter Michler[1] — [1]Universität Stuttgart, Institut für Halbleiteroptik und Funktionelle Grenzflächen und Research Center SCoPE, Allmandring 3, 70569 Stuttgart — [2]Universität Stuttgart, Institut für Strahlwerkezuge, Pfaffenwaldring 43, 70569 Stuttgart

Optically pumped semiconductor vertical-external-cavity surface-emitting lasers (OPS-VECSELs) provide the possibility of bandgap engineering in combination with the benefit of a near-diffraction-limited beam. By the use of AlGaInP material system, the emission wavelength in the red spectral range can easily adjusted around 640 nm to 680 nm depending on the material composition. Furthermore, the external cavity enables intra-cavity wavelength tuning, frequency doubling or mode locking. Previous AlGaInP OPS-VECSELs were pumped usually with green lasers at 532 nm to excite carriers in the barrier layers of the gain structure. The high quantum defect between the pump and the emission wavelength result in an elevated thermal input. In order to avoid degradation of the semiconductor structure and thermal rollover with increased pump power, we lower the quantum defect by carrier excitation in the quantum wells directly via pumping in the red spectral range. This causes challenges like low absorption efficiency and the lack of suitable pump sources. The present work is focusing on these challenges to achieve the quantum well-pumped VECSEL to a vest-pocket prototype.

HL 92.4 Thu 16:30 EW 202

Self-mode-locking vertical-external-cavity surface-emitting laser — Mahmoud Gaafar[1], •Philipp Richter[1], Hakan Keskin[2], Christoph Möller[1], Matthias Wichmann[1], Wolfgang Stolz[1,3], Arash Rahimi-Iman[1], and Martin Koch[1] — [1]Department of Physics and Materials Sciences Center, Philipps-Universität Marburg, Renthof 5, 35032 Marburg, Germany — [2]Department of Physics, Middle East Technical University, Ankara, 06800, Turkey — [3]NAsP III/V GmbH, Am Knechtacker 19, 35041 Marburg, Germany

Self-mode-locked (SML) optically-pumped semiconductor disk lasers emerged in recent years to become a promising alternative to their saturable-absorber-based pendants. Self-mode-locking has yet not only been shown for quantum-well systems, but also for quantum-dot ones. In this work, we present an SML quantum-well semiconductor disk laser at an emission wavelength of 1 micron. Green light originating from second-harmonic generation using the out-coupled laser beam is demonstrated using a BBO crystal outside the cavity. In addition, a long-time-span pulse train as well as an autocorrelation trace is presented for our sub-ps pulses at 500 MHz repetition rate. A beam-profile measurement reveals the excellent beam quality of our device with an M-square factor of less than 1.1 for both axes.

HL 92.5 Thu 16:45 EW 202

Spontaneous and stimulated emission dynamics of quantum dot high-Q micropillar structures — •Sören Kreinberg[1], Elisabeth Schlottmann[1], Steffen Holzinger[1], Janik Wolters[1], Sven Höfling[2,3], Martin Kamp[2], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany — [2]Lehrstuhl für Technische Physik, Universität Würzburg, 97074 Würzburg, Germany — [3]School of Physics & Astronomy, University of St Andrews, St Andrews, United Kingdom

Semiconductor microcavites are an ideal environment to study the fundamentals of light matter interaction down to the single emitter-single photon limit. Here, various effects like strong coupling or ultralow threshold lasing can be observed.

We present a comprehensive experimental study on the spontaneous and stimulated emission dynamics of InGaAs quantum dots embedded in high-Q micropillar cavities. While at low excitation powers the Purcell-enhanced spontaneous emission dominates the dynamics, a significant reduction of the emission lifetime indicates the onset of lasing at higher excitation powers.

Our results promise a better understanding of high-beta few-quantum-dot laser.

HL 92.6 Thu 17:00 EW 202

Finite-size high-contrast gratings for VCSELs — •Anjin Liu and Dieter Bimberg — Institut für Festkörperphysik und Zentrum für Nanophotonik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany

Vertical-cavity surface-emitting lasers (VCSELs) are attractive low-cost light sources e.g. for optical interconnects in computer networks or optical sensors, providing high modulation bandwidth, lower power consumption, and symmetric beam properties. High-speed, energy-efficient, and temperature-stable VCSELs for data transmission with increasing link lengths have been demonstrated in the last few years. Nanoscale photonic structures like high-contrast gratings (HCGs) provide novel opportunities for VCSEL design and are expected to exhibit

improved device performance like modulation speed, mode selectivity, and polarization control. Previous HCGs were designed with periodic boundary conditions using infinite-size plane incident waves. However, in a real device both the HCG and the incident wave are finite. Such modelling is presented here. The higher-order angular components of the finite-size incident wave are found to excite eigenmodes of the HCG causing reduced reflection and reduced reflection bandwidth. The in-plane and unidirectional transmission by the mode conversion in finite-size HCGs provide opportunities for novel applications like integrated VCSEL-based optical sensors and VCSEL-based on-chip optical interconnects.

HL 92.7 Thu 17:15 EW 202

Large frequency mode-locking of InP/InAs quantum-dot lasers — •Tagir Sadeev, Dejan Arsenijević, and Dieter Bimberg — Technische Universität Berlin Institut für Festkörperphysik

Passively mode-locked semiconductor lasers (MLL) are able to emit fs-short optical pulses at frequencies up to tens of GHz without any external frequency source. MLLs are of largest importance e.g. for ultra-high data rate optical transmission, clock sources and biomedicine. Significant improvements of the performance of MLL as well as continuous-wave lasers have been achieved in last decades, thanks to implementing zero-dimensional (quantum dot) structures into the active layer. Most advantages of QD MLL have been demonstrated for GaAs-based ones, operating at 1310 nm wavelength, targeting short-range telecom applications, where optical fiber exhibits zero dispersion. Long-haul optical transmission systems operate in the 1550 nm range, where fiber losses are minimal. At this wavelength InP based growth technology is common, but the brake-through results of QD MLLs are much scarcer as compared to their 1310 nm counterparts. In this work we investigate passive mode-locking of two-section QD MLL grown by metalorganic vapor phase epitaxy on InP substrate. We demonstrate monolithic two-section true QD MLLs at 1550 nm with better performance than yet reported: lowest optical pulse FWHM is 3.7 ps without any compression at 33.5 GHz repetition rate, which is noise-free and 300 MHz tuneable.

HL 92.8 Thu 17:30 EW 202

Gain compression induced polarization mode competition in quantum-dot micropillar lasers:A comparison of theoretical modeling via multi-mode rate equations and experimental measurements — •Christoph Redlich, Benjamin Lingnau, and Kathy Lüdge — Institut f. Theo. Physik, Sekr. EW 7-1, Technische Universität Berlin, Hardenbergstr. 36, 10623Berlin, Germany

We present a comparison of experimental results and theoretical modeling of the two-mode light emission of quantum-dot semiconductor micropillar lasers (QD micropillar VCSEL) subjected to optical feedback from a distant mirror. Using stochastic multi-mode rate equations with phenomenological gain compression parameters and spontaneous emission noise we show very good agreement in terms of intensity profiles and stochastic properties of the examined QD lasers. We further investigate intensity correlation functions and correlation times which can nicely be described by the semi-classical rate equation system. Even effects like superthermal bunching are reproduced, showing that this effect also finds its origin in spontaneous emission noise induced mode switching.

HL 93: III-V semiconductors (other than nitrides)

Time: Thursday 15:45–17:45 Location: EW 203

HL 93.1 Thu 15:45 EW 203

Bond stretching force constants in (In,Ga)P — •Stefanie Eckner[1], Martin Gnauck[1], Andreas Johannes[1], Tobias Steinbach[1], Helena Kämmer[1], Mark C. Ridgway[2], and Claudia S. Schnohr[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Department of Electronic Materials Engineering, Research School of Physics and Engineering, The Australian National University, Canberra ACT 0200, Australia

In order to exploit the full potential of mixed III-V-semiconductors for electronic and opto-electronic applications, a deeper understanding of their atomic scale structure and its relation to relevant properties such as the bandgap is necessary. The local atomic arrangement, which is crucial especially for strained thin films and nanostructures, strongly depends on the bond stretching force constants of the atomic pairs present in the material. In this study, (In,Ga)P grown by metal organic chemical vapour deposition was investigated using extended X-ray absorption fine structure spectroscopy. Measurements at the In- and Ga-K-edge were performed at ten different temperatures to determine the bond length variation as a function of temperature. As a result, bond stretching force constants of Ga-P- and In-P-bonds were determined in (In,Ga)P for varying indium content. These bond stretching force constants can be used in analyses of Raman spectra and in theoretical models of strained III-V thin films and nanostructures.

HL 93.2 Thu 16:00 EW 203

Capture cross sections from first-principles total energy calculations for oxygen in GaP as benchmark case — •Ying Cui, Christoph Freysoldt, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40627 Düsseldorf

Non-radiative recombination is of particular technological importance for optoelectronic devices. The mechanism is however far from well understood. The Shockley-Read-Hall model is usually applied to explain thermally activated recombination at deep defects. Capture cross sections are key parameters in this model. We present a theoretical approach to compute the capture cross sections by using density functional theory with hybrid functional (HSE). In our approach the transition state in the capture process is located by using defect level occupation as a natural reaction coordinate. To benchmark theory against experiment, we apply our method to substitutional oxygen in GaP for which accurate DLTS data is available. We find a good agreement for capture cross sections as well as optical transition energies. Our method to determine capture cross sections is universal and can be applied to materials beyond GaP.

HL 93.3 Thu 16:15 EW 203

Effect of localized boron states on the conduction band transport in n-type (B,Ga)P — •Lars Ostheim[1], Steve Petznick[1], Sven Liebich[2], Kerstin Volz[2], Wolfgang Stolz[2], and Peter J. Klar[1] — [1]I. Physikalisches Institut, Justus-Liebig-Universtität Gießen, Germany — [2]Department of Physics and Material Sciences Center, Phillips-Universität Marburg, Germany

(B,Ga)P:Te and GaP:Te samples are grown by MOVPE on a 300 nm GaP buffer layer under a Te-partial pressure of Te/Ga=5*10-4. While the incorporation of Te results in n-type doping of the samples, the incorporation of B into GaP leads to the formation of localized electronic states resonant with the conduction band. In order to investigate the influence of these localized states on the transport properties, magnetotransport measurements were performed in a temperature range from 1.5 K to 300 K and as a function of applied hydrostatic pressure up to 17 kbar using a non-magnetic pressure cell. The results obtained indicate that a boron-related density of localized states exists in the vicinity of the conduction band edge of the alloy, which act as electron traps as well as efficient scattering centers. By applying hydrostatic pressure the energetic positions of conduction band edge at the X-point and the localized boron states are shifted apart reducing the impact of boron on the electronic transport parameters of the alloy.

HL 93.4 Thu 16:30 EW 203

HR-XRD analysis on GaP rotational twin domains on Si(111) substrates — •Christian Koppka, Agnieszka Paszuk, Matthias Steidl, Katja Tonisch, and Thomas Hannappel — Technische Universität Ilmenau, FG Photovoltaik, 98693 Ilmenau, Deutschland

The combination of todays silicon technology with tunable III-V semiconductors is of great interest for future high-efficiency optoelectronic devices. Due to the small lattice mismatch GaP/Si is a suitable quasi-substrate to link non-polar silicon substrates and polar III/V layers. For the growth of nanowire-based semiconductor structures {111} oriented substrates are commonly used. Here, rotational twin domains are a major defect, which cannot easily be suppressed by the substrate surface structure. Low defect densities, however, are required for further III/V integration. A reliable quantification of the rotational domain ratio is essential in order to adjust the MOCVD process for

growth of single crystal GaP epilayers on Si(111). Here, we use high-resolution x-ray diffraction analysis for quantification and investigate the influence of various parameters, such as growth temperature, III:V ratio and surface terminations, on the twin domain ratio. We find that growth temperature and Si surface termination prior nucleation highly impact the GaP(111) epilayer growth.

HL 93.5 Thu 16:45 EW 203

Growth of (Ga,In)(As,Bi) layers on GaAs, InP and GaSb substrates by Molecular Beam Epitaxy — •Wolfgang Bennarndt, Gerhard Böhm, and Markus-Christian Amann — Walter Schottky Institut, Garching

The incorporation of Bi in III/V semiconductor alloys results in a strong band gap reduction and therefore has attracted considerable interest for long-wavelength optoelectronic applications. Theoretical calculations even revealed a negative band gap for the binary materials GaBi and InBi, which means that layers with metallic character could be epitaxially grown and can in principal act as a waveguide for lasers emitting in the THz wavelength range. In this work we present incorporation studies of Bi into (Ga,In)As grown on GaAs, InP and GaSb by molecular beam epitaxy. Smooth layers with Bi-contents as high as 20% were successfully grown and characterized by XRD and PL-measurements. The influence of growth parameters on Bi-incorporation such as In content, strain, temperature and the flux ratio of the Group V elements will be discussed.

HL 93.6 Thu 17:00 EW 203

Luminescence properties of green (InGaAl)P-GaP LED grown on different orientated GaAs substrates — •Sarah Schlichting[1], Nikolay N. Ledentsov[2], Vitaly A. Shukin[2], Jari Lyytikäinen[3], Oleg Okhotnikov[4], Yurri M. Shernyakov[4], Alexey S. Payusov[4], Nikita Gordeev[4], Michail V. Maximov[4], Felix Nippert[1], and Axel Hoffmann[1] — [1]TU Berlin, Germany — [2]VIS GmbH, Germany — [3]Tampere University of Technology, Finland — [4]Russian Academy of Science, Russia

$(Al_{0.5}Ga_{0.5})_{0.5}In_{0.5}P - (Al_{0.8}Ga_{0.2})_{0.5}In_{0.5}P$ LED with GaP barriers were investigated by means of EL and PL techniques. The structures were grown by MBE side-by-side on differently-oriented GaAs substrates: (100), (211) and (311). Through studies of the luminescence properties of the structures it was found that at room temperature at current densities of $\sim 500 A/cm^2$ and below the EL intensity is similar for all substrates. A shift towards shorter wavelengths is observed for the structures grown on high-index GaAs substrates. For higher current densities ($>1\ kA/cm^2$) the (211) and (311)-orientated substrates show a much higher EL intensity compared to the GaAs(100) substrate. A gradually saturation of integrated intensity of the (311)-grown structure occurs at current densities above 4 kA/cm^2, such saturation is not visible for the (211)-grown structure even for current densities up to 14 kA/cm^2. This effect is attributed to self-organized superlattice formation[1] and the GaP insertion-induced engineering of the conduction band structure on high-index surfaces[2]. [1] N. Cherkashin et al., to be published [2] Appl. Phys. Lett. 105, 181902 (2014)

HL 93.7 Thu 17:15 EW 203

Impact of growth temperature on structural and optical properties of GaAs quantum structures grown on GaP (100) substrate — •S. Dadgostar[1], J. Schmidtbauer[2], T. Boeck[2], M. Rodríguez[3], A. Torres[3], J. Jiménez[3], O. Martínez[3], W. T. Masselink[1], and F. Hatami[1] — [1]Department of Physics, Humboldt-Universität zu Berlin, Newton-Str. 15, D-12489 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, D-12489 Berlin, Germany — [3]GdS-Optronlab, Dpto. Fisica Materia Condensada, Univ. de Valladolid, Edificio I+D, Paseo de Belén 1, 47011, Valladolid, Spain

We describe impact of growth temperature on structural and optical properties of self-assembled GaAs/GaP quantum structures grown using GS-MBE. Formation of quantum structures is driven by the 3.6% lattice mismatch between GaAs and GaP. 2.7-ML of GaAs was deposited at temperatures between 450 and 530C on GaP(100) and capped by 50 nm GaP. Then, GaAs layer was grown again at the same conditions for AFM measurements. Morphology of deposited GaAs changes with increasing growth temperature from quantum dots to dashes. The dots have a density of e11 cm-2, diameter and height of 19, and 1.1 nm, while the dashes have a density of 7.0 e10 cm-2, length, width, and height of 58, 18, and 2.1 nm. Cathodeluminescence measurements indicate that the emission spectra of all samples contain two peaks between 1.99 and 1.84 eV, which we attribute to the recombination in wetting layer and in dot/dash structures. The peak position changes for samples due to different geometry of quantum structures.

HL 93.8 Thu 17:30 EW 203

High-power 1060-mn photonic band crystal lasers with narrow beam divergence and low astigmatism — •Md. Jarez Miah[1], Thorsten Kettler[1,2], Kristijan Posilovic[1,2], Vladimir P. Kalosha[1], Danilo Skoczowsky[2], Dieter Bimberg[1], Johannes Pohl[3], and Markus Weyers[3] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]PBC Lasers GmbH, Hardenbergstr. 36, 10623 Berlin, Germany — [3]Ferdinand-Braun-Institut für Höchstfrequenztechnik, Gustav-Kirchhoff-Str. 4, 12489 Berlin, Germany

High-power edge-emitting lasers are efficient and indispensable light sources for a wide range of scientific and commercial applications such as pump sources for solid-state lasers, frequency conversion, material processing, and medicine. High-power edge-emitting photonic band crystal lasers emitting in the commercially important 1060 nm wavelength range are investigated. Highest to date single transverse mode output power of 1.9 W is obtained from ridge waveguide lasers with 9 μm ridge width and 2.64 mm cavity length. Extended vertical waveguides result in a very narrow vertical far-field divergence below 14° (full width at half maximum) across full single mode operating regime. The corresponding lateral beam divergence is 9°. The lasers provide excellent beam quality with beam quality factor M^2 below 1.9 up to 1.9 W output power. A brightness as high as 72 $MWcm^{-2}sr^{-1}$ is achieved. The measured astigmatism varies only from 5 μm to 14 μm over the entire operating range, which means almost astigmatism-free.

HL 94: Poster IV A (Laser; Devices; Heterostructures; Surfaces, interfaces and defects)

Presenters are kindly requested to be near their poster for at least one hour in the time between 16:00-18:00 or to leave a note about their availability for discussions.

Time: Thursday 14:00–20:00 Location: Poster B

HL 94.1 Thu 14:00 Poster B

Towards AlGaInP-based electrically-pumped VECSELs emitting in the red spectral range — •Mona Stadler, Hermann Kahle, Roman Bek, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen and Research Center SCoPE, Allmandring 3, 70569 Stuttgart, Germany

Electrically-pumped vertical external-cavity surface-emitting lasers (EP-VECSELs) combine the advantages of optically-pumped semiconductor disk lasers with an external cavity and vertical cavity surface emitting lasers (VCSELs). Comparable to optically-pumped VECSELs, they exhibit for example scalable output powers and good beam qualities. The external cavity offers the use of elements within the cavity, which is helpful for further applications. In electrically-pumped devices there is no need of special and often expensive laser pump sources. Electrical pumping facilitates higher integration and further miniaturization and is an important step towards compact laser devices. The development of EP-VECSEL is challenging because of several reasons. The design should be as easy as possible, optical losses and Joule heating in doped layers is unavoidable but should be reduced. Therefore, a good thermal management, a suitable carrier distribution and a balance between the optical and electrical requirements is necessary. We present the first steps towards an electrically-pumped AlGaInP-based VECSEL emitting in the red spectral range.

HL 94.2 Thu 14:00 Poster B

Untersuchungen der Abstrahlcharakteristik von mehrmodigen Strahlquellen — •Inga-Maria Eichentopf, Sebastian Mam-

mitzsch und Martin Reufer — Institut Naturwissenschaften, Hochschule Ruhr West, Mülheim an der Ruhr, Deutschland

Zur Analyse der Strahlqualität von Laserquellen hat sich die Wellenfrontmessung mittels Shack-Hartmann Sensoren etabliert. Abweichungen in der Resonatorgeometrie und im Modenverhalten der Laserquellen können mit hoher Auflösung anhand der Deformation der Wellenfront analysiert werden. Breitstreifenlaserbarren im nahen Infrarot basieren auf dem Materialsystems GaAs. Sie emittieren aufgrund ihrer Resonatorgeometrie eine Vielzahl optischer Moden. Die Anzahl und Ausprägung der Moden wird dabei von thermischen und elektrischen Effekten im aktiven Medium beeinflusst. Aus diesem Grund kann die Emission dieser Bauteile stark mit den Betriebsbedingungen variieren. Von besonderer Bedeutung für die Anwendungen, bei denen das Laserlicht in Glasfasern eingekoppelt wird ist es, die räumlichen Abstrahlbedingungen für einen weiten Leistungsbereich konstant zu halten, um Effizienzeinbußen durch Koppelverluste zu minimieren. In unserer Arbeit untersuchen wir den Einfluss der Betriebsbedingung auf die Emission von Halbleiterdioden. Neben der Intensitätsverteilung der Laseremission im Nahfeld wird die Winkelverteilung im Fernfeld untersucht. Weiterhin liegt ein besonderer Fokus auf der Analyse der Veränderung der Phasenfronten des Lasers. Um Rückschlüsse auf die Modenstruktur zu ziehen zu können, werden die experimentellen Messergebnisse mit den Ergebnissen einer optischen Simulationssoftware korreliert.

HL 94.3 Thu 14:00 Poster B

Sub-Monolayer-Control in Epitaxial Growth of Quantum Cascade Lasers — •Michael Kwiatek[1], Negar Hekmat[1,2], Arne Ludwig[1], Nathan Jukam[2], and Andreas D. Wieck[1] — [1]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum — [2]AG Terahertz-Spektroskopie und Technologie, Ruhr-Universität Bochum

A quantum cascade laser (QCL) consists of multiple vertically stacked semiconductor modules including several well-dimensioned quantum wells. In QCLs intersubband transitions in the conduction band generate the laser light. Due to QCL's cascading structure, one electron generates multiple photons. The production of good QCLs sets high demands on the fabricating process, especially on the layer quality of the quantum wells and barriers, why QCL fabrication is often performed with Molecular Beam Epitaxy (MBE). A known problem in MBE is the shutter transient of the effusion cells (EC). When the EC-shutter is closed, the heat of the EC is reflected back in itself. If the shutter is opened, more power is needed to stabilize the temperature and hence the material flux of the EC. For QCLs, very thin material layers of only a few monolayers with high precision are crucial. The time the EC needs to stabilize leads to a change in the growth rate for those thin layers. Our goal is the reduction of the shutter transient effect and other growth related errors on the QCL's layer structure.

HL 94.4 Thu 14:00 Poster B

Selection of longitudinal modes in quantum cascade laser via narrow-band injection seeding — Hanond Nong[1], Shovon Pal[1,2], Sergej Markmann[1], •Negar Hekmat[1], Reshma A. Mohandas[3], Paul Dean[3], Lianhe Li[3], Edmund H. Linfield[3], Giles A. Davies[3], Andreas D. Wieck[2], and Nathan Jukam[1] — [1]Arbeitsgruppe THz Spektroskopie und Technologie, Ruhr-Universität Bochum, Germany — [2]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Germany — [3]School of Electronic and Electrical Engineering, University of Leeds, U.K.

Phase seeding is a technique to lock the phase of a quantum cascade laser (QCL) to the repetition rate of a fs laser, enabling access to the time-resolved THz-field of the QCL. In typical phase seeding all longitudinal modes in the gain region of a QCL are simultaneously seeded. We injection seed a THz QCL with narrow-band THz pulses which are generated in a periodically poled lithium niobate (PPLN) crystal. A THz seed pulse with a different frequency can be generated for each of the PPLN crystal's multiple poling periods. The seed pulses' FWHM are comparable to the longitudinal mode spacing of the QCL. When the longitudinal modes overlap the narrow-band seed spectrum they are selectively enhanced while other longitudinal modes are suppressed. When the narrow-band THz seed is shifted the QCL spectral emission also shifts to a higher longitudinal mode overlapping the seed. We study the dynamics of the QCL emission as a function of a round-trip time and a seed frequency. If the seed frequency is outside the gain maxima, a shifting to the preferential mode of a QCL is observed.

HL 94.5 Thu 14:00 Poster B

DFB-Master-Oscillator-Power-Amplifier system for high precision optical sensors — •Anja Kohfeldt[1], Mandy Krüger[1], Max Schiemangk[1,2], Andreas Wicht[1,2], Götz Erbert[1], Achim Peters[1,2], and Günther Tränkle[1] — [1]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Gustav-Kirchhoff-Str. 4, 12489 Berlin, Germany — [2]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin, Germany

We have developed hybrid integrated DFB-Master-Oscillator-Power-Amplifier modules (MOPA) for portable quantum optical sensors. This application typically requires the optical frequency of the laser to be stabilized to $\delta\nu/\nu = 10^{-10}$, in some cases even down to 10^{-15}. Frequency stabilization is commonly realized by controlling (modulating) the injection current of the laser diodes. In order to enable high servo bandwidths as mentioned above, the module hosts an electrical interface for a close-to-chip RF modulation.

We will present a MOPA module designed for rubidium spectroscopy at 780 nm achieving an optical output power >1 W (cw) and an intrinsic linewidth of <50 kHz. Furthermore, we discuss the transfer functions of the system for modulation of the injection current of both the master oscillator and the power amplifier.

This work is supported by the German Space Agency DLR with funds provided by the Federal Ministry for Economic Affairs and Energy (BMWi) under the grant numbers 50WM1134 and 50WM1240.

HL 94.6 Thu 14:00 Poster B

Quantum dot microlaser under external optical feedback. — •Leon Messner[1], Elisabeth Schlottmann[1], Sören Kreinberg[1], Steffen Holzinger[1], Christian Schneider[2], Sven Höfling[2,3], Martin Kamp[2], Janik Wolters[1], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Berlin, Germany — [2]Technische Physik, Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, Würzburg, Germany — [3]Present address: SUPA, School of Physics and Astronomy, University of St Andrews, United Kingdom.

To study the transition form linear to non-linear and chaotic behavior, semiconductor lasers under self feedback are an excellent and widely investigated model system. Similar, quantum dots embedded in photonic nanocavities provide an excellent platform for investigating the border between classical laser emission and quantum optical single photon emitters. In our experiments on feedback coupled micropillar lasers with only a few quantum dots in the active layer we combine both research fields, trying to reach the transition between the classical and the quantum regime of the involved nonlinear dynamics. We setup strong feedback-coupling of quantum dot micropillars while leaving options to explore changes in feedback strength and polarization. Our observations include changes in the second order autocorrelation function and intensity of the emitted light. Our studies promise not only novel insights into the underlying physics, but depending on emitter and feedback types a multitude of applications exist e.g. in quantum information science or cryptography.

HL 94.7 Thu 14:00 Poster B

Junction FETs based on n-ZnO/p-NiO heterojunctions — •Robert Karsthof, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstraße 5, 04103 Leipzig

In this work we present junction field-effect transistors (JFETs) based on an n-ZnO channel with p-NiO as gate material. The band gaps of both semiconductors lie in the UV spectral range, thus enabling the realization of visibly-transparent devices and subsequent application in electronic circuits, e.g. for transparent displays.

Both ZnO and NiO were deposited by the pulsed laser deposition (PLD) method. We investigated the influence of the channel layer thickness on the on-voltage, current on-off ratio, and sub-threshold slope of the transfer characteristics of our devices, and we show that by decreasing the ZnO thickness from 80 to 9.2 nm, the switching behavior of the transistors can be shifted from 'normally on' to 'normally off'. The best room-temperature values for current on-off ratio and sub-threshold slope were 3×10^7 and 67 mV/dec, respectively. We also investigated the influence of temperature on the device characteristics in the range between -20°C and 150°C.

HL 94.8 Thu 14:00 Poster B

pnCCD response for hard X-ray pulses — Mohammad Shokr[1], Alaa El Ghashi[1], Ali Abboud[1], Sebastian Send[1], Robert Hartmann[2], •Lothar Strüder[2], and Ullrich Pietsch[1] — [1]) University of Siegen, Solid State Physics, Siegen, Germany — [2]PNSensor GmbH, München, Germany

Differing from other CCD concepts, pnCCD can be used as a four-dimensional detector with two spatial coordinates,one energy coordinate, and a time coordinate running with fast frame rates (1000 images/sec), high quantum efficiency, high energy resolution and low electronic noise. Because the attenuation coefficient of photoelectric absorption is high enough at low energy (below 20keV),the interaction of X-ray photons takes place entirely within the silicon bulk material. This is not the case for hard X-ray radiation where the photoelectric attenuation coefficient become very low while the contribution of Compton scattering increases and starts to be the dominant interaction process. Due to inelastic scattering an incoming photon creates a bunch of scattered electrons which themselves may initiate additional multi scattering events leading to additional features in the detector response function. In this paper we show simulations of the detector response for high energy X-ray photons. The simulated data will be compared to data taken by means of a commercial high energy x-ray source using the pnCCD detector.

HL 94.9 Thu 14:00 Poster B

Electrical characteristics of semiconductor/electrolyte junctions — •Jairo Cesar Nolasco, Oliya Sadrillaevna Abdullaeva, Manuela Schiek, and Jürgen Parisi — Energy and Semiconductor Research Laboratory, Department of Physics, Carl von Ossietzky University of Oldenburg, D-26111, Germany

Recently, organic semiconductor/electrolyte junctions have been investigated in diverse fields, such as artificial photoreceptors for retinal implants, biological sensors, and hydrogen production by organic photo electrochemical cells. The further developing of these technologies require a fundamental understanding of the electrostatic and the current-transport mechanism occurring at such junctions. Towards such understanding, here we present the electrical characteristics of the P3HT (poly-3-hexylthiophene)/electrolyte and the Squarine dye (2,4-Bis[4-(N,N-diisobutylamino)-2,6-dihydroxyphenyl)]squaraine/electrolyte system, specifically the illuminated current voltage characteristics and the illuminated capacitance voltage characteristics are studied.

HL 94.10 Thu 14:00 Poster B

Local Droplet Etching on GaAs (111)A substrates — •Julian Ritzmann[1], Rüdiger Schott[1], Nandlal Sharma[2], Dirk Reuter[1,2], Arne Ludwig[1], and Andreas D. Wieck[1] — [1]Ruhr-Universität Bochum, Universitätstraße 150, D-44780 — [2]Universität Paderborn, Warburger Straße 100, D-33098

The generation of entangled photon pairs is a key to practical quantum communications. In the case of biexcitons in Stranski-Krastanov-grown quantum dots, the fine structure splitting (FSS) of the energy levels causes the transition paths of biexciton and exciton transitions 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 quantum dots exhibit a strong distribution in size, resulting in rather broad photoluminescence 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 first results for different parameters on the LDE and LDE QD process on GaAs (111)A surfaces using atomic force microscopy and photoluminescence measurements.

[1] T. Mano et al., Appl. Phys. Express 3, 065203 (2010).
[2] Ch. Heyn et al., Appl. Phys. Lett. 94, 183113 (2009).

HL 94.11 Thu 14:00 Poster B

Photoluminescence and microstructure of porous silicon doped by gallium — •Mehrnoosh Naderi[1], Wafaa Al-khayat[2], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Germany — [2]Baghdad,Iraq

Silicon itself has been the most important and widely used variable semiconductor in silicon based optoelectronics. Crystalline silicon has an indirect band gap of 1.1 eV, which limits its application in optoelectronics while porous silicon (PSi), due to its recent discovery of visible light emission at room-temperature may open a new field combining Si integrated technology and optoelectronics. On the other hand, doping is the most widely used method in semiconductor materials to obtain the required properties. For fast optoelectronics applications, blue photoluminescence (PL) is important. However, this specific PL has been less investigated in doped-PSi materials. In this contribution, the results obtained on Ga doped n-type porous silicon is reported. The Ga doping process was carried out by physical vapour deposition. The surface morphology and microstructure was observed by scanning electron microscopy (SEM) and transmission electron microscopy (TEM). Photoluminescence measurements illustrate that the luminescence behavior of Ga-doped PSi changes strongly from the red to the blue part of the spectrum by Ga doping.

HL 94.12 Thu 14:00 Poster B

Deep level transient spectroscopy of hydrogen-generated traps in nanoporous titanium dioxide — •Laurin Schnorr[1], Mihai Cerchez[1], Thomas Heinzel[1], and Dieter Ostermann[2] — [1]Solid State Physics Laboratory (IPkM), Heinrich-Heine-Universität Düsseldorf, 40204 Düsseldorf, Germany — [2]ODB-Tec GmbH & Co. KG, Bussardweg 12, 41468 Neuss, Germany

Deep level transient spectroscopy was carried out on Pt / nanoporous TiO_2 Schottky diode hydrogen sensors to investigate whether in addition to a shallow donor level deep traps get formed during hydrogen exposure. Therefore the sensor was exposed to different doses of molecular hydrogen using a H_2 in N_2 gas mixture with hydrogen concentrations in the ppm regime to allow time resolved measurements. A defined initial state of the sensor was achieved by exposing it to dry air at hight temperatures until the current-voltage characteristics became purely diodic. The DLTS measurements revealed two hydrogen-independent deep levels at 0.4eV and 0.6eV below the bottom of the conduction band. A third level at about 0.6eV with a significantly smaller emission rate could only be observed after exposures to high doses of H_2 and was reversible by oxygen exposure, suggesting that this level is related to hydrogen atoms interacting with oxygen vacancies.

HL 94.13 Thu 14:00 Poster B

Continuous composition spread method for amorphous zinc-tin-oxide — •Sofie Bitter, Peter Schlupp, Heiko Frenzel, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für ExperimentellePhysik II, Germany

Amorphous zinc-tin-oxide (ZTO) is a close-to-ideal candidate for low cost transparent devices. It consists of naturally abundant, non-toxic materials only and can be deposited at room temperature. It was shown that electron densities as high as $10^{19}\,\mathrm{cm}^{-3}$ and mobilities as high as $10\,\mathrm{cm}^2/\mathrm{Vs}$ are possible [1]. With that ZTO is a suitable material for transparent transistors and thus for transparent electronic applications.

It is of great interest to acquire knowledge about the optimal Zn/Sn ratio in order to tune electrical and optical properties as desired. Up to now, only a few different Sn/Zn ratios were realized experimentally [2]. We present ZTO thin films deposited by pulsed laser deposition using a method of continuous composition spread (ccs) [3] and a ccs thin film produced by co-sputtering. The films were deposited on $50 \times 50\,\mathrm{mm}^2$ glass substrates. Using energy dispersive X-ray analysis the spatial dependence of the Zn/Sn ratio was mapped. Subsequently the samples were divided along the compositional gradient into stripes and their electrical and optical properties were compared. Both types of properties show a systematic dependence on the Zn/Sn ratio.

[1] Jayaraj et al. J. Vac. Sci. Technol. B, **26(2)** 2008
[2] Görrn et al. Applied Physics Letters, **91** , 193504 (2007)
[3] von Wenckstern et al. , CrystEngComm, **15**, 100 20, 2013

HL 95: Poster IV B (Quantum dots and wires: Prepration, characterization, optical properties, and transport)

Presenters are kindly requested to be near their poster for at least one hour in the time between 16:00-18:00 or to leave a note about their availability for discussions.

Time: Thursday 14:00–20:00 Location: Poster B

HL 95.1 Thu 14:00 Poster B

Nanowire junctions grown on Si substrates — •Daniil Vakulov, Torsten Rieger, Sebastian Heedt, Daniel Rosenbach, Mihail Ion Lepsa, Thomas Schäpers, and Detlev Grützmacher — Peter Grünberg Institute (PGI-9) and JARA-Fundamentals of Future Information Technology, Forschungszentrum Jülich, 52425 Jülich, Germany

Nowadays nanowire junctions are attracting much attention due to many reasons, for example the search of Majorana fermions. We present the growth, structural characteristics and room temperature transport measurements of these junctions. InAs nanowires have been grown without the use of Au catalysts on Si (100) substrates patterned with V-grooves. The V-grooves have been produced by KOH etching. The nanowires grow perpendicular to the {111} side facets of the V-grooves. When two nanowires are grown on opposing V-groove facets, they can cross, grow together and form a nanowire junction. In this case three different basic configurations of nanowire junctions are obtained: a tip-to-tip junction (L-shape), tip-to-side junction (T-shape) and a side-to-side junction (X-shape). The junctions exhibit a uniform crystal structure. They have zinc blende crystal structure while the remaining parts of the nanowires show the expected high density of stacking faults. Preliminary room temperature transport measurements demonstrate that the resistivity across the junctions is similar to the resistivity of single InAs nanowires. The results demonstrate the excellent suitability of Au-free nanowire junctions for future nanoelectronic devices.

HL 95.2 Thu 14:00 Poster B

Growth of site-controlled InAs nanowires induced by focused ion beam — •Sven Scholz, Rüdiger Schott, Arne Ludwig, and Andreas D. Wieck — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum

We have grown single localized Au seeded InAs NWs on GaAs(111)B substrate by molecular beam epitaxy, to investigate the morphology, structure and behavior of individual one-dimensional nanostructures, so called nanowires (NWs). The Au-seeds are implanted by focused ion beam (FIB) technology. Optimizing the growth process due to the growth parameter and material we were able to create monocristalline NWs with nearly no stacking faults and on the other hand control the morphology down to a region of 20 nm in diameter. Furthermore we investigate the axial and radial growth of heterostructures in our NWs, which leads to a promising approach for band gap modulation in single NWs. We studied the morphology of the NWs by SEM imaging and the crystalline structure with TEM imaging.

HL 95.3 Thu 14:00 Poster B

Focused ion beam induced growth of single GaAs nanowires on arbitrarily arranged sites — •Rüdiger Schott, Sven Scholz, Arne Ludwig und Andreas D. Wieck — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum

Semiconductor nanowires (NWs) are used as building blocks for a new generation of advanced devices intended for different applications in the field of nanoelectronics, nanophotonics and nanomechanics. NWs are near one-dimensional structures that typically have a high length-to-width ratio. This is the base of fascinating structural properties. Heterostructures of highly lattice mismatched materials can be combined without dislocations and metastable phases, unattainable in bulk materials like wurtzite GaAs, are feasible. We present focused ion beam (FIB) induced molecular beam epitaxy (MBE) grown single GaAs nanowires from site selectively deposited Au seeds. The possibility of maskless patterning makes focused ion beam lithography a powerful tool and an alternative to conventional lithography based methods in semiconductor processing. With an FIB system, equipped with an ExB filter and a liquid metal alloy ion source (LMAIS), most of the elements of the periodic table are accessible for ion implantation and patterning. Structural and optical properties of the nanowires are investigated by secondary electron microscopy, transmission electron microscopy, X-ray diffraction and photoluminescence spectroscopy.

HL 95.4 Thu 14:00 Poster B

Focused ion beam patterning of Si substrate for the growth of GaAs nanowires — •danial bahrami[1], heiko schäfer-eberwein[2], hanno küpers[3], faebian bastiman[3], lutz geelhaar[3], and ullrich pietsch[1] — [1]University of Siegen, Solid State physics, Siegen, Germany — [2]University of Siegen, Electronic and Information department, Siegen, Germany — [3]Paul Drude Institut für Festkörperelektronik, Berlin, Germany

Semiconductor nanowires (NWs) have been employed as light emitting diodes, transistors, anti-reflecting coating and other applications. For all of these applications, it is demanding to control density and position of NWs in a technically and economically efficient way. In most cases, NWs growth in Molecular Beam Epitaxy (MBE) onto silicon (111) substrates is realized onto a thin native silicon oxide throughout native openings providing a random distribution of NWs. Here we report on results of patterning the silicon substrates using a Focused Ion Beam (FIB) technique to define nucleation sites for further NWs growth. In particular, we created a 2D dot pattern of 1μm spacing. Optimum conditions for NWs growth are achieved by changing dose of the Gallium ions implantation. Implantation depth and the shape of implantation dots have been inspected by SEM and compared with the results of MBE NWs growth.

HL 95.5 Thu 14:00 Poster B

Site-controlled InAs quantum dots on pre-patterned GaAs substrates: Growth and characterizations — •Patrick Krawiec, Mohammed Usman, Johann Reithmaier, and Mohamed Benyoucef — Institute of Nanostructure Technologies and Analytics (INA), Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Germany

The selective epitaxial growth through the use of the seeded self-ordering technique leads to the formation of quantum dots (QDs) at determined nucleation sites. Here, we present the fabrication and characterization of site-controlled (SC) InAs QDs on pre-patterned GaAs substrates. The nanoholes on GaAs substrate were obtained using electron beam lithography (EBL). The growth of SCQDs was realized by solid-source molecular beam epitaxy. Highly ordered InAs QDs with periodicities ranging from 0.5 μm to 4 μm and negligible dot formation between the nanoholes are realized. Relatively narrow light emission from single SCQDs down to 150 μeV is measured by micro-photoluminescence.

HL 95.6 Thu 14:00 Poster B

Altering the luminescence properties of self-assembled quantum dots in GaAs by focused ion beam implantation — •Charlotte Rothfuchs, Markus K. Greff, Arne Ludwig, and Andreas D. Wieck — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum

In the growing field of quantum information and technology there is an increasing demand on semiconductor quantum structures. Especially single quantum dots (QD) were shown to be promising for the generation of single photons for quantum information processes [1]. Thus, there is a need for the controlled fabrication of those QDs. One approach is the combination of molecular beam epitaxy (MBE) and focused ion beam (FIB) implantation. While the former enables the growth of well-defined self-assembled quantum dots in great quantity [2], FIB implantation is on the one hand shown to be a suitable method to initialize a site-selective growth of QDs [3]. On the other hand it could be a proper method for the post-selecting of the latter. We anticipate the mechanism for eliminating QD luminescence by introducing lattice disorders in the irradiated regions. As a first approach, we present a study on the parameter space allowing the alteration of QD luminescence in GaAs by FIB implantation. Different sets of ion species, their energies and fluences are investigated by photoluminescence measurements on the QDs before and after FIB implantation.

[1] I. Robert-Philip et al., J. Lumin. 102-103, 67-71, (2003).
[2] D. Reuter et al., Physica E 40(6), 1961-1964, (2008).
[3] M. Mehta et al., Physica E 40, 2034-2036, (2008).

HL 95.7 Thu 14:00 Poster B

Cadmium Selenide / Cadmium Sulfide Core-Shell Quantum Dots in Titanium Dioxide — •Beate Horn[1], Svenja Herbertz[1], Thomas Heinzel[1], and Klaus Schierbaum[2] — [1]Solid State Physics Laboratory, Heinrich-Heine-Universität Düsseldorf — [2]Material Science Laboratory, Heinrich-Heine-Universität Düsseldorf

Cadmium selenide (CdSe) quantum dots (QD) were synthesised following procedure described by[2]. The growth of the CdS-shell is done in another chemical reaction adapting the procedure from[1]. A red shift of about 20nm in the emission and absorption spectra and the enlargement of quantum yield from 6.7% to 51.2% prove shell formation around the QD-core. The CdSe/CdS QD's were redissolved in chloroform and inserted into porous titanium dioxide[4] using mercaptopropionic acid. Frontface-fluorescence spectroscopy indicated adsorption of CdSe/CdS QD's into the titanium dioxide . A lower fluorescence signal after annihilation of the CdSe/CdS titanium dioxide samples indicates direct contact between the titanium dioxide and the CdSe/CdS QDs. Photo current measurements further prove the adsorption of the CdSe/CdS QDs'. Finally the influence of the CdSe/CdS QDs' on hydrogen sensing is investigated (and compared to [3]), using a platinum-titanium dioxide Schottky barrier with inserted CdSe/CdS QDs. Moreover the effect of electroformation was investigated. [1] Yue Y., Chem. Res. Ch. Un. 2010, 26(6), 871-875 [2] Murray C., Norris D., J. Am. Chem. Soc. 1993, 115, 8706-8715 [3] Cerchez, M. Langer, H. El Achhab, M. Heinzel, T., Appl. Phys. 103, 033522 (2013) [4] Achhab E., Erbe A., 2014, Appl. Phys. A (2014) 116:20392044

HL 95.8 Thu 14:00 Poster B

Efficient calculaltion of the Coulomb coupling elements including monopole-monopole interaction and Förster transfer between quantum dots — •Anke Zimmermann and Marten Richter — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, EW 7-1, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany

Coulomb coupled semiconductor quantum dots provide a great flexibility for controlling their optical properties. Due to the couplings between the quantum dots the individual characteristics of separated quantum dots are modified and new collective states are formed. Examples include dipole induced Förster coupling transfer and the monopole-monopole interaction.

The calculation of the Coulomb coupling involves the evaluation of a six dimensional integral of the diverging Coulomb potential. For applications in materials with different permittivity (e.g. quantum dots in a solvent) the numerical complexity can be greatly reduced by using solutions of the modified Poisson equation.

To see the effects of Coulomb coupling on single excitons and biexcitons the double quantum coherence spectroscopy is used. It allows an investigation of the coupling mechanisms and a deeper insight into the involved processes. The characteristic optical signatures of quantum dots at different position with varying orientations can be calculated, for seeing more information about the spatial arrangement.

HL 95.9 Thu 14:00 Poster B

Optical Coupling of Whispering-Gallery Modes of Two Microdisks — •Tilmann John[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 Engeneering and Applied Sciences, Harvard University, 29 Oxford Street, Cambridge, MA 02138

Coupling dynamics between optical resonators generates much interest with possible applications e.g. in quantum information processing.

Microdisk dimers supporting high-quality and small mode volume whispering gallery modes are well suited candidates for the formation of photonic molecules.

Here, we investigate the coupling of two closely spaced GaInP microdisks with an inter disk separation below 100 nm. Local laser heating is used to overcome spectral mode detuning which results from the size mismatch of the two disks. To improve the local laser heating new structures with an additional heating layer are examined allowing the tuning of the cavity dimers independent of the excitation of single quantum dots coupled to the supermode.

In addition, by using a setup for imaging the dimers, we show an attractive way to observe the optical mode profile immediatedly.

To improve the coupling of the evanescent field of the WGMs between the disks, a new approach is to deform the disks to a more rectangular shape with rounded corners. We numerically investigate this approach using the Finite-difference time-domain method.

HL 95.10 Thu 14:00 Poster B

Two-photon interference measurements on photons from quantum dots excited via a two-photon excitation scheme — •Hüseyin Vural, Eva Schöll, Sascha Kolatschek, Markus Müller, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

Indistinguishable photons are basic building blocks for quantum information processing and quantum communication. As single-photon sources, semiconductor quantum dots (QDs) are promising candidates for the generation of highly indistinguishable photons. In this work we investigate photons emitted by the biexciton state of a single InGaAs QD, which are generated via a pulsed, coherent and resonant two-photon excitation. The theory predicts the visibility of the two-photon interference to be given by the coherence time of the photons and the lifetime of the state. The measured two-photon interference of the biexciton photons provides a value of the visibility which fits the theory. Furthermore, the influence of the excitation laser pulse width on the visibility is investigated.

HL 95.11 Thu 14:00 Poster B

Single-Photon Emission of MOVPE-grown InGaAs-Quantum Dots at Telecom Wavelengths — •Katharina Zeuner, Fabian Olbrich, Jan Kettler, Matthias Paul, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Allmandring 3, 70569 Stuttgart, Deutschland

Semiconductor quantum dots (QDs) are promising candidates to be employed as single-photon sources for fiber-based communication networks. Although already established by molecular beam epitaxy (MBE), it has been challenging to achieve metal organic vapor phase epitaxy (MOVPE)-grown low-density InAs QDs with emission wavelengths suitable for widespread optical glass fibers.

In this contribution, we report on low-density MOVPE-grown InGaAs-QDs that are assembled on a GaAs substrate and on top of a 15-pair AlAs/GaAs distributed Bragg reflector (DBR). We demonstrate single-photon emission at the telecom O-band (1.3 μm). Furthermore, we investigate time-resolved and polarization-dependent photoluminescence to give an estimation of carrier lifetimes and fine-structure splittings.

HL 95.12 Thu 14:00 Poster B

Pressure-induced shift of energy levels and structural phase transition in CdSe/ZnS quantum dots — Jonas Tauch[1], •Johannes M. Braun[2], Janine Keller[1], Christopher Hinz[1], Johannes Haase[1], Denis V. Seletskiy[1], Alfred Leitenstorfer[1], and Alexej Pashkin[1,2] — [1]Department of Physics and Center for Applied Photonics, University of Konstanz, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Electronic band structure of CdSe/ZnS quantum dots under high pressures is studied using fluorescence spectroscopy. We observe a strong blue shift of about 40 meV/GPa for the emission line at 655 nm. At moderate pressures (below 3 GPa) this shift is linear and it is dominated by increase of the fundamental band gap of CdSe under pressure [1,2]. In contrast to bulk CdSe where the fluorescence is quenched above 3 GPa as a result of the phase transition into the rock-salt structure [3,4], the CdSe/ZnS quantum dots remain structurally stable up to 6.5 GPa. This structural robustness together with the high fluorescence yield and the large pressure-induced line shift, exceeding that of bulk ruby crystals by a factor of 40, make CdSe quantum dots a promising candidate for precise pressure calibration at moderate pressures.

[1] W. Shan et al., Appl. Phys. Lett. **84**, 67 (2004).
[2] B. S. Kim et al., J. Appl. Phys. **89**, 8127 (2001).
[3] S. H. Tolbert and A. P. Alivisatos, J. Chem. Phys. **102**, 4642 (1995).
[4] S. H. Tolbert and A. P. Alivisatos, Science **265**, 373 (1994).

HL 95.13 Thu 14:00 Poster B

The role of band mixing for excitons and biexcitons in semiconductor quantum dots — •Matthias Holtkemper, Doris E. Reiter, and Tilmann Kuhn — Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

A detailed understanding of the electronic structure in semiconductor

quantum dots (QD) is a prerequisite to model dynamical processes in QDs relevant for quantum information processing. We analyse the structure of excitons and biexcitons by studying theoretically the influence of different coupling mechanisms. To be specific, we model the QD using a harmonic confining potential and consider valence band mixing using a four band Luttinger theory, direct Coulomb interaction as well as long- and short-range Coulomb exchange interaction. We discuss the dependence of specific coupling mechanisms on the QD size and shape. We find a different scaling of Luttinger and Coulomb couplings depending on the QD size, while varying the QD shape leads to jumps in Coulomb exchange couplings. Furthermore we extend our studies to a QD doped with a single Mn, where a six line signature on the lowest absorption line appears. The calculated spectrum shows additional features due to the consideration of Luttinger couplings which are in good agreement with experimental findings.

HL 95.14 Thu 14:00 Poster B

Temperature-dependent quantum optical properties of In(Ga)As quantum dots with emission wavelength above 1μm — •Fabian Olbrich, Katharina Zeuner, Jan Kettler, Matthias Paul, Michael Jetter, and Peter Michler — Universität Stuttgart, Institut für Halbleiteroptik und Funktionelle Grenzflächen (IHFG), Allmandring 3, 70569 Stuttgart

Promising single photon sources for the realization of fiber-based quantum communication networks are provided by semiconductor quantum dots (QDs). For this purpose QDs with emission wavelengths above 1 μm, in this case targeting the telecom O-band (1,3 μm), would provide the advantage of minimal absorption and dispersion of the transmitted signal.

Furthermore for the implementation of these QDs, an operation at higher temperatures is desirable, because of the reduced amount of required cooling and simpler handling.

In this work we study (quantum) optical properties of long-wavelength In(Ga)As-QDs at elevated temperatures such as the spectral behaviour, e.g. spectral broadening or the addressability of a single QD, the single photon emission via cw autocorrelation measurements and time-correlated photon counting measurements to gather information about decay times and refilling effects.

HL 95.15 Thu 14:00 Poster B

Ultrafast Dual Color Transient Absorption Spectroscopy with synchronized GHz-Oscillators — •Christian Dicken[1], Alexander Neufeld[1], Christian Wolpert[2], and Markus Lippitz[1] — [1]Experimental Physics III, University of Bayreuth, Germany — [2]Solid State Spectroscopy Group, Kyoto University, Japan

Nanooptics heads towards coherently coupled single emitters as ingredients in numerous applications. Knowledge of the coherent properties and optical control of the quantum state of the emitters are crucial points in designing such systems.

We demonstrated[1] recently that it is possible to detect, analyze and control a single semiconductor quantum dot in an optical far-field experiment, utilizing spectrally resolved transient absorption spectroscopy and coherent manipulation of the quantum dot state.

As a next step, we present an approach to increase the signal-to-noise ratio by an order of magnitude by switching to a fs-Ti:Sapphire oscillator with GHz repetition rate and acquisition of spectroscopic data with frame rates up to 126 kHz.

[1] *C. Wolpert et al, Nano Lett., 2012, 12 (1), pp 453-457.*

HL 95.16 Thu 14:00 Poster B

Inspection of Relaxation by Coherent Spectroscopy and Nanoplasmonics — •Markus Krecik, Mario Schoth, Sven M. Hein, and Marten Richter — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany

Coherent multidimensional spectroscopy allows for analysis of exciton-phonon relaxation. Nanoplasmonics allows to dynamically induce gradient fields, which relax dipole selection rules.

Through the combination of coherent spectroscopy and nanoplasmonics, we provide a way for studying relaxation between dipole-forbidden and dipole-allowed states: A quantum emitter is placed in a plasmonic structure, an excitation pulse controls electric field gradients and thus excitation of dipole-forbidden states. Multidimensional spectroscopy with an appropriate choice of gradient and non-gradient pulses gives us enhanced control over the relaxation process.

The possibilities are illustrated on a CdSe quantum dot using photoelectron-emission detection.

HL 95.17 Thu 14:00 Poster B

GaAs/GaP Quantenpunkt-LEDs — •Christian Golz — Humboldt-Universität zu Berlin, Berlin, Germany

Im Rahmen der hier vorzustellenden Arbeit wird die Optimierung der Prozessierung von Leuchtdioden basierend auf GaAs Quantenpunkten eingebettet in einer GaP-Matrix präsentiert. Die hier verwendeten Proben wurden mittels Gasquellen-Molekularstrahlepitaxie hergestellt. Die ausreichende Gitterfehlanpassung von 3,6% zwischen GaAs und GaP ermöglicht die selbstorganisierte Bildung von Quantenpunkten im Stranski-Krastanow-Wachstumsmodus auf GaP. Die GaAs/GaP Quantenpunkte sind in einen p-n-Übergang eingebettet und zeigen optische Emission zwischen 1,8 und 2 eV. Untersucht wurden dabei insbesondere die Mikrostrukturierung und Kontaktierung der Probe zur Optimierung der Elektrolumineszenzausbeute. Mit Photolithographie- und Ätzschritten wurden dabei der Halbleiter und auch die Kontakte nach einem für diese Proben entworfenen Muster strukturiert. Auch die Optimierung der Kontaktierung durch Metallaufdampfen und Annealing der Proben wurde untersucht.

HL 95.18 Thu 14:00 Poster B

Theory of a QD-phonon laser — •Leon Droenner and Julia Kabuss — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Berlin, Germany

The research area of nanophononics involves the investigation and manufactoring of phononic devices such as acoustic cavities, designed to confine a single acoustic phonon mode. These solid state based phonon cavities form the basis for different applications, such as the phonon laser or imaging.

External optical manipulation of the harmonic oszillator mode of the acoustic cavity can result in optical cooling or vibrational amplification. The proposed phonon laser is realized as a a two-level quantum dot-acoustic cavity-system, which is optically driven by a frequency detuned laser at the anti-Stokes resonance. This leads to a effective stimulated phonon emission based on the induced Raman-process.

Our study is focused on the generalisation of the one-quantum dot limes to an N-emitter system which can be reduced to an intuitive analytical treatment.

HL 95.19 Thu 14:00 Poster B

Metal-enhanced luminescence of CdSe and Au nanoparticles in colloidal solution — •Evelyn Röder, Nils Rosemann, Beatriz Pelaz, Wolfgang J. Parak, Sangam Chatterjee, and Nadeem Sabir — Faculty of Physics and Materials Science Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany

Cadmium selenide semiconductor nanoparticles (SNP) show a strong photoluminescence (PL) that can be tuned either by doping or changing the structure of the SNP [1]. Their emission is further enhanced by plasmonic effects in the vicinity of metals [2,3]. We investigate the origin of this interaction by studying a series of CdSe-SNPs mixed with Au-based metallic nanoparticles (MNP) in solution with varying concentration ratio of SNP and MNP by UV/VIS absorption and time-resolved photoluminescence (PL) spectroscopy. We find a non-linear dependence of the PL intensity on the concentration ratio along with a photon-energy-dependent quenching of the absorption.

[1] Gaponik et al., 2010, 2010, 6, 1364-1378
[2] Kulakovich et al., 2002, Nanoletters Vol.2, No. 12 1449-1452
[3] Okamoto et al., 2006, J. Opt. Soc. Am. B/Vol. 23, No. 8

HL 95.20 Thu 14:00 Poster B

Single-photon emission from a partly stimulated two-photon emission in semiconductor quantum dots — •Dominik Breddermann, Dirk Heinze, Artur Zrenner, and Stefan Schumacher — Physics Department and Center for Optoelectronics and Photonics Paderborn (CeOPP), University of Paderborn, Warburger Strasse 100, 33098 Paderborn, Germany

In the context of designing efficient single-photon sources, semiconductor quantum dots are widely studied. Besides the established cascaded biexciton-exciton emission - underlying most of the recent studies -, also a direct two-photon transition from the biexciton to the ground state is optically allowed. We show that this higher-order transition is a promising alternative starting point to realize a single-photon source. In our scheme, an external laser field excites the system into a virtual intermediate state located in the band gap. As the quantum dot relaxes to its electronic ground state via this virtual state, a single photon is spontaneously emitted (here into a cavity mode). The properties of the single photon can be controlled all-optically by the classical laser field

enabling the emission. In this contribution we introduce the scheme and focus on the calculation of photon correlation functions and investigate the spectral properties of the single photon emission.

HL 95.21 Thu 14:00 Poster B

Time-resolved photoluminescence of silicon nanoparticles — •Robert Niemöller, Daniel Braam, Günther M. Prinz, Martin P. Geller, and Axel Lorke — Experimentalphysik und CENIDE, Universität Duisburg-Essen

Bulk silicon is a poor light emitter, due to its indirect band-gap, hindering optical device integration into today's CMOS technology. Silicon nanoparticles could overcome this problem, as they exhibit bright luminescence and high quantum yield.

The time-resolved photoluminescence (PL) of silicon nanoparticles with different functionalisations such as fluor or dodecene is studied using micro-photoluminescence. We performed PL-measurements at low temperatures to determine the line width of single nanoparticles, which was found to be in the range of several millielectron volts. In time resolved measurements on particle ensembles, this enables us to address a sub-set with a specific diameter by taking into account only a small spectral range of the inhomogeneously broadened Pl spectrum.

We present data of such sub-sets of particles for different laser excitation powers and temperatures and find PL decay characteristics, which can be fitted by bi-exponential or stretched exponential functions. We observe decay-times of up to 300 μs, decreasing below 50 μs for increasing PL energy, an effect, which we attribute to an increasing quantum confinement for smaller nanoparticles. This shows the high technological potential of silicon nanoparticles as their lifetime can be controlled by size.

HL 95.22 Thu 14:00 Poster B

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.

To fully understand and control these processes one has to understand the electronic structure of the coupled systems as well as the excitation dynamics within these systems. We investigate single particle eigenenergies and eigenstates by means of k·p-theory with the nextnano^3 software package [4]. Results from these calculations are then used as input paramters for Heisenberg equations of motion for a reduced density operator.

[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 95.23 Thu 14:00 Poster B

Spin switching in Mn-doped quantum dots using detuned and chirped laser pulses — •Sebastian Lüker[1], Doris E. Reiter[1,2], Vollrath Martin Axt[3], and Tilmann Kuhn[1] — [1]Institut für Festkörpertheorie, WWU Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [2]Blackett Laboratory, Imperial College, London, UK — [3]Theoretische Physik III, Universität Bayreuth

When a manganese (Mn) ion is doped into a CdTe quantum dot (QD), the photoluminescence spectrum shows six lines corresponding to the six Mn spin states. This is caused by the exchange interaction which couples the Mn spin to the spin of the exciton in the QD. This coupling enables the control of the Mn spin via the optical manipulation of the exciton. For excitation with circularly polarized laser pulses, the complete system can be reduced to a bunch of three level systems, consisting of the ground state with Mn spin in a given orientation, the bright exciton state with unchanged Mn spin, and the dark exciton state with flipped Mn spin.

We present a theoretical analysis of two different switching protocols for the Mn spin. The first one uses an ultrashort resonant laser pulse which excites the exciton. By applying a second pulse, which is detuned from the exciton transition energy, the relevant states are shifted into resonance, resulting in an occupation transfer between the Mn spin states. An alternative switching protocol uses chirped, i.e., frequency modulated laser pulses. In this case, one pulse is sufficient to manipulate the Mn spin. During the pulse, the state of the system is driven adiabatically into the desired Mn spin state.

HL 95.24 Thu 14:00 Poster B

Computational analysis of CdSe and PbS quantum dot structures — •Farzana Aslam and Christian von Ferber — Coventry University, UK

We analyse small structures of potential quantum dot material applying computational time dependent density functional techniques. In particular we focus on the optical properties of these dots observing the effects of clustersize, cluster composition, capping ligands and complexation.

HL 95.25 Thu 14:00 Poster B

Electrical properties of free-standing GaAs nanowires by multi-tip scanning probe microscopy — •Ilio Miccoli[1,2], Frederik Edler[1], Nico Lovergine[2], Paola Prete[3], Christoph Tegenkamp[1], and Herbert Pfnür[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, DE — [2]Dept. Innovation Engineering, Salento University, IT — [3]IMM-CNR, Lecce, IT

Free-standing III-V nanowires (NWs) represent the forefront of materials science, and it is expected they will impact several technological fields, ranging from nanoelectronics to nano-photonics. Huge progress has been made in the vapour-liquid-solid growth by MOVPE technology of III-V NWs. However, further efforts are needed for the precise control of their electrical properties, especially in terms of dopant concentration and distribution profiles. Even more critical, the NW current-voltage (I-V) analysis usually requires the multi-step and time-consuming EBL/FIB-assisted fabrication of NW-based FET devices, which often alter the genuine NW transport properties. Recently, single-tip scanning tunnelling microscope (STM) has proven to be a versatile tool for the structural and electrical characterization of free-standing NWs, although the I-V characteristic is often dominated by the metal-catalyst/NW Schottky interface. Here, we show that the use of a multi-probe STM allows for the rapid sub-nanometric placement of three probe tips on free-standing n-/p-doped GaAs NWs. The NW transport properties are studied as function of NW diameter and along the NW lateral facet, and finally correlated with growth conditions.

HL 95.26 Thu 14:00 Poster B

Resonant tunneling current through energy levels of strain induced quantum dots — •Daming Zhou, Andreas Beckel, Martin Geller, and Axel Lorke — Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany

Strain-induced quantum dots (SIQD) confine electrons and holes to a lateral potential minimum within a nearby quantum well (QW) layer. The potential minimum can be introduced by a self-assembled quantum dot layer. SIQD have a much weaker confining potential than the self-assembled quantum dots. Their discrete energy levels have been demonstrated by optical measurements previously.

In this experiment, we pattern a two-dimensional electron gas with adjacent quantum dots into a field-effect transistor structure, in which a pair of metal split gates define the conduction channel in the QW layer. We observe a group of resonant current peaks when the free electrons in the constriction are depleted completely by application of deep negative voltage. Firstly, we can determine the SIQD space locations between the slit, by scanning the active area from one side to another using an antisymmetric bias contribution applied to the sides of the split gates. Furthermore, by varying the symmetric gate voltage contribution we can align the energy levels in the SIQD with the Fermi energy to allow transport through the SIQD. This way, we can study not only how one resonant energy level follows the two side gates, but also, from the energy level space, it is possible to learn about the Coulomb blockade effect of electrons inside the dot.

HL 95.27 Thu 14:00 Poster B

Determination of the inelastic diffusion length in GaAs/AlGaAs heterostructures by hot electron thermopower — •Oliver Kreiter[1], Ulrich Wieser[1], Arne Ludwig[2], Andreas Dirk Wieck[2], and Ulrich Kunze[1] — [1]Lehrstuhl für Werkstoffe und Nanoelektronik, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Precise determination of material parameters such as the charge carrier scattering length gain a growing interest in theoretical modelling of nanostructures for reliably predicting the appropriate device characteristics. On GaAs/AlGaAs (electron density $n = 3.04 \cdot 10^{11}\mathrm{cm}^{-2}$, mobility $\mu = 7.70 \cdot 10^5\mathrm{cm}^2(\mathrm{Vs})^{-1}$ at 4.2 K), we measured hot-electron thermopower (HETP) in quantum point contacts (QPCs). The sample consists of a symmetric cross junction of 600 nm wide channels, one supplied by a heating current and the other equipped with a series of split-gate contacts forming QPCs at distances ranging from 625 nm to several microns. We recorded the HETP signal at fixed heating current while one of the QPCs is tuned from positive gate voltages into pinch-off and all the others are kept open. At $T = 4.2$ K apart from quantum oscillations reflecting the QPC subband structure the HETP signal exhibits a maximum close to the threshold voltage. From the exponential decay of this maximum as a function of distance we extract the inelastic diffusion length. At temperatures above 10 K this length rapidly decreases due to lattice vibrations.

HL 95.28 Thu 14:00 Poster B

Signal addition in a dual-stage ballistic rectifier — •Joeren von Pock[1], Sandra Rudnik[1], Ulrich Wieser[1], Thomas Hackbarth[2], and Ulrich Kunze[1] — [1]Lehrstuhl für Werkstoffe und Nanoelektronik, Ruhr-Universität Bochum, D-44780 Bochum — [2]DaimlerChrysler Forschungszentrum Ulm, D-89081 Ulm

We investigate a ballistic rectifier consisting of 220 nm wide channels on a high mobility Si/SiGe heterostructure ($\mu_{2\mathrm{D}} = 18.3\ \mathrm{m}^2\mathrm{V}^{-1}\mathrm{s}^{-1}$, $n_{2\mathrm{D}} = 6.3 \cdot 10^{15}\ \mathrm{m}^{-2}$ at 1.4 K). The rectifier geometry is formed by a straight voltage stem with contacts U and L and two pairs of injector branches (contacts 1-2 and 3-4) inclined with respect to the stem by 45°. A Pd gate electrode covers the whole structure. At $T = 4.2$ K, under gate voltages $V_\mathrm{G} \geq 0.3$ V solely ballistic transport determines the output voltage [1]. Each of the rectifier stages nearly exhibit a parabolic characteristic, i.e. $V_{\mathrm{UL},ij} = (\alpha_{ij} \cdot I_{ij})^2$, where ij refers to the contacts 12 or 34, respectively, and $\alpha_{12} \approx \alpha_{34}$ represents the individual rectifier sensitivities. If the injector pairs are separated by at least 450 nm the individual output voltages add up, $V_{\mathrm{UL,tot}} = V_{\mathrm{UL},12} + V_{\mathrm{UL},34}$. At smaller separation $V_{\mathrm{UL,tot}}$ exceeds the sum by up to 80%. We interpret this synergy gain by a gradual transition from voltage to current addition. Pure current addition should occur if both injector pairs are connected to the stem at the same position leading to $V_{\mathrm{UL,tot}} = (\alpha_{12} \cdot I_{12} + \alpha_{34} \cdot I_{34})^2$, which is twice that of pure voltage addition.

[1] D. Salloch *et al.*, Appl. Phys. Lett. **94**, 203503 (2009).

HL 95.29 Thu 14:00 Poster B

Capacitance-Voltage Spectroscopy of InAs Quantum Dots Under External Applied Strain — •Sascha R. Valentin[1], Arne Ludwig[1], Dirk Reuter[2], and Andreas D. Wieck[1] — [1]Angewandte Festkörperphysik, Ruhr-Universität-Bochum — [2]Optoelektronische Materialien und Bauelemente, Universität Paderborn

Self-assembled InAs quantumdots (QDs) are integrated in a variety of interesting optical and electronical devices and are also highly interesting from a fundamental point of view. Electric fields are often used to tune the optical and electronical properties of QDs. Recently it has been shown that external applied strain can reversibly shift the optical emission energy of QDs. Theoretical calculations indicate that the shift in the emission energy originates in the changed coulomb interaction between the charge carriers as well as in the shift of the energy levels themselves. In this project we want to measure the dependence of the interaction energies of the carriers on externally applied strain using capacitance voltage (CV) spectroscopy. In the device we present, a thin electrically contacted CV-membrane is bonded to a PMNPT-piezoelectric actuator. This allows to apply strain to the QDs and at the same time it enables electrical measurements on a QD ensemble.

HL 95.30 Thu 14:00 Poster B

Narrow-gap semiconductor nanstructures in the quantum Hall regime — •Olivio Chiatti[1], Chistian Riha[1], Johannes Boy[1], Christian Heyn[2], Wolfgang Hansen[2], and Saskia F. Fischer[1] — [1]Neue Materialien, Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Institut für Angewandte Physik, Universität Hamburg, 20148 Hamburg, Germany

One of the most prominent phenomena in modern solid state physics is the quantum Hall effect (QHE). The quantum Hall edge channels (QHECs) are central to our understanding of the underlying physics of the QHE. Most research has been directed at GaAs/AlGaAs heterostructure systems, but there has been little work directed at understanding the role of spin-orbit interaction (SOI) in this phenomenon. We have combined quantum point contacts (QPCs) with in-plane gates and Hall-bars in a narrow-gap semiconductor heterostructure with strong SOI. The constriction was fabricated by micro-laser photolithography and wet-chemical etching from an InGaAs/InAlAs quantum well with an InAs-inserted channel [1]. The two-dimensional electron gas (2DEG) is at about 53 nm depth and has a carrier density of about $3 \cdot 10^{11}\ \mathrm{cm}^{-2}$ and mobility of about $7.5 \cdot 10^4\ \mathrm{cm}^2/\mathrm{Vs}$, in the dark. We have performed transport measurements of the combined QPC and Hall-bar structures in magnetic fields perpendicular to the 2DEG. We observe conductance quantization through the QPC when QHECs are formed. We discuss the transmission and reflection of QHECs as a function of symmetric and asymmetric in-plane gate voltages.

[1] Chiatti *et al.*, arXiv:1410.8588v2 [cond-mat.mes-hall] (2014).

HL 95.31 Thu 14:00 Poster B

Controlling ballistic heat conduction in a four-terminal nanoring — Christoph Kreisbeck[1], •Tobias Kramer[1,2], Christian Riha[1], Olivio Chiatti[1], Sven S. Buchholz[1], Andreas D. Wieck[3], Dirk Reuter[3,4], and Saskia F. Fischer[1] — [1]Neue Materialien, Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Mads-Clausen Institute, University of Southern Denmark, 6400 Sonderborg, Denmark — [3]Angewandte Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany — [4]Optoelektronische Materialien und Bauelemente, Universität Paderborn, 33098 Paderborn, Germany

The transport in a one-dimensional (1D) waveguide is dominated by the wave-like character of electrons. In simple ballistic 1D waveguides electric and thermal conductance are quantized and follow the Wiedemann-Franz law. The question is how the mode-dependent heat transfer evolves in networks of extended 1D waveguides, such as Aharonov-Bohm rings.

We show experimental data and theoretical calculations for ballistic heat transfer in a four-terminal nanodevice. By applying a gate voltage, the heat flux is distributed to different leads according to the scattering states at the wire junctions. The theoretical analysis relies on a computationally efficient wavepacket technique to model the flux through the device over a large transport window. At finite temperatures and Fermi energies we identify a strong ballistic component of the electric and heat currents, which opens the prospects to actively control the heat flux close to the quantum threshold.

HL 96: Poster III C (III-V Semiconductors incl. Nitrides)

Presenters are kindly requested to be near their poster for at least one hour in the time between 16:00-18:00 or to leave a note about their availability for discussions.

Time: Thursday 14:00–20:00 Location: Poster B

HL 96.1 Thu 14:00 Poster B

Use of In-Plane-Gate transistors for sensing of dielectrics — •Benjamin Gerd Feldern, Arne Ludwig, and Andreas Dirk Wieck — Angewandte Festkörperphysik, Ruhr Universität Bochum, Germany

The Idea of this work is to examine the ability of In-Plane Gate field effect transistors (IPG-FET)[1] based on GaAs/$Al_xGa_{1-x}As$ to sense dielectrics and to determine the dielectric function from the measurements. The work is motivated by the observation that organic IPG-FETs were shown to be able of sensing different organic molecules[2]. The change of the transconductance on presence of dielectrics is supposed from the shielding of the electric field between gate and source contact. This is assumed from polarization of the molecules due to the electric field. Additionally, an ac-gate-source field might be able to excite resonant modes of the molecule, thus leading to additional polarization. The measurements shown address the question of effect of an ac-gate voltage in the kHz region.

[1] J. Nieder, A D. Wieck, P. Grambow, H. Lage, D. Heitmann, K. v. Klitzing, and K. Ploog, "One-dimensional lateral field-effect transistor with trench gate-channel insulation", Appl. Phys. Lett . **57**, 2695 (1990). [2] J. Kettle, S. Whitelegg, A.M. Song, D.C. Wedge, L. Kotacka, V. Kolarik, M.B. Madec, S.G. Yeates, and M.L. Turner; Nanotechnology **21** 075301 (2010).

HL 96.2 Thu 14:00 Poster B

Fabrication of nanopattern arrays of gold dots for nanowire arrays on GaP substrates by electron-beam lithography — •Emad H. Hussein[1,2], Vanesa Hortelano[1], M. P. Semtsiv[1], and W. T. Masselink[1] — [1]Institut für Physik, Humboldt Universtät zu Berlin, Newtonstrasse 15, 12489 Berlin, Germany — [2]Department of Physics, college of Science, Al-Mustansiriyah University, Iraq

Fabrication of high-density and uniformly distributed gold dots on GaP (100) substrates using electron-beam lithography (EBL) was carried out. A positive EBL resist of PMMA (polymethyl methacrylate -600k) with a nominal thickness about 300 nm was spun onto the substrate and immediately baked on a hotplate at 160 $^{\circ}C$ for 3 min. The pattern on the PMMA resist was written using a Raith nanolithography system connected to a JEOL JSM- 6360 scanning electron-microscopy. Arrays of 100 × 100 μm^2 including holes patterns have been printed on the resist. We optimized the electron beam acceleration voltage to less than 15 kV and exposure doses between 150 and 220 $\mu c/cm^2$ that are needed to generate a high-contrast pattern. A gold layer with thickness of 35 nm was evaporated onto the produced pattern and lifted off. The resulting nanopattern of gold dots with diameter about 130 nm and density of 3 × 10^7 cm^{-2} has been fabricated on the substrates. These patterns are used either to directly etch nano-columns in the GaP substrate or as etch masks for initiating organized arrays of GaP nanowires grown by gas-source molecular-beam epitaxy. Results of the pattering and of resulting nanowires will be discussed.

HL 96.3 Thu 14:00 Poster B

Rabi Oscillations of Photon Echo in (In,Ga)As Quantum Dots — •Matthias Salewski[1], Lukas Langer[1], Sergey V. Poltavtsev[1,2], Irina A. Yugova[1,2], Dimitri R. Yakovlev[1,3], Christian Schneider[4], Martin Kamp[4], Ilya A. Akimov[1,3], and Manfred Bayer[1,3] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Spin Optics Laboratory, St. Petersburg State University, 198504 St. Petersburg, Russia — [3]A.F. Ioffe Physical-Technical Institute, 194021 St. Petersburg, Russia — [4]Technische Physik, Universität Würzburg, 97074 Würzburg, Germany

We perform four-wave-mixing spectroscopy on an ensemble of inhomogeneously broadened (In,Ga)As quantum dots which are embedded into a cavity with low quality factor Q∼200. Enhancement of light-matter interaction in studied structures allows us to observe strong photon echo (PE) signals.

In our experiments we studied the dependence of the PE amplitude on the pulse area of ps-laser pulses for different polarization configurations. The oscillatory behavior of the PE amplitude as function of the first and second pulse areas is attributed to Rabi oscillations. We observe different envelopes for oscillations in various polarization configurations which is explained due to different contributions of exciton and trion sub-ensembles.

HL 96.4 Thu 14:00 Poster B

Optical properties of Bi-containing nanostructures on GaAs — •Julian Veletas, Nils Rosemann, Lukas Nattermann, Kerstin Volz, and Sangam Chatterjee — Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany

Incorporating bismuth (Bi) into well studied GaAs-based devices leads to a promising way of tuning the band gap to telecom wavelength. Because of the large covalent radius of Bi the incorporation into the GaAs lattice is hindered and it tends to form nanoscaled structures at the substrate surface. Due to their metallic character these structures show interesting properties e.g., strong plasmonic effects. To investigate those nanostructures, we studied a series of Bi-containing nanostructures grown on GaAs substrates using photo modulated reflection spectroscopy.

HL 96.5 Thu 14:00 Poster B

Increase of efficiency of photoelectric transformers of solar concentrated energy on the basis of III-V semiconductor compounds — •Ia Trapaidze[1], Rafael Chikovani[1], Gela Goderdzishvili[1], Temur Khachidze[1], and Lia Trapaidze[2] — [1]Dep. of Physics, Georgian Technical University, 77 Kostava, 0175 Tbilisi, Georgia — [2]Dep. of Physics, Tbilisi State University, 3 Chavchavadze Ave., 0179 Tbilisi, Georgia

Georgia, as the Southern country is rich of solar energy. It is located in the Sun's belt. Using of solar energy for receiving the electrical and thermal energies is very important for Georgia. To increase the efficiency of using of solar element there are used the concentrators of optical radiation. They provide with concentration of incident beam energy on a wide area (on the surface of a concentrator) on relatively small area of a semiconductor crystal, which increases the power of electronic energy generated (labored out) by the photocell. And this means the increase of efficiency of using of the solar cells.

For the purpose to make more effective the removal of heat from the photocells, we consider it expedient to develop a new system for using to heat relieved from the photocell for heating the water.

HL 96.6 Thu 14:00 Poster B

Optical properties of GaN and InGaN/GaN microrods — •Christian Tessarek[1], George Sarau[1], Martin Heilmann[1], Robert Röder[2], Carsten Ronning[2], and Silke Christiansen[1,3] — [1]Max-Planck-Institut für die Physik des Lichts, Erlangen — [2]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena — [3]Helmholtz Zentrum Berlin für Materialien und Energie

Self-assembled GaN microrods on sapphire substrates have been grown by metal-organic vapor phase epitaxy. The smooth and straight sidewall facets and the regular hexagonal shape of the rods facilitate the use as microresonators. Respective whispering gallery modes (WGMs) can be observed in cathodo- (CL) and photoluminescence (PL) investigations [1].

A route towards an improvement of the optical activity in the GaN near band edge emission range will be discussed. Excitation density dependent PL investigations will show lasing activity in these microrods between 365 and 380 nm [2].

Finally, optical properties of GaN microrods covered with InGaN quantum wells (QWs) will be presented. An emission wavelength gradient along the microrod can be observed in spatially resolved CL measurements. The InGaN emission in the range between 400 and 500 nm is in superposition with WGMs having quality factors up to 1200.

[1] C. Tessarek et al., Opt. Express **21**, 2733 (2013).
[2] C. Tessarek et al., ACS Photonics **1**, 990 (2014).

HL 96.7 Thu 14:00 Poster B

Oxygen and hydrogen profiles and electrical properties of unintentionally doped n-GaN grown by HVPE — •Valentin Garbe[1,2], Barbara Abendroth[1], Hartmut Stöcker[1], Arkadi Gavrilov[2], Doron Cohen-Elias[2], Shlomo Mehari[2], Dan Ritter[2], and Dirk C. Meyer[1] — [1]Institute for Experimental Physics, TU Bergakademie Freiberg, Leipziger Str. 23, 09599 Freiberg, Germany — [2]Department of Electrical Engineering, Technion, Israel Institute of Technology, Haifa 32000, Israel

During hydride vapor phase epitaxy (HVPE) growth of GaN, oxygen and hydrogen are easily incorporated. Oxygen is an n-type dopant, while hydrogen may passivate some of the donors. In this work, we attempt to characterize commercially available 5 μm thick HVPE grown (0001) GaN (deposited on sapphire), which is unintentionally n-doped. On the basis of secondary ion mass spectrometry profiles provided by the manufacturer Kyma Inc., electrical (capacitance–voltage, Hall), structural (high resolution X-ray diffraction) and optical (polarized infrared spectroscopy) methods were utilized to derive a GaN layer model of the wafer, including doping profile and mobility. The model contains two different layers, a smooth GaN surface layer which exhibits lower carrier concentration but higher mobility, while a bottom layer shows higher background carrier concentration and lower mobility, because of high impurity incorporation. Oxygen seems to be the donor, substitutionally filling the positions of nitrogen vacancies, leading to the overall n-doping. Surprisingly, the effect of hydrogen passivation seems to play no role here.

HL 96.8 Thu 14:00 Poster B

Optical investigations on the effect of hydrogen on the internal quantum efficiency of GaInN LED structures — •Silke Wolter, Fedor Alexej Ketzer, Heiko Bremers, Torsten Langer, Uwe Rossow, and Andreas Hangleiter — Institut für Angewandte Physik, Technische Universität Braunschweig

GaInN based light emitting diodes being grown via low pressure MOVPE are investigated regarding the impact of hydrogen from the buffer layer on the active zone. So far hydrogen is used as carrier gas during the growth of the buffer layer. Therefore it is present in the reactor as also in the structure and may influence recombination of carriers and the efficiency of the LED in several ways. Hydrogen is known to influence incorporation as well as electrical activity of defects in GaN.
We compare structures having different surroundings of the quantum well with additional use of hydrogen and silane fluxes during the growth for raising the hydrogen content within the n-GaN buffer layer. The comparison is based on excitation power and temperature dependent photoluminescence (PL) spectroscopy. From the data we determine the internal quantum efficiency and compare it with time-resolved PL measurements to understand the influence of hydrogen on radiative and nonradiative recombination. Our results show that the growth of the layers close to the quantum well highly affects the efficiency of the LED. While low temperature PL shows high intensity, room temperature efficiency is decreased which may be attributed to a change in the density of background carriers.

HL 96.9 Thu 14:00 Poster B

In-situ UHV cathodoluminescence of MQW samples grown by MBE and MOVPE — •Kim Sandra Degener, Christopher Hein, Andreas Kraus, Heiko Bremers, Uwe Rossow, and Andreas Hangleiter — Institute of Applied Physics, TU Braunschweig, Germany

A special point of interest concerning the characterization of group-III-nitride heterostructures are their luminescence properties. Therefore in situ techniques are desired to analyze the optical quality and structure of group-III-nitride quantum films, in particular piezoelectric characteristics of samples without accumulated surface charge. Our experimental setup consists of a RIBER 32P MBE machine equipped with a STAIB instruments RHEED gun which we use as the excitation source for cathodoluminescence studies. The luminescence of the samples is then collected by an optical fibre cable positioned outside the chamber, sent into a Spex double spectrometer and measured by a photodiode. We compare the luminescence properties of MBE and MOVPE grown samples. MBE grown samples enable us to measure the luminescence properties of samples which have never been exposed to air. During air exposure an adsorption or oxide layer develops on the samples. The influence of such a layer on optical properties can be investigated by removing it in UHV conditions via heating combined with in-situ CL measurements.

HL 96.10 Thu 14:00 Poster B

Effects of rapid thermal annealing on the disorder and composition of Ga(N,As,P) quantum wells on silicon for laser application — •Sebastian Gies, Sarah Karrenberg, Martin Zimprich, Tatjana Wegele, Andreas Beyer, Wolfgang Stolz, Kerstin Volz, and Wolfram Heimbrodt — Faculty of Physics and Material Science Center, Philipps University Marburg, D-35032 Marburg, Germany

Realizing suitable light sources for optical data transmission on silicon is one of the major goals of optoelectronic integration nowadays. The quaternary Ga(N,As,P) is a promising candidate for this. Here, we present an analysis of the annealing effects on Ga(N,As,P) quantum wells (QWs) on silicon using PL, PL excitation and raman spectroscopy as well as transmission electron microscopy (TEM). The growth was performed using metal-organic vapor-phase epitaxy. After growth the samples underwent rapid thermal annealing for ten seconds at annealing temperatures between 800 °C and 1000 °C. Combining PL and raman spectroscopy an As-P-exchange could be revealed. Furthermore, we could quantify this exchange by conjunction of PLE experiments and QW calculations to be 5-10% at highest annealing temperatures. To further analyze the interplay of removing defects by annealing and creating new ones by As-P-exchange we studied the disorder of the Ga(N,As,P) QW. A two scaled disorder common for these materials was found. The behavior of the disorder was compared with the QWs morphology obtained by TEM measurements.

HL 96.11 Thu 14:00 Poster B

Type-II Excitons in (Ga,In)As/Ga(N,As)-quantum wells on GaAs — •Carsten Kruska, Sebastian Gies, Philip Hens, Wolfgang Stolz, Kerstin Volz, and Wolfram Heimbrodt — Faculty of Physics and Material Science Center, Philipps University Marburg, D-35032 Marburg, Germany

Quantum Well (QW) structures are used in many semiconductor devices. These systems inevitably contain interfaces, that influence the charge carriers. Since the recombination of type-II excitons takes place across the interface their properties are influenced by the interface, making type-II excitons an excellent probe to study internal interfaces. Here, we present an analysis of the recombination of spacially indirect (type-II) excitons in (Ga,In)As/Ga(N,As)-MQWs on GaAs.

The MQW structures under investigation were grown epitaxially using metal-organic vapor-phase epitaxy and consist of a (Ga,In)As-QW and a Ga(N,As)-QW separated by a GaAs interlayer of varying thickness. By adjusting the N-content the type-I or type-II behavior is achieved. The type-II transition between the electron in the Ga(N,As)-QW and the heavy hole in the (Ga,In)As-QW was observed and investigated depending on the interlayer thickness. Conjuction of experiment and QW-calculation using the transfer matrix method reveal the hetero-offset between the conduction bands of Ga(N,As) and GaAs to be 600 meV. For the heavy hole band within the errorbars no offset was found. Furthermore, time resolved measurements were performed to reveal the recombination dynamics of the type-II transitions and their interplay with the interface.

HL 96.12 Thu 14:00 Poster B

Study of Optical Emission Properties of InGaN Quantum Wells on Semipolar (20-21) and (20-2-1) orientations — •Nikolay Ledentsov Jr.[1], Ingrid Koslow[1], Christian Mounir[3], Tim Wernicke[1], Tore Niermann[1], Ulrich T. Schwarz[3], Markus Weyers[2], and Michael Kneissl[1,2] — [1]TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Ferdinand-Braun-Institut, Gustav-Kirchhoff-Str. 4, 12489 Berlin, Germany — [3]Universität Freiburg, Georges-Köhler-Allee 106, 79110 Freiburg, Germany

Semipolar quantum wells (QW) exhibit polarized surface emission in contrast to polar QWs grown on the (0001) plane. This is caused by anisotropic and shear strain, leading to the mixing of the A,B and C valence bands. In this work we investigate the optical polarization of $In_{0.16}Ga_{0.84}N$ and $In_{0.25}Ga_{0.75}N$ 3.5nm single QWs grown on bulk GaN substrates with (20-21) and (20-2-1) orientation. Polarization resolved temperature- and excitation-dependent photo- (PL) and electro- (EL) luminescence measurements were performed on these samples. On (20-2-1) QWs we observe polarization ratios of 0.8-0.9 and band distances (ΔE) of 20-30meV at room temperature. These values agree with $k \cdot p$ simulations and literature. We found a strong dependency of ΔE on excitation power in PL measurement which could explain discrepancies between EL and PL measured ΔE values in the literature. (20-21) QWs exhibit low polarization ratios and do not correspond

with $k \cdot p$ simulations, a trend observed by many groups. This discrepancy is addressed by TEM measurements and their interpretation in connection with the PL results.

HL 96.13 Thu 14:00 Poster B

Spectroscopic characterization of Lanthanide-doped AlN and AlInN — •Sebastian Bauer[1], Miao Yang[2], Niklas Bayrle[1], Murat Yildirim[1], Matthias Hocker[1], Horst P. Strunk[2], and Klaus Thonke[1] — [1]Institute of Quantum Matter / Semiconductor Physics Group, University of Ulm, 89081 Ulm, Germany — [2]Institute of Materials Science, Chair of Materials Physics, University of Stuttgart, 70569 Stuttgart, Germany

Radiative electron transitions in the $4f$ shell of rare earth ions are of great interest for applications in optoelectronics as temperature-stable emitters of sharp spectral lines. Due to the wide band gap of the host semiconductor AlN, a wide range of the rare earth internal transitions is accessible.

We investigate polycrystalline rare earth doped AlN and AlInN layers with grain sizes in the nanometre regime. They were deposited by magnetron co-sputtering on Si(100) substrates, and doped with Praseodymium, Neodymium, Samarium, Terbium, and Thulium. The emission features recorded in temperature dependent photoluminescence using above or below bandgap excitation are assigned to their corresponding $4f$ states split by the hexagonal crystal field. Despite the polycrystalline nature of the samples, line widths below 0.5 nm were observed in the spectra. Furthermore, the influence of indium as a constituent in the host crystal, and of different annealing processes applied after deposition is discussed.

HL 96.14 Thu 14:00 Poster B

Combined and spatially correlated measurements by SEM-CL and EBIC on semiconductor microstructures — •Manuel Knab[1], Matthias Hocker[1], Ingo Tischer[1], Pascal Maier[1], Junjun Wang[2], Ferdinand Scholz[2], and Klaus Thonke[1] — [1]Institute of Quantum Matter/Semiconductor Physics Group, University of Ulm — [2]Institute of Opotoelectronics, University of Ulm

Among the crucial aspects for the successful realization of semiconductor-based light emitting diodes is the quality of both the pn-junction and the quantum well. The cathodoluminescence (CL) measurement technique provides important information about the radiative recombination in the semiconductor structure, especially in the quantum well. With the electron beam induced current (EBIC) setup we are able to gain access to the pn-junction quality. Both measurement techniques are applied in a scanning electron microscope yielding high spatial resolution. The investigations were performed on the identical spot of semipolar InGaN/GaN microstructures. The results show both correlation and anti-correlation of the respective signal intensities. These are discussed regarding the crystal quality, the quality of the pn-junction and of the quantum well. In conclusion we can provide a powerful tool for the analysis of the light emitting diode structures by the combination of CL and EBIC.

HL 96.15 Thu 14:00 Poster B

GaN quantum dot ensembles for capacitance-voltage measurements — •Carlo A. Sgroi, Arne Ludwig, and Andreas D. Wieck — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum, Germany

GaN and its alloys have excellent properties regarding thermal stability at ambient conditions, high thermal conductivity and wide bandgap energies, thus making it an ideal candidate for high power and high temperature microelectronic devices.

The aim of this study is to design a heterostructure by MBE growth for measuring self-assembled GaN QDs on $Al_xGa_{1-x}N$ by capacitance-voltage (C-V) spectroscopy. Whereas InAs - QDs on GaAs cease to exhibit their quantum character above a temperature of about T = 20 K, the higher bandgap of GaN will lead to a substantial higher working temperature of GaN - QDs.

$GaN/Al_xGa_{1-x}N$ heterostructure layers in the wurzite structure have deformed band structures due to polarization effects induced by doping and strain which complicates the prediction about the band structure and electrical properties.

Band structure simulations were run to calculate a decent tunneling barrier for C-V measurements capitalizing on the polarization effect and the quantum dot conduction band minimum close to the Fermi energy. Therefore, different Al-contents in the adjacent heterostructure layers are required. To establish a lower polarization effect and the demanded band structure, the Al-content is graded linearly. C-V measurements will be presented for different configurations.

HL 96.16 Thu 14:00 Poster B

Achieving step flow AlN growth by MOVPE — •Konrad Bellmann, Tim Wernicke, Markus Pristovsek, Frank Mehnke, Christian Kuhn, and Michael Kneissl — Technische Universität Berlin, Institute of Solid State Physics, Secretariat EW6-1, Hardenbergstrasse 36, 10623 Berlin, Germany

Wide bandgap devices based on nitride materials like UVC-LEDs and GaN QDs rely on smooth AlN base layers. Depending on the growth conditions the surface morphologies of AlN layers can vary between step bunches, step flow or spiral hillocks. The V/III ratio during growth has an important impact on the surface reconstruction resulting in a change in surface energy. This work will present a systematic study of AlN growth by metal organic vapor phase epitaxy(MOVPE). The growth of AlN at 1080 °C is investigated for different V/III ratios from 15 to 250. Depending on the V/III ratio a clear transition in surface morphology can be observed. For high V/III ratios AlN growth exhibits spiral growth. At low V/III ratio smooth surfaces with step flow growth are obtained. The data is interpreted with a kinetic model considering the balance between terraces width and diffusion length.

HL 96.17 Thu 14:00 Poster B

Experimental verification of electron scattering simulations for depth-resolved cathodoluminescnece — •Matthias Hocker[1], Pascal Maier[1], Ingo Tischer[1], Oliver Rettig[1], Robert A.R. Leute[2], Kamran Forghani[2], Ferdinand Scholz[2], and Klaus Thonke[1] — [1]Institute of Quantum Matter, Semiconductor Physics Group, University of Ulm, Ulm, Germany — [2]Institute of Optoelectronics, University of Ulm, Ulm, Germany

Scanning electron microscope cathodoluminescence (SEM-CL) has a high lateral resolution. However, the depth of the origin of the luminescence signal cannot be determined directly. By varying the primary electron (PE) energy and comparing the measurement results with Monte Carlo simulations of the PE scattering process inside the semiconductor material, depth-resolved SEM-CL measurements are possible. We applied this investigation method to different nitride semiconductor layer systems. In order to verify the validity of the simulation model, cross sectional SEM-CL measurements were perfomed as well.

HL 96.18 Thu 14:00 Poster B

Photoluminescence of Si-doped $Al_xGa_{1-x}N$ with aluminum mole fractions beyond 80% — •Dimitri Henning, Christoph Reich, Frank Mehnke, Tim Wernicke, Christian Kuhn, Harald Pingel, and Michael Kneissl — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

For the realization of deep ultraviolet light emitting diodes, highly conductive n-doped layers are needed. In this study we investigate the photoluminescence of Si-doped doped n-$Al_xGa_{1-x}N$ ($0.8<x<1$) layers grown by metal organic vapor phase epitaxy on epitaxially laterally overgrown AlN/sapphire templates. We found the resistivity is highly dependent on the SiH_4/III ratio leading to a narrow growth window. Si-doped n-$Al_xGa_{1-x}N$ layers with resistivites as low as 0.026 Ω cm have been realized. The n-AlGaN layers were excited by an ArF-excimer laser (193 nm) in a range between 5 K-300 K. Low temperature PL spectra show near band gap emission as well as different defect bands depending on the SiH_4/III ratio. Three major defect luminescence bands were identified as impurity transitions using assignments from literature as $(V_{III}\text{-complex})^{1-}$, $(V_{III}\text{-complex})^{2-}$, $(V_{III})^{3-}$ (listed high to low energy position). For SiH_4/III ratio below the optimum condition the emission related to the $(V_{III}\text{-complex})^{1-}$ appears to be the strongest defect luminescence band. At the optimum condition intensity of all defect luminescence bands reaches a minimum in comparison to the band edge luminescence. A higher SiH_4/III ratio leads to a strong increase of $(V_{III})^{3-}$ related defect luminescence.

HL 96.19 Thu 14:00 Poster B

Non-Classical Light Emission From GaN Quantum Wires — S. Kalinowski[1], G. Callsen[1], J. Teubert[2], J. Arbiol[3], P. Becker[2], G. Hönig[1], D. Bostanjoglo[1], •A. Bokov[1], A. Schliwa[1], M. Eickhoff[2], and A. Hoffmann[1] — [1]Technische Universität Berlin, Institut für Festkörperphysik,10623 Berlin, Germany — [2]Justus Liebig-Universität Gießen, I. Physikalisches Institut, 35392 Gießen, Germany — [3]ICREA and ICMAB-CSIC, Campus de la UAB, 08193 Bellaterra, Spain

Studying quantum effects in nitride-based nanowires with diameters scaling down to a few hundred nanometers is hindered by their still mostly bulk-like properties. A drastic diameter reduction towards the domain of the so-called quantum wires (QWRs) facilitates true one- dimensionality of the structures exhibiting confinement in two directions, while the third direction can straightforwardly be tailored. If the QWR length is sufficiently reduced one can approach the transitional regime between one- and zero-dimensional structures with drastic effects on the observed emission line characteristics and photon statistics.

Our results summarize the particular optical properties of novel GaN QWRs with special regard on the photon statistics. By tuning the QWR length as most vital parameter we can tune the emission characteristics yielding a natural transition between the optical properties of one- to zero-dimensional structures with strong perspectives for future photonic applications.

HL 96.20 Thu 14:00 Poster B

External Pressure on GaN/GaInN Quantum Wells: Influence of Strain on Internal Fields — •Hendrik Kuhn[1], Torsten Langer[2], Jens Hübner[1], Andreas Hangleiter[2], and Michael Oestreich[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, Abteilung Nanostrukturen, Appelstrasse 2, D-30167 Hannover, Germany — [2]Technische Universität Braunschweig, Institut für Angewandte Physik, Mendelssohnstrasse 2, D-38106 Braunschweig, Germany

Group III nitride based heterostructures are of strong interest since their versatile tunability in emission energy that is especially interesting for optical devices e.g. the blue LED [1]. However, as a piezoelectric material they contain an internal electric field that results in a small overlap of the wavefunctions of electron and hole and is the reason for a reduced quantum efficency. We examine GaN/InGaN quantum wells (QW) and apply external stress in order to vary the internal piezoelectric fields and thereby influence the optical properties of the QWs [2,3]. We measure time resolved photoluminescence and perform pump probe experiements on single and multiple GaN/InGaN QW under varied strain that is applied uniaxial and along the growth direction with a pressure cell. Additionally we measure the spin dynamics via Kerr rotation to gain information on the internal electric fields since the spin dephasing rate is directly related to the field via Rashba effect.

[1] Y. Nanishi, Nat. Photonics (2014). [2] S.L. Chuang and C.S. Chang, Semicond. Sci. Technol. 12, (1997). [3] A. Hangleiter et al., Phys. Status Solidi 216, (1999).

HL 96.21 Thu 14:00 Poster B

Optimization of Ohmic contacts of GaN HEMTs with AlN spacer — •Teresa Baur[1,2], Sebastian Mansfeld[2], Helmut Jung[2], Manfred Madel[2], Hervé Blanck[2], Jan Grünenpütt[2], Bernd Schauwecker[2], and Klaus Thonke[1] — [1]Institute of Quantum Matter / Semiconductor Physics Group, Ulm University, 89081 Ulm, Germany — [2]United Monolithic Semiconductors GmbH, 89081 Ulm, Germany

As a promising candidate for future microwave and millimeter-wave power devices, AlGaN/GaN high-electron mobility transistors (HEMTs) have attracted much research interest. In order to realize the full potential of AlGaN/GaN HEMTs as high-power, high-frequency, and high-temperature devices Ohmic contacts with low specific resistance are essential. The electron mobility in the two-dimensional electron gas (2DEG) can be increased by inserting a thin Aluminum Nitride spacer at the AlGaN-GaN interface, which reduces alloy scattering. This AlN spacer lowers the sheet resistance, but also typically leads to undesirable higher ohmic contact resistance.

A possible way to circumvent this disadvantage is to reduce the distance between the contact and the 2DEG by creating a recess prior to the metallization step. Electrical data extracted from the Transmission Line Measurement (TLM) confirm this theory.

In order to better understand the physical conduction mechanisms at the metal/semiconductor interface, temperature-dependent $I(V)$ measurements were undertaken for different sample configurations.

HL 96.22 Thu 14:00 Poster B

Strain and surface morphology in AlGaN-based UV-C laser heterostructures — •F. Krueger[1], C. Kuhn[1], F. Mehnke[1], M. Martens[1], P. Schneider[1], V. Kueller[2], J. Park[3], A. Knauer[2], J. Rass[1,2], T. Wernicke[1], M. Weyers[2], M. Lehmann[3], and M. Kneissl[1,2] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Germany — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Berlin, Germany — [3]Technische Universität Berlin, Institut für Optik und Atomare Physik, Germany

UV laser diodes would be superior to conventional UV lasers in cost, size and robustness. However the realization of UV lasers has proven to be challeging due to insufficient n- and p-type doping as well as high dislocation densities in AlGaN/ sapphire heterostructures. In this work optically pumped AlGaN MQW lasers grown on defect reduced AlN/sapphire templates with lasing wavelengths between 250 nm and 280 nm are investigated. The surface morphology is strongly dependent on the growth conditions and exhibits step bunches, hillocks and V-pits. It was found, that the V-pit density correlates with the strain state of the QWs. By increasing the aluminum content in the QWs less strain is induced which leads to a reduced V-pit density and therefore less non-radiative recombination centers and mode losses. Additionally, the optimized QWs were embedded into a p-n-junction for current injection. For the p-side we investigated AlGaN:Mg cladding layers with an average aluminum content between 34%-81%. All heterostructures show electro-luminescence near 270 nm and increasing operation voltage with increasing aluminum content in the AlGaN cladding.

HL 96.23 Thu 14:00 Poster B

C-doped GaN buffer layers with CBr_4, C_3H_8 and Fe-doped GaN for breakdown voltage enhancement of HEMTs — •Andreas Lesnik, Jonas Hennig, Armin Dadgar, Jürgen Bläsing, Hartmut Witte, and Andrè Strittmatter — Institut für Experimentelle Physik / Abteilung Halbleiterepitaxie, Otto-von-Guericke-Universität Magdeburg

We investigated C-doped and Fe-doped GaN buffer layers grown on Si (111) substrates using metalorganic vapour-phase epitaxy (MOVPE). For the intentional C-doping a high purity 10% propane in hydrogen mixture and carbon tetrabromide (CBr_4) were used as precursors. For Fe-doping ferrocene was used as iron source. Secondary ion mass spectroscopy measurements were performed to quantify the incorporation behaviour of carbon and iron. X-ray diffraction and atomic force microscopy (AFM) were used to characterize the structural quality of the buffer layers. The horizontal and vertical buffer breakdown voltage in dependence of carbon and iron incorporation was investigated.

HL 97: Quantum dots and wires: Pillars and cavities

Time: Friday 9:30–11:00 Location: ER 164

HL 97.1 Fri 9:30 ER 164

Control of spontaneous emission by shaping the vacuum field in coupled cavity systems — •Robert Johne[1], Chao-Yuan Jin[2], Milo Y. Swinkels[2], Ron Schutjens[2], Sartoon Fattah poor[2], Thang B. Hoang[2], Leonardo Midolo[2], Peter J. van Veldhoven[2], and Andrea Fiore[2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]COBRA Research Institute, Eindhoven University of Technology, P.O. Box 513, NL-5600MB Eindhoven, The Netherlands

The real-time control of spontaneous emission (SE) is needed to harness cavity quantum electrodynamics processes for quantum information processing. Here we report an approach to the control of spontaneous emission via the ultrafast moulding of the vacuum field in two or three coupled cavities. We provide a first demonstration of this concept in a two-cavity structure where the injection of free carriers in a control cavity changes the mode volume and quality factor seen by semiconductor quantum dots sitting in a target cavity, and report a change in SE intensity by over a factor of two over a 200 ps timescale [1]. In the three-cavity system, tuning of the cavity resonances allows for on/off switching of the light-matter interaction [2] paving the way towards advanced applications in quantum information processing as well as for a new class of gain modulated lasers.

[1] C.-Y. Jin et al., Nature Nanotechnology 9, 886 (2014)
[2] R. Johne et al., submitted

HL 97.2 Fri 9:45 ER 164

Light matter coupling between a site controlled quantum dot and a resonant laser field — •Sebastian Unsleber[1], Michael Dambach[1], Sebastian Maier[1], Sven Höfling[2], Christian Schneider[1], and Martin Kamp[1] — [1]Technische Physik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Present address: SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, KY16 9SS, United Kingdom

Many new applications in the field of quantum information technology and photonics require single and indistinguishable photons. Since quantum dots act inherently as emitters of such photons, they are basically predestinated for this schemes. A much higher scalability can be achieved if these quantum dots have a controlled nucleation position. Furthermore, the indistinguishability of the emitted photons is directly linked to their coherence properties, which means that the quantum dot should be excited resonantly in order to suppress e.g. spectral diffusion and time-jitter effects. As a step towards the generation of indistinguishable photons out of resonantly pumped site controlled quantum dots, we present in this work fundamental effects that occur for the coupling of the QD-exciton to the driving laser field. This coupling splits the two excitonic states into four dressed states. Transitions between these states give rise to the well-known Mollow-triplet. Furthermore, we investigate the temperature depended splitting of the two sidepeaks and their dephasing properties.

HL 97.3 Fri 10:00 ER 164

Non-classical Light Emission from an On-chip Excited Quantum Dot Micropillar Cavity — •Pierce Munnelly[1], Matthias Karow[1], Tobias Heindel[1], Matthias Lermer[2], Christian Schneider[2], Sven Höfling[2], Martin Kamp[2], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany — [2]Technische Physik and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Nanophotonics has been rapidly developing in recent years as the quest for integrated devices enabling the generation, manipulation and detection of single photons for light-based quantum information processing and cryptography is heavily pursued. A huge step forward in this regard is the monolithic integration of an electrically driven excitation source driving a non-classical light source on a single chip. We report on recent progress with a novel device incorporating semiconductor quantum dots embedded in micropillar cavities, which can be excited optically through the in-plane whispering gallery mode laser emission of a nearby electrically driven micropillar. The feasibility of such an approach for on-demand single and indistinguishable photon generation utilizing cavity-quantum electrodynamic effects as well as on-chip resonance fluorescence is clearly demonstrated by recent results.

HL 97.4 Fri 10:15 ER 164

Single quantum dot lasing in the strong coupling regime — •Fabian Gericke[1], Steffen Holzinger[1], Leon Messner[1], Tobias Heindel[1], Janik Wolters[1], Andreas Löffler[2], Martin Kamp[2], Sven Höfling[2,3], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany — [2]Technische Physik, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [3]Present address: School of Physics and Astronomy, University of St Andrews, St Andrews KY16 9SS, United Kingdom

Light-matter interaction of single semiconductor quantum dots coupled to optical modes of microcavities enables one to study different regimes of cavity quantum electrodynamics in solid state. Of particular interest is the coherent coupling regime which is crucial for a variety of applications in quantum information processing and for exciting effects such as single photon nonlinearities. In this contribution, we experimentally demonstrate the onset of laser oscillation in a quantum dot micropillar laser which operates in the strong coupling regime. Single quantum dot lasing effects are demonstrated within comprehensive optical studies comprising power dependent first order and second order photon autocorrelation measurements, and a comparison between axial and lateral emission of the micropillar. Our work has high potential to trigger further progress on experiments with single dot lasers, as well as their theoretical modeling.

HL 97.5 Fri 10:30 ER 164

Statistical study on strong coupling of single and multiple quantum dots in micropillar cavities — •Anna Musial[1,2], Caspar Hopfmann[1], Micha Strauss[3], Christian Schneider[3], Sven Höfling[3,4], Martin Kamp[3], and Stephan Reitzenstein[1] — [1]Institute of Solid State Physics, Berlin University of Technology, 10623 Berlin, Germany — [2]Laboratory for Optical Spectroscopy of Nanostructures Department of Experimental Physics, Wrocław University of Technology, 50-370 Wrocław, Poland — [3]Technische Physik, University of Würzburg, 97074 Würzburg, Germany — [4]Present address: SUPA, School of Physics, and Astronomy, University of St Andrews, United Kingdom

Coherent photonic coupling of multiple quantum dots (QDs) in micropillar cavities is a very promising platform for the realization of coherent interaction between distant qubits. We performed a statistical study on various cases of strong coupling (SC) from isolated QDs coupled to cavity mode (CM) to multiple QDs interacting coherently via the CM. Experimental results are supported by the results of calculations in the framework of a coupled oscillator model. A characteristic triple peak spectral feature, increased effective coupling constant and double anticrossing, beeing a fingerprint of coherent coupling between 3 quantum states (hybrid states of two excitons and a CM), have been observed at resonance in agreement with the Tavis-Cummings description. Moreover, the hybridization of the coupled states is also reflected in a characteristic change of their polarization properties.

HL 97.6 Fri 10:45 ER 164

Influence of acoustic phonons on strong coupling phenomena in quantum-dot micro pillars — •Max Strauss[1], Anna Musial[1,2], Caspar Hopfmann[1], Micha Strauss[4], Andreas Barth[3], Martin Gläßl[3], Christian Schneider[4], Sven Höfling[4,5], Martin Kamp[4], Vollrath Martin Axt[3], and Stephan Reitzenstein[1] — [1]Technische Universität Berlin, Germany — [2]Wroclaw University of Technology, Poland — [3]Universität Bayreuth, Germany — [4]Universität Würzburg, Germany — [5]University of St Andrews, United Kingdom

Coupled quantum dot (QD)- microcavity systems are of great interest with respect to both, the fundamental study of cavity quantum electro dynamics (cQED) and possible applications (e.g. quantum information processing). In such systems, phonon-induced losses have recently become comparable to cavity losses and it is thus desirable to understand their influence on cQED phenomena. We investigate the influence of acoustic phonons on the exciton-photon interaction in the strong coupling regime. Examining more than 90 QD-micropillars, we comprehensively study the phonon-induced renormalization of the Rabi frequency in an extraordinary wide temperature range of up to 60 K.

HL 98: Nitrides: Bulk material, films, surfaces and quantum wells

Time: Friday 9:30–12:30 Location: EW 201

HL 98.1 Fri 9:30 EW 201

Valence band tomography in wurtzite GaN — •Martin Feneberg, Karsten Lange, Michael Winkler, Matthias Wieneke, Hartmut Witte, Jürgen Bläsing, Armin Dadgar, and Rüdiger Goldhahn — Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg

Effective masses describe the curvature of the conduction and valence bands. These masses are extremely important input parameters for device design, understanding optical or transport phenomena, and evaluating theoretical results. However, especially the hole masses are experimentally largely unexplored.

Here, we present valence band tomography performed by analyzing spectroscopic ellipsometry data of a-plane wurtzite GaN with free electron concentrations up to $10^{20}\mathrm{cm}^{-3}$. The conduction band curvature of the same set of samples is already known from infrared studies [1]. By taking into account Burstein-Moss shift and band gap renormalization, the onset of the anisotropic interband absorption reveals the valence band edges for $k > 0$ in certain directions. This analysis yields the valence band curvature for the upper two valence bands.

[1] M. Feneberg, K. Lange, C. Lidig, M. Wieneke, H. Witte, J. Bläsing, A. Dadgar, A. Krost, and R. Goldhahn, Appl. Phys. Lett. 103, 232104 (2013).

HL 98.2 Fri 9:45 EW 201

Interaction of GaN(0001) surfaces with potassium and water — •Marcel Himmerlich, Vladimir Irkha, Anja Eisenhardt, Stephanie Reiss, and Stefan Krischok — Institut für Physik and Institut für Mikro- und Nanotechnologien, TU Ilmenau, Germany

Due to its high physical and chemical stability, gallium nitride (GaN) is a promising material for the use in chemical or biological sensor devices. For device optimization and clarification of degradation mechanisms, a profound understanding of the interaction between the GaN surface and the species of the surrounding environment that are aimed to be analysed is essential. Here we present a study on the interaction of GaN(0001) surfaces with potassium and water, motivated by K ions in aqueous environment being important for biosensor applications due to its involvement in fundamental cell metabolism processes. Changes in the chemical and surface electronic properties during the adsorption and coadsorption of K and water on the epitaxial grown GaN surfaces were in-situ characterized by X-ray and ultraviolet photoelectron spectroscopy. The measurements show the formation of K and oxygen related electron states as well as significant changes in the sample work function Φ and surface band bending V_{bb}. Water adsorption leads to a slight increase in Φ, while K adsorption and coadsorption of K and water induce a pronounced work function decrease. Furthermore, K increases the surface upward band bending of GaN(0001), while during the interplay of K with water a reduction in V_{bb} is observed. The interplay between surface and adsorbate electron states and the occurring chemical and charge transfer processes will be discussed.

HL 98.3 Fri 10:00 EW 201

Ultrafast to slow time-resolved defect luminescence studies of rare earth doped AlN — •Tristan Koppe[1], Oliver Beck[1], Takashi Taniguchi[2], Hans Hofsäss[1], and Ulrich Vetter[1] — [1]2. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]National Institute for Materials Science, Namiki 1 - 1, Tsukuba, Ibaraki 305-0044, Japan

We report on studies of fast and slow defect luminescence processes in undoped and rare earth doped AlN. It was synthesized by the temperature gradient method in a belt-type HP-HT apparatus using e.g. Li_3AlN_2 as solvent which was then mixed with EuF_3 before synthesis for rare earth doped AlN.

In this work a general overview is given on the known defect types in AlN reported in literature so far, and the interaction of defects and rare earth ions in the host are discussed based on luminescence studies. Time-resolved luminescence studies were performed using a Coherent MIRA 900-F Ti:Sa laser in combination, a pulse picker and an APG HarmoniXX FHG 3+1 harmonics generator with the luminescence light collected with a 0.3 m spectrograph and a streak camera.

Two distinct luminescence bands at 2.7 eV and 3.9 eV in undoped AlN with lifetimes in the range from several ps to several μs are found and their origin is discussed. In rare earth doped AlN energy transfer between rare earth ion and defects in the AlN host is discussed based on temperature dependent time-resolved luminescence measurements.

HL 98.4 Fri 10:15 EW 201

Aberration-corrected-STEM investigation of epitaxial GaN thin films formed by ion-beam based post-nitridation of Ga droplets — •David Poppitz, Andriy Lotnyk, Jürgen W. Gerlach, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstr. 15, D-04318 Leipzig

GaN is a widely used semiconductor material in optoelectronics applications due to its optical properties. By increasing the crystalline quality, the emission efficiency for light emitting devices can be improved. Here, GaN thin films were produced in a system usually used for ion-beam assisted molecular-beam epitaxy (IBA-MBE) on 6H-SiC-, Al_2O_3- and γ-$LiAlO_2$-substrates. In the first step of the deposition process, Ga-droplets were deposited on the substrates. In the second step, a post-nitridation process of Ga droplets by a hyperthermal nitrogen ion beam with ion energies less than 25 eV was used to form the GaN thin films.

The thin films characterization was done by using a state of the art FEI Titan^3 G2 60-300kV probe aberration-corrected scanning transmission electron microscope (STEM). It was found that coalesced GaN thin films with film thicknesses less than 30 nm can be achieved by this preparation method. The detailed investigation shows different types of defects such as grain boundaries and stacking faults in the epitaxial, differently oriented films. However, the crystalline quality of GaN thin films was dependent on the substrate material.

HL 98.5 Fri 10:30 EW 201

Towards an understanding of (11$\bar{2}$2) InGaN quantum wells — •Markus Pristovsek, Tongtong Zhu, Yisong Han, and Colin J. Humphreys — Department of Materials Science and Metallurgy, University of Cambridge, 27 Charles Babbage Road, Cambridge, CB3 0FS, UK

InGaN quantum wells (QWs) are at the heart of every light emitting diode. The drop of their photoluminescence (PL) emission towards green is mostly attributed to the piezo-electric fields which separate electron and hole wave functions. Semi- and non-polar orientations are investigated since the resulting fields are strongly reduced. Especially the stable (11$\bar{2}$2) orientation offers high indium incorporation.

We have grown and characterized (11$\bar{2}$2) InGaN QWs from 400 to 600 nm and compared with (0001) QWs. The indium desorption on the (11$\bar{2}$2) is slightly higher, hence QW growth rates and temperatures have a stronger influence and indium concentration are slightly lower. The critical thickness for full relaxation was comparable to (0001).

A QW thickness series showed indeed less wavelength shift for (11$\bar{2}$2) QWs from 2.0 to 4.5 nm. However, all the wavelengths were not close to the expected positions. Furthermore, the PL intensities of all QWs were less than a third of that of simultaneously grown (0001) QWs. Systematic variation of the barrier width showed that carriers generated more than ≈3 nm away from the (11$\bar{2}$2) QWs do not contribute to the PL. Electroluminescence is currently under investigation.

We acknowledge funding from EU-FP7 ALIGHT NMP-2011-280587 and the UK EPSRC EP/I012591/1.

Coffee break

HL 98.6 Fri 11:00 EW 201

Growth and characterization of InN on Si (111) by molecular beam epitaxy — •Saskia Weiszer, Andreas Zeidler, Fabian Schuster, and Martin Stutzmann — Walter Schottky Institut and Physics Department, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany

Multi-junction solar cells have received wide attention as the energy conversion efficiency can be increased significantly compared to single-junction solar cells. Theoretical considerations show that an InGaN/Si tandem solar cell could be an optimal implementation of a double-junction solar cell, as two different wavelength regions of the broad solar spectrum can be utilized by each junction connected via a resonant tunnel junction which is expected to form at an indium content of 46 %. As a first step towards such an InGaN/Si tandem solar cell, the growth of high quality InN directly on Si (111) substrates by molecular

beam epitaxy (MBE) has been investigated. First attempts of growing InN as a homogeneous thin film suffered from an insufficient quality. The obtained layer-like structures showed high surface roughness in atomic force microscope and various epitaxial orientations measured by high resolution X-ray diffraction. A possible alternative to layer growth is the growth of nanowires to reduce structural defects, since the lattice mismatch induced strain can relax through the nanowire sidewalls. By a varying the applied growth parameters, namely substrate temperature and III/V-ratio, the InN nanowire growth has been optimized and recent results will be presented.

HL 98.7 Fri 11:15 EW 201

Molecular beam epitaxy of GaN quantum dots — •Christopher Hein[1], Andreas Kraus[1], Heiko Bremers[1], Fedor Alexej Ketzer[1], Kamran Forghani[2], Uwe Rossow[1], Ferdinand Scholz[2], and Andreas Hangleiter[1] — [1]Institute of Applied Physics, TU Braunschweig, Germany — [2]Institute of Optoelectronics, Universität Ulm, Germany

Quantum dots are desired nanostructures for laser diodes and non classical light generation. The III-nitride material system constitutes a valuable material for such applications due to their high bandgap and thermal stability. Our samples are grown in a RIBER 32P molecular beam epitaxy system in Stranski-Krastanov self assembled growth. Templates are c-oriented 300μm sapphire substrates on top of which MOVPE GaN (2.5μm) or AlN (500nm) is grown. Our experiments cover temperature dependent (675-725°C) deposition and subsequent characterization of uncapped and capped GaN QD. Growth on MOVPE GaN started with a 100 nm tick AlN (700°C) buffer. Afterwards 2 min GaN was deposited during which in situ RHEED developed from streaky to a dotty pattern, indicative for Stranski-Krastanov growth. AFM of the samples showed dots with 1.4 nm (700°C) up to 2 nm height with densities ranging from $1.3 \cdot 10^{10}/\mathrm{cm}^2$ (725°C) up to $6.0 \cdot 10^{10}/\mathrm{cm}^2$ (675°C). At higher temperatures dots reorganize in a way such that smaller dots coalesce due to higher mobility thus reducing the overall density. The QD sample grown at 700°C was reproduced on MOVPE AlN and capped with a 30 nm AlN layer to allow for optical characterization.

HL 98.8 Fri 11:30 EW 201

Investigation of the optical properties of Zn doped GaN/AlGaN quantum wells for future single photon applications — •Johannes Dühn[1], Matin Mohajerani[2], Xue Wang[2], Andreas Waag[2], Kathrin Sebald[1], and Jürgen Gutowski[1] — [1]Institute for Solid State Physics, University of Bremen, Germany — [2]Institute for Semiconductor Technology, Technical University of Braunschweig, Germany

Efficient single photon sources are a fundamental requirement for experimental quantum optics and cryptography. Established single photon sources often provide low intensities and have to be operated at cryogenic temperatures. A promising approach to this problem is the usage of bound excitons in wide-band-gap materials, because they possess large exciton binding energies and are therefore applicable at elevated temperatures. The position of the bound exciton emission is only determined by the type of defect and the emission exhibits a narrow line width, as it is favourable for device applications. In this work we investigate the micro-photoluminescence of a quantum well of zinc doped GaN embedded in AlGaN. Incorporation of zinc dopants is proven by identifying the acceptor bound exciton emission line at 3.455eV. To reveal the properties of individual emitters we investigate the luminescence properties of mesa etched structures on the sample. The single-photon properties of these emitters will be characterised by using a Hanbury-Brown-Twiss interferometer.

HL 98.9 Fri 11:45 EW 201

Optical investigations of anisotropic strain of nonpolar GaInN quantum wells grown on AlInN/GaN buffer layers — •Fedor Alexej Ketzer, Ernst Ronald Buss, Philipp Horenburg, Holger Jönen, Heiko Bremers, Torsten Langer, Uwe Rossow, and Andreas Hangleiter — Institut für Angewandte Physik, Technische Universität Braunschweig

We investigate the effect of different buffer layers on the anisotropic strain of nonpolar GaInN quantum well (QW) structures. Therefore we examine optical properties of QWs grown via low pressure MOVPE. We compare fully strained QWs grown on m-plane pseudobulk GaN substrates with similar samples with AlInN buffer layers of different composition. The effect of the strain of the active zone is investigated by temperature dependent and polarization resolved resonant photoluminescence spectroscopy. Since high strain is prominent in GaN/GaInN heterostructures, AlInN buffer layers provide a good possibility of changing overall strain and relaxation. Due to the deformation potentials which strongly affect the band energies, changing the indium content and relaxation of the buffer layer can further tune the emission wavelength and the degree of polarization of the emitted light. Our samples show good optical properties with narrow spectra but strong differences in the degree of polarization and transition energy compared to samples with regular GaN buffer. This is in good agreement with our calculations of the strain and valence band energies.

HL 98.10 Fri 12:00 EW 201

Photoluminescence of GaN grown by high temperature vapor phase epitaxy — •Friederike Zimmermann[1], Jan Beyer[1], Gleb Lukin[2], Olf Pätzold[2], Christian Röder[1,3], Michael Stelter[2], and Johannes Heitmann[1] — [1]Institut für Angewandte Physik, TU Bergakademie Freiberg, Leipziger Str. 23, D-09599 Freiberg, Germany — [2]Institut für Nichteisenmetallurgie und Reinststoffe, TU Bergakademie Freiberg, Leipziger Str. 34, D-09599 Freiberg, Germany — [3]Institut für Theoretische Physik, TU Bergakademie Freiberg, Leipziger Str. 23, D-09599 Freiberg, Germany

High temperature vapor phase epitaxy (HTVPE) is a promising process for chlorine-free growth of GaN. We report on a photoluminescence study on GaN samples grown in a modified HTVPE reactor, which was designed to overcome some of the drawbacks of HTVPE growth. All samples show an overall high luminescence efficiency increasing with III/V-ratio. At 15 K the spectra are dominated by a DAP-like transition at 3.27 eV indicating the presence of acceptors. The near band edge region shows two broad excitonic features which can be ascribed to the common residual donor bound excitons at 3.473 eV and an acceptor bound exciton at 3.462 eV. A carbon contamination cannot be ruled out. The HTVPE samples generally show a much lower variety of radiative defects compared to GaN grown by other methods.

HL 98.11 Fri 12:15 EW 201

Influence of off-cut on the surface morphology and defect distribution of epitaxial laterally overgrown (ELO)-AlN — •Johannes Enslin[1], Frank Mehnke[1], Tim Wernicke[1], Konrad Bellmann[1], Arne Knauer[2], Viola Kueller[2], Anna Mogilatenko[2], Markus Weyers[2], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Gustav-Kirchhoff-Str. 4, 12489 Berlin, Germany

Smooth AlN layers on sapphire with low defect densities are essential for efficient light emitters in the UV-C spectral region between 200 nm and 280 nm. By growing AlN on patterned sapphire substrates (ELO) the threading dislocation density can be significantly reduced from $10^{10}\mathrm{cm}^{-2}$ to $< 10^{9}\mathrm{cm}^{-2}$. However, the ELO-AlN surfaces often suffer from macrosteps with heights of 22 nm for an off-cut angle of 0.25° to the sapphire m-plane. In this paper, we study the influence of the sapphire substrate off-cut angle on the occurrence of macrosteps on ELO-AlN. For this purpose sapphire wafers with off-cut angles between $0.08° \pm 0.008°$ and $0.23° \pm 0.008°$ were overgrown. AFM analysis of the ELO-AlN surfaces revealed macrosteps for off-cut angles between 0.16° and 0.23° with step heights of 19 nm. For substrate off-cuts of $< 0.12°$ the surface exhibits a wavelike surface morphology with the periodicity of the ELO pattern and a peak to bottom ratio of 4 nm. The influence of the surface morphology on the defect distribution will be discussed.

HL 99: Invited Talk Werner Wegscheider

Time: Friday 9:30–10:00 Location: EW 202

Invited Talk HL 99.1 Fri 9:30 EW 202

Fractional quantum Hall effect states in ultrahigh mobility two-dimensional electron systems — •Werner Wegscheider[1], Christian Reichl[1], Jun Chen[2], Werner Dietsche[1,2], Stephan Baer[1], Lars Tiemann[1], Szymon Hennel[1], Clemens Rössler[1], Thomas Ihn[1], and Klaus Ensslin[1] — [1]Solid State Physics Laboratory, ETH Zürich, CH-8093 Zürich, Switzerland — [2]Max-Planck-Institute for Solid State Research, D-70569 Stuttgart, Germany

We report on the fabrication as well as on low-temperature transport investigations of AlGaAs/GaAs heterostructures hosting exotic fractional quantum Hall (FQH) systems. The FQH state which can be observed at the filling factor ν =5/2 is a very exceptional one as it is predicted that its quasiparticle excitations are of anyonic character and obey non-Abelian statistics. Although this property, in principle, paves the way for fault-tolerant quantum computing, the extreme fragility of this state undermines this endeavour. Molecular beam epitaxial growth strategies will be discussed that allow the realization of samples with enhanced 5/2 gap energies. By identifying the most suitable growth and doping schemes, we demonstrate how quantum point contacts (QPCs) can be defined without destroying this fragile FQH state. The investigation of quasiparticle tunnel properties using such structures represents a crucial step towards future interference experiments. Time-resolved measurements performed with the QPC filling factor tuned to $\nu = 2/3$ show periodic oscillations with a period of several minutes. These can be described as a consequence of dynamic nuclear polarization around the corresponding spin phase transition.

HL 100: ZnO and its relatives

Time: Friday 9:30–12:15 Location: EW 203

HL 100.1 Fri 9:30 EW 203

First-principles Evidence for Intermediate Hole Polarons in ZnO — •Honghui Shang[1], Christian Carbogno[1], Patrick Rinke[1,2], Matthias Scheffler[1], Hikmet Sezen[3], Fabian Bebensee[3], Chengwu Yang[3], Maria Buchholz[3], Alexei Nefedov[3], Stefan Heissler[3], and Christof Woell[3] — [1]Fritz-Haber-Institut der MPG, Berlin, DE — [2]Aalto University, Helsinki, Fi — [3]Karlsruhe Institute of Technology, Karlsruhe, DE

We performed density functional theory calculations at the hybrid-functional level (HSE06) to investigate the nature of the polaronic states in ZnO. Our calculations confirm that neither small (i.e., strong coupling) electron nor hole polarons are stable in ZnO, in agreement with previous studies [1]. The binding energy of large polarons (i.e., weak coupling) was determined by evaluating the renormalization of the band edges due to the zero-point motion of the atoms [2]. However, for intermediate polarons at intermediate coupling strength, the harmonic approximation breaks down, and there is currently no first-principle theory. We use the HSE06 effective masses to calculate the Fröhlich coupling constants α. Feynman's path integral technique then yields an intermediate hole polaron, whose binding energy of 245 meV and associated peaks in the optical absorption spectrum are consistent with infrared reflection absorption spectroscopy. [1] J. B. Varley *et al.*, Phys. Rev. B **85**, 081109(R)(2012), [2] G. Antonius *et al.*, Phys. Rev. Lett. **112**, 215501 (2014)

HL 100.2 Fri 9:45 EW 203

Characterization of the p-GaAs / n-ZnO tunnel contact system for opto-electronic applications — •Christian Koppka, Andreas Nägelein, Katja Tonisch, and Thomas Hannappel — Technische Universität Ilmenau, FG Photovoltaik, 98693 Ilmenau, Deutschland

Nanowire based concepts for optoelectronic applications such as LEDs, sensors and solar cells are current global research areas. In contrast to axial structures, the front contacting of nanowire structures with radial configuration is more challenging. In this regard, we examine the contacting of p-doped GaAs nanowire shells using AlOx and ZnO:Al to realize a tunnel junction at the interface. To achieve a good contact system we investigate a ALD type growth of AlOx and ZnO:Al layers for the homogeneous coating of non-planar surfaces in a conventional MOCVD reactor (AIX 200). Due to the very limited analysis methods for coated nanowires structures, the characterization of the p-GaAs/AlOx/n-ZnO system was carried out on planar samples. Current-voltage measurements reveal an ohmic behavior between TCO and III-V material and confirm the applicability of the contact system. By depth-resolved auger electron spectroscopy measurements no diffusion processes of Al or As were found. Accordingly, a sharp interface is assumed. Our ALD process was used successful on nanowire structures and reveal a homogeneous coating.

HL 100.3 Fri 10:00 EW 203

Low temperature PLD-growth of ZnO nanowires on $Zn_xAl_{1-x}O$ films — •Alexander Shkurmanov, Chris Sturm, Helena Franke, Holger Hochmuth, and Marius Grundmann — Inst. f. Exp. Phy. II, Universität Leipzig, Leipzig, Germany

Self-organized grown ZnO micro- and nanostructures exhibit high crystallinity and good electronic properties which makes them interesting to be implemented in devices. In order to integrate these nanostructures in CMOS technology, a growth temperature of less than 450°C is required. For nanowires (NW) prepared by pulsed laser deposition (PLD) typically temperatures of about 900°C are used [1] and a reduction of temperature is quite challenging. In this work, we present the impact of the Al concentration of the ZnO seed layer on the NW growth and as a function of temperature in the range from 400°C to 950°C. At high temperatures (950°C), the Al concentration has a strong influence on the morphology of the NWs as well as on the NW density. The highest NW density we observed for an Al concentration of about 1.5% within the seed layer whereas for larger values, no NW growth was observed. By reducing the temperature down to 400°C a decrease of the density and length of NWs can be observed. This can be attributed to the reduced surface mobility of the incoming particles due to the reduced temperature and a possible change of the polarity of the seed layer by the Al incorporation [2]. [1] C.P. Dietrich, M. Grundmann in *Wide Band Gap Semiconductor Nanowires 1*, V. Consonni, G. Feuillet eds., (Wiley-ISTE, 2014). [2] S. Käbisch et al., Appl. Phys. Let. **103**, 103106 (2013).

HL 100.4 Fri 10:15 EW 203

Influence of mechanical destruction on phonons and excitonic transition on polar and non-polar ZnO crystals — •Nadja Jankowski[1], Christian Nenstiel[1], Mark Berkahn[2], Matthew Phillips[2], and Axel Hoffmann[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Berlin, Germany — [2]School of Physics and Advanced Materials, University of Technology, Sydney, Australia

As Zinc Oxide (ZnO) is a very soft material it is very sensitive towards destruction during handling, thus it is interesting to study the influence of mechanical destruction on optical and structural properties. Therefore polar (c-orientated) and non-polar (a- and m-orientated) ZnO crystals where locally destroyed with a spherical indenter with a diameter of 1 μm and an applied load of 100 mN.

The influence of the destructed area on strain fields and crystal quality was investigated in detail by the means of Raman map scans. The shift of the E_2^{high}-mode revealed complex strain fields with hexagonally arranged strain fields for the polar plane and elongated V-shaped bands of strain for the non-polar plains.

The influence on the excitonic recombination due to destruction was investigated by micro photoluminescence at about 10 K. In general the excitonic transition shows a shift according to the strain fields. On the non-polar planes a change of the intensity ratio between high and low energy neutral bound excitons and the ionized bound ones can be observed in the compressive and tensile strained regions. Therefore a clear connection between the change of excitonic transition and the indentation induced strain fields can be observed.

HL 100.5 Fri 10:30 EW 203

Room-temperature fabricated amorphous oxide heterodiodes on glass and flexible substrates — •Peter Schlupp, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für experimentelle Physik II, Leipzig, Germany

Beside the lower energy input, room-temperature (RT) fabrication of semiconductors has the advantage that thermally unstable but flexible substrates can be used. The amorphous oxides *n*-type zinc-tin oxide (ZTO) and *p*-type zinc-cobalt oxide (ZCO) show promising semiconducting properties even though they are fabricated at RT [1,2]. Furthermore they contain abundant materials only.

We present electrical properties of ZTO/ZCO heterodiodes fabricated entirely at RT by pulsed laser deposition. These diodes were deposited on corning glass substrates and on flexible plastic substrates. To enhance the rectification of the diodes, an ultrathin insulating ZTO layer was introduced at the heterointerface leading to bipolar diodes with a rectification ration of more than six orders of magnitude. The diode properties and the conduction mechanism will be derived from temperature dependend current voltage measurements. Furthermore we have investigated the influence of bending of the flexible substrates on the diode properties.

[1] Schlupp et al., MRS Proceedings **1633**, 101 (2014)
[2] Schein et al., Appl. Phys. Lett., **104**, 022104 (2014)

Coffee break

HL 100.6 Fri 11:00 EW 203

Selective Back Channel Passivation of ZnO TFTs Utilizing Oxiranes — •Marlis Ortel, Nataliya Kalinovich, Gerd-Volker Röschenthaler, and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Zinc oxide layers of 10nm film thickness were deposited by spray pyrolysis as active layer in TFT structures. They were utilized to investigate the influence of the surface at the back channel on the charge transport processes in ZnO TFTs by detailed IV analysis. A strong but reversible increase of shallow and deep trap states was found when the material was exposed to humid atmosphere. This results in a decrease in mobility, increase in hysteresis and shift of the threshold voltage during gate bias stress due to coulomb interaction of surface and active channel charges.

Oxiranes were selectively bound to hydroxyl groups at the metal oxide surface to gain information about the active sides at the surface which induce the change of the electronic surface structure. The binding of hexafluoropropylene oxide self-assembled monolayer (SAM) to the surface caused a significant decrease in hysteresis by a factor of 4. Furthermore, no shift of the on-set under negative gate bias stress was observed after oxirane treatment and the mobility remained stable. We conclude that hydroxyl surface groups act as active sides to induce mainly deep trap levels at the back channel of ZnO TFTs in humid atmosphere.

HL 100.7 Fri 11:15 EW 203

Blue shifting the photoluminescence of ZnO by doping with amino acids — •Marlene Lamers[1,3], Verena Baumann[1,3], Anastasia Brif[2], Guy Ankonina[4], Alexander Urban[1,3], Jessica Rodríguez-Fernández[1,3], Boaz Pokroy[2], and Jochen Feldmann[1,3] — [1]Photonics and Optoelectronics Group, Ludwig-Maximilians-Universität, Munich — [2]Department of Materials Science and Engineering and the Russell Berrie Nanotechnology Institute of Technology, Haifa, Israel — [3]Nanosystems Initiative Munich (NIM), Munich — [4]Photovoltaic lab, Department of Electrical Engineering, Technion Israel Institute of Technology, Haifa, Israel

Zinc oxide (ZnO) is an attractive semiconductor due to its wide and direct bandgap in the UV region (Eg = 3.4 eV), its large free-exciton binding energy (60 meV) and its strong photoluminescence even at room temperature. Bandgap tuning is of special interest to extend the spectral range of ZnO based devices. Recently, it has been demonstrated by optical reflection spectroscopy that the bandgap of zinc oxide can be engineered by intracrystalline incorporation of amino acids due to an increased lattice strain [1]. We have performed photoluminescence and absorption experiments, which reveal a controlled blue-shift of the bandgap emission for amino acid doped ZnO vs. pure ZnO. Additionally, the ratio of band-edge-to-defect emission can be significantly enhanced by post-synthetic heat treatment. Morphological changes will be discussed as a possible reason for these observations.

[1] A. Brif, G. Ankonina, C. Drathen, B. Pokroy, Adv. Mater. (2014) 26, 477.

HL 100.8 Fri 11:30 EW 203

Influence of Fe impurities on the annealing of OH-Li complexes in ZnO — •Frank Herklotz, Klaus Magnus Johansen, Augustinas Galeckas, and Bengt Gunnar Svensson — University of Oslo, Department of Physics/Centre for Materials Science and Nanotechnology, N-0318 Oslo, Norway

The annealing behavior of the OH-Li_{Zn} center in ZnO, which leads to a local vibrational mode at 3577 cm^{-1}, has been studied. Infrared absorption measurements confirm the previous findings that the center dissociates already at about 450 °C and an apparent stability up to 1250 °C is due to efficient retrapping of H by Li_{Zn}. Secondary ion mass spectrometry data strongly indicate that Fe impurities prevent a reformation of OH-Li_{Zn} after dissociation. The formation of Fe-Li complexes is proposed as a mechanism for this behavior. Absorption lines due to Fe in as-grown and intentionally doped ZnO crystals are studied.

HL 100.9 Fri 11:45 EW 203

Effects of the growth temperature on the properties of RF sputtered $Zn_{1-x}Mg_xO$:Al thin films — •Philipp Schurig[1], Benedikt Kramm[1], Shengqiang Zhou[2], Angelika Polity[1], and Bruno K. Meyer[1] — [1]1. Physikalisches Insitut, Justus-Liebig-Universität Giessen, Deutschland — [2]Functional Materials, Helmholtz-Zentrum Dresden-Rossendorf, Germany

Transparent conductive materials (TCMs) are of major interest for optoelectronic or photovoltaic applications, i.e. ZnMgO:Al can be used as a window layer material or transparent electrode in solar cell applications. ZnMgO:Al can be tuned by variation of the magnesium content concerning the band gap or electrical properties, respectively. The thin films were deposited by RF sputtering on c sapphire and soda lime glass substrates. A ceramic ZnMgO:Al target was used as sputtering source.

The influence of the growth temperature on the structural, optical and electrical properties is investigated using various methods, e.g. XRD, SEM, XPS, UV-Vis NIR and Hall measurements. With increasing growth temperature the structure of the films changes from wurzite (low temp.) to rock salt-phase (high temp.), whereas the wurzite phase was the main interest in this research. With higher temperatures the ZnO (0 0 2) diffraction peak shifts to higher angles which indicates a higher magnesium content. The band gap also shifts to higher values, from 3.9 to 4.1 eV. The growth temperature influence on the electrical properties couldn't be determined, because other aspects do influence these as well, e.g. the grain size or the Mg content, respectively.

HL 100.10 Fri 12:00 EW 203

The influence of Al and Ga dopants on the structural, electrical and optical properties of (Mg,Zn)O thin films grown by PLD — •Abdurashid Mavlonov, Steffen Richter, Holger von Wenckstern, Rüdiger Schmidt-Grund, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig, Germany

We have investigated structural, electrical and optical properties of Al- and Ga-doped (Mg,Zn)O thin films in dependence on the doping and alloy concentration. For this purpose, the samples have been prepared with two perpendicular, lateral composition gradients (Mg composition is varied in one direction whereas the Al/Ga concentration is varied in a perpendicular direction) [1]. The thin films were grown by pulsed-laser deposition (PLD) using a threefold segmented PLD target, a growth temperature of 600°C and 2-inch in diameter $c-$plane sapphire substrates. With increasing free charge carrier concentration N_{Hall} in a range from 1×10^{19} to 3×10^{20} cm^{-3}, the dielectric functions (DF) of the films show drastic changes due to increased (a) free-carrier absorption in the infrared region and (b) the Burstein-Moss effect in the ultraviolet region [2]. It has been found that the dopant efficiency and mobility tend to decrease with increasing Mg content, showing significant dependence in the case of Ga-doped films which can be explained with increasing the density of acceptor like compensating defects.

[1] H. von Wenckstern *et al.*: CrystEngComm 15, 10020 (2013).
[2] H. Fujiwara and M. Kondo, PRB 71, 075109 (2005).

HL 101: Frontiers of electronic structure theory: Many-body effects on the nano-scale

Time: Friday 9:30–12:15 Location: H 0105

Invited Talk HL 101.1 Fri 9:30 H 0105
Excitations and charge transfer phenomena in C based systems — •Elisa Molinari — University of Modena and Reggio Emilia, Modena, Italy — CNR, Istituto Nanoscienze, Modena, Italy

Excitonic effects control excitations and optical spectra in graphene-based nanostructures and related polymers [1], as well as in interacting C-based molecular systems of relevance for photovoltaics [2]. I will show results from ab-initio many body perturbation theory and discuss their implications for spectroscopies and for a realistic description of ultrafast charge separation phenomena.

[1] R. Denk et al, Nat Commun 5, 4253 (2014); A. Batra et al, Chem Sci 5, 4419-4423 (2014); L. Massimi et al, J. Phys. Chem C, in press. [2] S. M. Falke et al, Science 344, 1001-1005 (2014).

Invited Talk HL 101.2 Fri 10:00 H 0105
Towards optimal correlation factors for many-electron perturbation theories — •Andreas Grüneis — Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — Universität Wien, Vienna, Austria

Many electron perturbation theories such as the coupled-cluster method form a hierarchy of increasingly accurate approximations to the electronic ground state wave function. This presentation will overview recent progress in applying coupled-cluster methods to solids and techniques to reduce their computational cost such as explicit correlation methods [1,2]. Furthermore applications to archetypal solid state systems as well as the uniform electron gas model system will be discussed [3].

[1] G. H. Booth, A. Grüneis, G. Kresse and A. Alavi, Nature 493, 365-370 (2013).

[2] A. Grüneis, J.J. Shepherd, A. Alavi, D.P. Tew, G.H. Booth, The Journal of chemical physics 139 (8), 084112 (2013).

[3] J.J. Shepherd, A. Grüneis, Physical Review Letters 110 (22), 226401 (2013).

Invited Talk HL 101.3 Fri 10:30 H 0105
Towards an ab-initio description of high temperature superconductivity — •Garnet Chan — Department of Chemistry, Princeton University, United States NJ08544

I will describe our continued efforts in developing ab-initio many-body theory in the condensed phase with a view to a first principles description of a cuprate phase diagram.

Coffee break

Invited Talk HL 101.4 Fri 11:15 H 0105
Correlation effects in unconventional superconductors: from micro- to nano- and macroscales. — •Roser Valenti — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Strasse 1, 60438 Frankfurt am Main, Germany

The combination of ab initio density functional theory with dynamical mean field theory (DFT+DMFT) has been proven to be a powerful approach for describing correlation effects in solid state systems at the microscopic level. In this talk we will focus on recent progress on this method and its application to unconventional superconductors such as Fe-pnictides, organic charge-transfer salts as well as correlated Dirac metals [1,2,3]. Further, we shall discuss the manifestation of such effects at the nano- and macroscales.

[1] I. I. Mazin *et al.* Nature Communications 5, 4261 (2014)
[2] S. Backes *et al.* New J. Phys. 16, 083025 (2014)
[3] J. Ferber *et al.* Phys. Rev. B 89, 205106 (2014)

Invited Talk HL 101.5 Fri 11:45 H 0105
Stochastic density functional and GW theories scaling linearly with system size — •Roi Baer[1], Daniel Neuhauser[2], and Eran Rabani[3] — [1]Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, The Hebrew University of Jerusalem, 91904 Israel. — [2]Department of Chemistry and Biochemistry, University of California, Los Angeles Los Angeles, CA 90095-1569 USA. — [3]Department of Chemistry, University of California, Berkeley, Berkeley, CA 94720 USA.

Kohn-Sham density functional theory (KS-DFT) is formulated as a statistical theory in which the electron density is determined from an average of correlated stochastic densities in a trace formula. Method allows reliable estimates of the electronic band structure, forces on nuclei, density and moments etc. "Self-averaging" leads to sublinear scaling. An embedded fragment stochastic DFT greatly decreases statistical fluctuations. Based on stochastic DFT a GW method is developed scaling linearly with system size. We demonstrate the results on silicon nanocrystals and large water clusters. References: *Phys. Rev. Lett. 111, 106402 (2013). *Phys. Rev. Lett. 113, 076402 (2014). *J. Chem. Phys. 141, 041102 (2014).

HL 102: Organic electronics and photovoltaics: Devices (CPP with HL/TT)

Time: Friday 9:30–12:00 Location: C 130

Invited Talk HL 102.1 Fri 9:30 C 130
Strong and switchable magnetic couplings in molecular semiconductor films — •Michele Serri[1], Wei Wu[1,2], Luke Fleet[1], Cyrus Hirjibehedin[2], Nicholas Harrison[1], Chris Kay[2], Andrew Fisher[2], Gabriel Aeppli[2], and Sandrine Heutz[1] — [1]London Centre for Nanotechnology, Imperial College London, UK — [2]London Centre for Nanotechnology, University College London, UK

Polyaromatic molecular thin films are well established as alternative semiconductors, but their magnetic properties have received less attention. This presentation will focus on phthalocyanines (Pc), archetypal molecular semiconductors that can ligate spin-bearing transition metals at their centre. They can be processed as thin films and nanowires [1] from the vapour phase and crystallise as a range of polymorphs. This leads to the formation of spin chains, and may give rise to magnetic exchange whose sign and magnitude depends on the nature of the transition metal and crystal structure [2]. A recent milestone was reached by CoPc, which exhibits antiferromagnetic coupling, with an exchange energy reaching 100 K [3]. This interaction is up to two orders of magnitude larger than in other first-row transition metal Pcs and can be obtained on flexible plastic substrates.

[1] Wang et al. ACS Nano 4 (2010) 3921. [2] Heutz et al. Adv. Mater. 19 (2007) 3618. [3] Serri et al. Nat. Commun. 5 (2014) 3079.

15 min. break

HL 102.2 Fri 10:15 C 130
Effects of Coulomb repulsion on conductance switching in organic molecules — •Irina Petreska[1,2] and Gertrud Zwicknagl[1] — [1]Institut für Mathematische Physik, Technische Universität Braunschweig, 38 106 Braunschweig, Germany — [2]Faculty of Natural Sciences and Mathematics, Ss. Cyril and Methodius University, 1 000 Skopje, Republic of Macedonia

Charge transfer in phenylene ethynylene oligomers (OPEs), using realistically estimated effective model parameters from first principles is studied by a combined, ab initio and model approach. The aim of our work is to investigate the Coulomb correlation effects on conductance switching in OPEs. In the proposed model, molecular electronic system is restricted to one-level coupled to metallic leads, described by a two-site Hubbard Hamiltonian. Comparison of the current-voltage curves, obtained from rate equations, for the planar and perpendicular conformer, clearly demonstrates enhancement of the switching process due to two-particle correlations.

HL 102.3 Fri 10:30 C 130
Enhanced performance of polymeric electron injection layers for OLEDs by the use of a solvent-additive. — •Sebastian Stolz[1,5], Martin Petzoldt[2,5], Naresh Kotadiya[1,5], Eric Mankel[3,5], Manuel Hamburger[2,5], Uli Lemmer[1,4], Norman Mechau[1,5], and Gerardo Hernandez-Sosa[1,5] — [1]Karlsruhe

Institute of Technology, Light Technology Institute — [2]University of Heidelberg, Institute of Organic Chemistry — [3]Technische Universität Darmstadt, Materials Science Institute, Surface Science Division — [4]Karlsruhe Institute of Technology, Institute of Microstructure Technology — [5]InnovationLab GmbH, Heidelberg

In this work, we investigate an amino-functionalized polyfluorene as electron injection layer in OLEDs. We demonstrate that its performance can be considerably increased by adding a functionalized alkane to the polyfluorene solution. X-ray photoelectron spectroscopy shows that the polymer thickness decreases with increasing additive concentration which indicates a better packing of the polymers. At the same time, Ultraviolet photoelectron spectroscopy reveals that the cathode work-function decreases with increasing additive concentration. Finally, we solution process OLEDs that use a PPV derivative commonly known as Super-Yellow as emitting layer and the polyfluorene in combination with silver as cathode layer. OLEDs, that use a mixture of functionalized alkane and polyfluorene, exhibit an about 0.8 eV lower turn-on voltage while the maximum luminance is almost doubled compared to OLEDs without additive. Furthermore, operational lifetimes are improved by a factor of two.

HL 102.4 Fri 10:45 C 130

Modeling of organic semiconductors: from molecular to device properties — Pascal Kordt[1], Mustapha Al Helwi[2,3], Wolfgang Kowalsky[3], Falk May[4], Alexander Badinski[5], Christian Lennartz[4], and •Denis Andrienko[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]BASF SE, GVE/M-B009, 67056 Ludwigshafen, Germany — [3]IHF Institut, Technische Universität Braunschweig, Brunswick, Germany — [4]BASF SE, GVE/M-B009, 67056 Ludwigshafen, Germany — [5]BASF SE, GVM/S-B009, 67056 Ludwigshafen, Germany

We review the progress in modeling of charge transport in disordered organic semiconductors on various length-scales, from atomistic to macroscopic. This includes evaluation of charge transfer rates from first principles, parametrization of coarse-grained lattice and off-lattice models, and solving the master and drift-diffusion equations. Special attention is paid to linking the length-scales and improving the efficiency of the methods. All techniques are illustrated on an amorphous organic semiconductor, DPBIC, a hole conductor and electron blocker used in state of the art organic light emitting diodes (OLEDs). The outlined multiscale scheme can be used to predict OLED properties without fitting parameters, starting from chemical structures of compounds.

HL 102.5 Fri 11:00 C 130

Combined electrical and optical analysis of the efficiency roll-off in phosphorescent organic light-emitting diodes — Sebastian Wehrmeister[1], •Tobias D. Schmidt[1], Lars Jäger[1], Thomas Wehlus[2], Andreas F. Rausch[2], Thilo C. G. Reusch[2], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg, 86153 Augsburg — [2]OSRAM OLED GmbH, 93049 Regensburg

We present a method for a comprehensive analysis of the efficiency roll-off with current density in phosphorescent organic light-emitting diodes (OLEDs). By combining electrical and optical excitation in time-resolved spectroscopic experiments we are able to measure the excited states lifetime for different driving conditions. It is thus possible to correlate changes of the triplet lifetime with a decrease of the radiative quantum efficiency of the emitting system due to exciton quenching processes. As compared to the conventional analysis of the measured external quantum efficiency (EQE) in dependence of the applied current density, the lifetime analysis is not affected by changes of the charge carrier balance with current, which can have a significant impact on the interpretation of the results. With this method we show that triplet-polaron quenching is the dominating quenching mechanism for the red phosphorescent emitter $Ir(MDQ)_2(acac)$ doped into an α-NPD matrix up to current densities of $100\,mA/cm^2$.

HL 102.6 Fri 11:15 C 130

Influence of Molecular Orientation on the Coupling of Excitons to Surface Plasmons in Semitransparent Inverted Organic Solar Cells — •Mark Gruber, Michael Mayr, Björn Gallheber, and Wolfgang Brütting — Institute for Physics, University of Augsburg, Germany

To prove the principle of coupling between surface plasmons (SPs) and excitons, we investigated semi-transparent organic solar cells, in which SPs are excited at interfaces of thin metal films and a dielectric medium by using a Kretschmann configuration setup. Therefore it is essential, that the dielectric medium has a smaller refractive index than glass, e.g. LiF or air.

To compare the SP coupling to different orientations of the transition dipole moment, two donor materials were used, diindenoperylene (DIP) and dibenzo-tetraphenyl-periflanthen (DBP). Both molecules have the transition dipole moment along the long axis. While DIP crystallizes with nearly upright standing molecules on the underlying PCBM film, DBP grows amorphous with predominantly lying molecules.[1,2] To locate the angular position of the SP resonance the reflectance of the OPVC is measured angle dependent. A simultaneously measured photo current reveals the impact of SPs in these OPVCs. The use of different donors shows, that coupling from SPs to excitons only leads to a positive effect for upright-standing transition dipole moment orientation.

[1] Wagner et al., Adv. Func. Mater. **20**, 4295, 2010.
[2] Grob et al., Appl. Phys. Lett. **104**, 213304, 2014.

Invited Talk HL 102.7 Fri 11:30 C 130

Excitonic phenomena in molecular semiconductors — •Jens Pflaum — Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ZAE Bayern, 97074 Würzburg

Excitons constitute the primary electron-hole excitation in organic solid states and offer a broad range of photo-physical phenomena. In this talk we will address two key aspects of excitonic states in molecular semiconductors: i) their sensitivity to structural ordering on various length scales and ii) their implementation as recombination sites yielding access to microscopic current characteristics.

In case of i), we will discuss the impact of molecular packing on the exciton motion [1] and how long-range exciton diffusion enables access to boundary-induced trap states that might lead to suppression of otherwise prominent singlet exciton decay channels [2]. Regarding ii), the non-invasive optical read-out of molecular recombination dynamics will be demonstrated to provide information on the local current density [3]. As a consequence, by utilizing the triplet emission of suited molecules this approach paves the way towards electrically driven single photon sources operating at room temperature [4]. Financial support within the DFG research programme SPP1355 and FOR1809 is acknowledged.

[1] A. K. Topczak, et al., Phys. Rev. B 89, 201203(R) (2014).
[2] B. Gieseking, et al., Phys. Rev. B 90, 205305 (2014).
[3] B. Stender, et al., Adv. Mater. 25, 2943 (2013).
[4] M. Nothaft, et al., Nature Comm. 3, 628 (2012).

HL 103: Spintronics incl. quantum dynamics (MA with HL/TT)

Time: Friday 9:30–12:00 Location: EB 202

Invited Talk HL 103.1 Fri 9:30 EB 202

Antiferromagnetic spintronics — •Tomas Jungwirth — Institute of Physics v.v.i., ASCR, Prague, Czech Republic

Atiferromagnets (AFMs) have for decades played a passive role in conventional spin-valve structures where they provide pinning of the reference ferromagnetic layer. This implies that on one hand, incorporation of some AFM materials in common spintronic structures is well established. On the other hand, limiting their utility to a passive pinning role leaves a broad range of spintronic phenomena and functionalities based on AFMs virtually unexplored. Apart from the insensitivity to magnetic fields and the lack of stray fields, AFMs are common among metals, semiconductors, and insulators and can have orders of magnitude shorter spin-dynamics timescales, to name a few immediate merits of the foreseen concept of AFM spintronics. Several non-relativistic and relativistic spin-transport phenomena have been proposed for AFMs to complement or replace ferromagnets in active parts of spintronic devices. We will focus on the theory of relativistic phenomena and their utility in experimental AFM magneto-resistors, memories, and structures in which AFMs are employed to control ferromagnets electrically.

J. Zelezny et al., Phys. Rev. Lett. 113 (2014) 157201 I. Fina et al., Nature Commun. 5 (2014) 4671 X. Marti et al., Nature Mater. 13 (2014) 367 P. Wadley et al., Nature Commun. 4 (2013) 2322 B.G. Park et al., Nature Mater. 10 (2011) 347

HL 103.2 Fri 10:00 EB 202

Stability of a single spin against readout — •Christoph Hübner[1], Benjamin Baxevanis[1,2], Alexander A. Khajetoorians[3,4], and Daniela Pfannkuche[1] — [1]I. Institute for Theoretical Physics, Hamburg University, Hamburg, Germany — [2]Lorentz Institute, Leiden University, Leiden, The Netherlands — [3]Institute of Applied Physics, Hamburg University, Hamburg, Germany — [4]Institute of Applied Physics, Radboud University Nijmegen, Nijmegen, The Netherlands

A magnetic atom or cluster is extremely sensitive to interactions with a scanning tunneling microscope (STM), that is used to read and write the magnetic state [1]. On the other hand the symmetry of the substrate allows magnetic adatoms to retain their magnetization for minutes, which is extremely long on an atomic time scale [2]. We systematically study this protection against magnetization fluctuations in the presence of a magnetic field and scattering with electrons from the STM and substrate with a non-equilibrium master equation. A combination of spin and substrate symmetry is proposed that produces a stable magnetic orientation even in the presence of a magnetic field [3]. Additionally characteristic features are presented that allow to deduce the spin and substrate symmetry by measurement.

[1] A. A. Khajetoorians et al., Science 339, 55 (2013)
[2] T. Miyamachi et al., Nature 503, 242 (2013)
[3] C. Hübner et al., Phys. Rev. B 90, 155134 (2014)

HL 103.3 Fri 10:15 EB 202

Electric field as a tool for tuning quantum entanglement in supported clusters — •Oleg O. Brovko, Oleg V. Farberovich, and Valeri S. Stepanyuk — Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

Electric field has been recently gaining in reputation as a versatile tool for tuning adsorption, electronic and magnetic properties of nanostructures. In the present contribution we show that using this tool it is also possible to tune quantum entanglement of spins in small clusters on metallic surfaces. Relying on a combination of ab initio and Heisenberg-Dirac-Van Vleck quantum spin Hamiltonian calculations we show by the example of a typical transitional metal dimer (Mn) on Ag(001) surface, that in an inherently unentangled system, electric field can "switch on" the entanglement and change its critical temperature parameter by orders of magnitude. The physical mechanism allowing such rigorous control of entanglement by electric field is shown to be the field- induced change in the internal coupling of the supported nanostructure.

HL 103.4 Fri 10:30 EB 202

Transmission through correlated Cu_nCoCu_n heterostructures — •Liviu Chioncel[1], Cristian Morari[2], Ivan Runger[3], Andrea Drogetti[3], Andreas Oestlin[4], Ulrich Eckern[5], and Andrei Postnikov[6] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D - 86135 Augsburg, Germany — [2]National Institute for Research and Development of Isotopic and Molecular Technologies, 65-103 Donath, RO-400293 Cluj Napoca, Romania — [3]School of Physics and CRANN, Trinity College, Dublin 2, Ireland — [4]Department of Materials Science and Engineering, Applied Materials Physics, KTH Royal Institute of Technology, Stockholm SE - 100 44, Sweden — [5]Theoretical Physics II, Institute of Physics, University of Augsburg, D - 86135 Augsburg, Germany — [6]LCP-A2MC, Institute Jean Barriol, University of Lorraine 1, Bd Arago, F - 57078 Metz, France

We study the effects of local electronic interactions and finite temperatures upon the transmission across the Cu_4CoCu_4 metallic heterostructure in a combined density functional and dynamical mean field theory. We show that the total transmission at the Fermi level is reduced as the electronic correlations are taken into account via a local but dynamic self-energy, whereby such a reduction is more pronounced in the minority spin channel. Consequently, the spin polarization of the transmission increases. Our results also demonstrate that the enhancement in spin contrast is in mainly driven by interaction rather than finite temperature fluctuations.

HL 103.5 Fri 10:45 EB 202

Tricky details of tunnel magnetoresistance — •Christian Franz, Michael Czerner, and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University, Giessen, Germany

The basic mechanism responsible for the large TMR in coherent tunnel junctions has already been clarified in the first publications [1,2]. These predictions initiated a broad investigation continuing for more than a decade. Nevertheless, the quantitative understanding of TMR is still incomplete. In particular, the agreement between experiments and calculations remains deficient. The reason for these shortcomings is a complicated interplay of many effects, several of which are not yet fully understood.

We contribute by investigating several effects in great detail using advanced *ab initio* methods [3]. In particular, we discuss the effects of disorder, several interface resonance states and bulk states of different materials. These effects are illustrated by the example of $Fe_{1-x}Co_x$ alloys as ferromagnetic layers [4] which show substitutional disorder for finite concentrations, a complicated concentration dependence of the interface resonance states and variety of bulk states which become available via band filling.

[1] W.H. Butler, X.-G. Zhang, T.C. Schulthess, J.M. MacLaren, Phys. Rev. B 63, 054416 (2001)
[2] J. Mathon, A. Umerski, Phys. Rev. B 63, 220403 (2001).
[3] C. Franz, M. Czerner, C. Heiliger, J. Phys.: Condens. Matter 25, 425301 (2013).
[4] C. Franz, M. Czerner, C. Heiliger, Phys. Rev. B 88, 094421 (2013).

HL 103.6 Fri 11:00 EB 202

Electronic transport in carbon nanotube quantum dots functionalized with magnetic molecules — •Carola Meyer[1,2], Claire Besson[1,2], Michael Schnee[1,2], Henrik Flötotto[3], Robert Frielinghaus[1,2], Lothar Houben[2,4], Paul Kögerler[2,3], and Claus M. Schneider[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA - Fundamentals of Future Information Technologies, Germany — [3]RWTH Aachen University, Institute for Inorganic Chemistry, 52074 Aachen, Germany — [4]Ernst Ruska-Center for Microscopy and Spectroscopy with Electrons, Forschungszentrum Jülich, 52425 Jülich, Germany

Transport devices built from individual functionalized carbon nanotubes (CNTs) show great potential for instance in spintronics applications. We graft magnetic complexes to CNTs [1]. The route for the CNT functionalization is very general, based on ligand exchange, and can be applied for different molecules, in particular SMMs. We present first quantum transport measurements on individual functionalized CNTs that prove only weak distortion of the electron wave function by the covalent functionalization. The g-factor of the chemically modified CNT quantum dot (QD) is much smaller compared to pristine CNT QDs indicating spin interaction between the QD and the attached molecules. A clear random telegraph signal is recorded de-

pending on the states of the QD. Origin of timescale and energy of the signal are discussed. [1] Meyer, C. et al., Phys. Status Solidi B 249, 2412(2012)

HL 103.7 Fri 11:15 EB 202

Spin transport and its gate-induced modulation in non-degenerate Si at room temperature — •Masashi Shiraishi[1], Tomoyuki Sasaki[2], Yuichiro Ando[1], Makoto Kameno[1], Hayato Koike[2], Toshio Suzuki[3], and Tohru Oikawa[2] — [1]Kyoto Univ., Japan — [2]TDK Corporation, Japan — [3]AIT, Akita Prefectural Industrial Center, Japan

Si spintronics has been collecting tremendous attention, because of its long spin lifetime and achievement of spin transport at room temperature (RT) [1,2]. In the course of our study in Si spintronics, we have revealed that the so-called 3-terminal method [3] cannot completely preclude spurious signals [4], which is now widely recognized [5-7]. Here, we introduce some methods enabling to avoid detection of spurious signals, and report on reliable RT spin transport in non-degenerate n-type Si and gate-induced modulation of spin signals [8]. This is the first experimental demonstration of spin MOSFET at RT, which can pave a way to establish spin-based logic systems.

[1] T. Suzuki, T. Sasaki, M. Shiraishi et al., Appl. Phys. Express 4, 023004 (2011). [2] E. Shikoh, M. Shiraishi et al., Phys. Rev. Lett. 110, 127201 (2013). [3] S. Dash et al., Nature 462, 491 (2009). [4] Y. Aoki, M. Shiraishi et al., Phys. Rev. B86, 081201(R) (2012). [5] O. Txoperena et al., Appl. Phys. Lett. 102, 192406 (2013). [6] T. Uemura et al., Appl. Phys. Lett. 101, 132411 (2012). [7] O. Txoperena, H. Dery et al., Phys. Rev. Lett. 113, 146601 (2014). [8] T. Sasaki, M. Shiraishi et al., Phys. Rev. Applied 2, 034005 (2014).

HL 103.8 Fri 11:30 EB 202

Spin transfer by pure spin current at magnetic interfaces — •Wei Chen[1], Manfred Sigrist[2], Jairo Sinova[3], and Dirk Manske[1] — [1]Max Planck Institute for Solid State Research, Stuttgart — [2]ETH-Zurich, Zurich, Switzerland — [3]Johannes Gutenberg University-Mainz, Mainz

We present a microscopic theory for the spin transfer torque, spin pumping, spin mixing conductance, and Onsager relation caused by the pure spin current in the normal metal/ferromagnetic insulator bilayer (such as Pt/YIG) and normal metal/ferromagnetic metal/oxide trilayer (such as Pt/Co/AlO_x). The spin Hall effect in the normal metal generates a pure spin current which, upon quantum tunneling into the ferromagnet, causes the magnetization dynamics. The field-like and damping-like component of these spin-transfer quantities are expressed in terms of characteristic energy scales such as the insulating gap and $s-d$ hybridization, which are applicable to a wide range of materials, hence the result can guide the search for materials that have a particular function in spin transport.

HL 103.9 Fri 11:45 EB 202

Spin pumping experiments in Gadolinium Iron Garnet/Pt thin films — Johannes Lotze[1], •Kathrin Ganzhorn[1], Stephan Geprägs[1], Francesco Della Coletta[1], Rudolf Gross[1,2,3], and Sebastian T. B. Goennenwein[1,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, TU München, Garching, Germany — [3]Nanosystems Initiative Munich, München, Germany

Magnetically compensated rare earth garnets, such as Gadolinium Iron Garnet ($Gd_3Fe_5O_{12}$, GdIG), exhibit a pronounced temperature dependence of the sublattice magnetizations, leading to a magnetization compensation temperature $T_{\mathrm{comp,\,M}}$. The investigation of spin currents in GdIG/Pt heterostructures thus can give important insight into the processes involved in the spin current generation in ferrimagnetic insulator/Pt bilayers. Temperature dependent spin Seebeck effect experiments have recently been performed in GdIG/Pt thin film samples [1], revealing two sign changes of the spin Seebeck voltage, a first one at $T_{\mathrm{comp,\,M}}$ and a second one at a lower temperature. We have performed microwave heating induced spin Seebeck together with spin pumping measurements as a function of temperature in doped GdIG/Pt heterostructures. Our experiments confirm the temperature dependent evolution of the spin Seebeck voltage reported in Ref. [1]. We critically discuss this evolution and compare it to the temperature dependence of the spin pumping voltage observed.

Financial support by DFG via SPP 1538 is gratefully acknowledged.

[1] S. Geprägs *et al.*, arXiv 1405.4971 (2014)

HL 104: Transport: Molecular electronics (TT with CPP/HL/MA/O)

Time: Friday 9:30–12:15 Location: H 0110

HL 104.1 Fri 9:30 H 0110

Phononic and thermoelectric properties of π-stacked molecular junctions — •Thomas Hellmuth[1,3], Marius Bürkle[2], and Fabian Pauly[1] — [1]Theorie der Nanostrukturen, Universität Konstanz, 78457 Konstanz, Germany — [2]Nanosystem Research Institute, National Institute of Advanced Industrial Science and Technology, Japan — [3]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, 76131 Karlsruhe,Germany

We present our newly developed approach to compute phonon thermal transport through nanosystems from first principles using density functional theory combined with non-equilibrium Green's function techniques. Combining both electron and phonon transport, we analyze the heat transport and thermoelectric properties of π-stacked paracyclophane molecules contacted to gold electrodes [1]. We show that, depending on temperature, the phononic contribution to the heat conductance is a factor of about 5 larger than the electronic one. By calculating the thermoelectric coefficients in linear response, we estimate the figure of merit ZT of the single-molecule junctions for different molecular lengths and substituents.

[1] M. Bürkle, T. J. Hellmuth, F. Pauly, Y. Asai, submitted.

HL 104.2 Fri 9:45 H 0110

Conductance and thermopower of C_{82} and endohedral metallofullerene molecular junctions with Au electrodes — •Marius Buerkle[1], See Kei Lee[2], Ryo Yamada[2], Hirokazu Tada[2], and Yoshihiro Asai[1] — [1]AIST, NRI, Tsukuba, Japan — [2]Graduate School of Engineering Science, Osaka University, Japan

By combining STM based conductance and thermopower measurements with first-principle transport calculations we investigate the thermoelectric properties of single C_{82} molecules, and its endohedral metallofullerene (EMF) derivatives Gd@C_{82} and Ce@C_{82} bridging Au electrodes. All three molecular junctions show a comparable conductance of around 0.2 G0 and a negative thermopower indicating electron-like transport through the lowest unoccupied molecular orbital (LUMO). However, for the EMF junctions a much larger thermopower is observed which we can relate to changes in the electronic structure induced by the lanthanide atoms.

HL 104.3 Fri 10:00 H 0110

A scaling relation in the vibronic contribution to the current noise — •Yoshihiro Asai — AIST, Tsukuba, Japan

The electron-phonon coupling effect on the electric current noise is studied based on the fully self-consistent theory of electron and phonon currents (SCEPC) given in terms of the Keldysh Greens function method [1], which has been successful in describing the local heating phenomena [2] and the temperature dependence of the electric conductance [3,4]. Based on the theoretical result on the noise accompanying the vibronic current, we will discuss a scaling relation between the two quantities derived from the current noise and the electric conductance at finite bias voltage. We found that the scaling relation holds when the dynamics of the electron satisfies a specific condition. We will describe these in the talk.

[1] Y. Asai, Phys. Rev. B 78, 045434-1-24 (2008).
[2] Y. Asai, Phys. Rev. B, 84, 085436-1-7 (2011).
[3] S.-K. Lee, R. Yamada, S.Tanaka, G.-S. Chang, Y. Asai, and H. Tada, ACS Nano, 6, 5078-5082 (2012).
[4] Y. Asai, Phys. Rev. B 86, 201405(R)-1-4 (2012).

HL 104.4 Fri 10:15 H 0110

Thermo-voltage of nano-thermocouples — •Ayelet Ofarim, Bastian Kopp, Johannes Boneberg, Paul Leiderer, and Elke Scheer — University of Konstanz, Department of Physics, Konstanz,

Germany

As the down-scaling of electronic components continues, engineering the devices has become a challenge, in particular in view of energy and heat management. Study of thermoelectric effects in nanostructures gives important additional information about charge transport, also regarding possible life-time limiting phenomena and applications for the conversion of light energy via heat into electrical energy. The scope of this presentation is to gain deep insight into the charge transport mechanism, by studying thermo-voltage effects of metallic atomic-sized contacts [1]. We present the concept for determination of the thermo-voltage of nano-thermocouples, using a novel mechanically-controlled break junction (MCBJ) mechanism. A technique to create and detect a temperature gradient, using laser irradiation, is also presented.

[1] B. Kopp, Z. Yi, D. Benner, F. Q. Xie, C. Obermair, T. Schimmel, J. Bonenberg, P. Leiderer and E. Scheer, Beilstein J. Nanotechnol. 3, 703 (2012).

HL 104.5 Fri 10:30 H 0110

Quantum interference in thermoelectric molecular junctions: A toy model perspective — •Daijiro Nozaki[1], Stas. M. Avdoshenko[2], Haldun Sevinçli[3], and Gianaurelio Cuniberti[1,4,5] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany — [2]Department of Chemistry and Institute for Computational Engineering and Sciences, University of Texas at Austin, USA — [3]Department of Materials Science and Engineering, Izmir Institute of Technology, Turkey — [4]Dresden Center for Computational Materials Science (DCCMS), TU Dresden, Germany — [5]Center for Advancing Electronics Dresden (cfAED), TU Dresden, Germany

In order to reveal the relationship between the line shape of the transmission spectra affected by quantum interference and the electronic structures, we consider a homogeneous toy model where all on-site energies are identical and model four types of molecular junctions due to their topological connectivities. We systematically analyze their transmission spectra, density of states, and thermoelectric properties. Even without the degree of freedom for on-site energies an asymmetric Fano peak could be realized in the homogeneous systems with the cyclic configuration. We also calculate the thermoelectric properties of the model systems with and without fluctuation of on-site energies. Even under the fluctuation of the on-site energies, the finite thermoelectrics are preserved for the Fano resonance, thus cyclic configuration is promising for thermoelectric applications.

[1] D. Nozaki, H. Sevinçli, S. M. Avdoshenko, G. Cuniberti, J. Appl. Phys. 117, 074308 (2014).

HL 104.6 Fri 10:45 H 0110

Effect of nonadiabatic electronic-vibrational interactions on the transport properties of single-molecule junctions — •André Erpenbeck[1], Rainer Härtle[2], and Michael Thoss[1] — [1]Institut für Theoretische Physik und Interdisziplinäres Zentrum für Molekulare Materialien (ICMM), Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany — [2]nstitut für theoretische Physik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany

The interaction between electronic and vibrational degrees of freedom in single-molecule junctions may result from the dependence of the electronic energies or the electronic states of the molecular bridge on the nuclear displacement. The latter mechanism leads to a direct coupling between different electronic states and is referred to as nonadiabatic electronic-vibrational coupling. Employing nonequilibrium Green's functions in combination with the self-consistent Born approximation, we study the influence of nonadiabatic electronic-vibrational coupling in model molecular junctions. Thereby we distinguish between systems with well separated and quasi-degenerate electronic levels. Our results show that the nonadiabatic electronic-vibrational interaction can have a significant influence on the transport properties [1]. The underlying mechanisms are analyzed with respect to the different signatures of nonadiabatic and adiabatic electronic-vibrational coupling, the relevant transport channels, negative differential resistance and quantum interference effects.

[1] A. Erpenbeck et. al., arXiv:1411.5844 (2014)

15 min. break.

HL 104.7 Fri 11:15 H 0110

Significant role of end groups in electrical transport through molecules — •Karthiga Kanthasamy[1], Markus Ring[2], Fabian Pauly[2], Christoph Tegenkamp[1], and Herbert Pfnür[1] — [1]Institut für Festkörperphysik, Leibniz Universität, Hannover, Germany — [2]Fachbereich Physik, Universität Konstanz, Germany

Mechanically controllable break junction (MCBJ) technique is used to investigate the electronic properties of ferrocene and phenyl based molecules with different end groups. Stepwise changes in conductance are observed below 1Go after insertion of the molecules. The junctions are opened in vacuum and IV curves are measured for various distances between the electrodes. Detailed analysis of IV curves shows characteristic peaks in the first-order derivative for ferrocene dithiol (FDT) molecules, which are absent in ferrocene diamine (FDA) and biphenyl dithiol (BPDT). For FDT, in the range of 0.56Go to 0.09Go, there are two symmetric peaks, whose energy difference increases from 60 meV to 160 meV with increasing contact distance. Above 0.56Go or below 0.01Go, symmetric peaks are absent. The FDT molecules show typically a one order of magnitude higher conductance than FDA and BPDT. The IV graph for FDT is linear, i.e., it has metallic characteristics, while FDA and BPDT are dominated by tunneling. Theoretical calculations for the molecules in different configurations between the gold electrodes are performed based on density functional theory and the non-equilibrium Green's function formalism. Both elastic transport properties and inelastic electron tunneling spectra are studied to explain the experimental observations.

HL 104.8 Fri 11:30 H 0110

Photoinduced transient current through a molecular junction: Effects of lead excitation — •Yaroslav Zelinskyy[1,2], Yoram Selzer[3], and Volkhard May[1] — [1]Institut für Physik, Humboldt Universität zu Berlin, Newtonstraße 15, D-12489 Berlin, Germany — [2]Bogolubov Institute for Theoretical Physics, National Academy of Science of Ukraine, 14-b Metrologichna str., UA-03683, Kiev, Ukraine — [3]School of Chemistry, Tel Aviv University, Ramat Aviv, 69978 Tel Aviv, Israel

Laser pulse induced transient currents through a molecular junction are studied in the framework of a density matrix theory. By focusing on the sequential transport regime two types of lead excitation are considered. Firstly, effects of collective plasmon excitations of the leads and their resonant coupling to molecular excitations are investigated. If such a resonant coupling cannot be realized a second excitation regime would be of interest. Now, the nonequilibrium dynamics of individual lead electrons affect the transient current formation. While a resonant coupling to lead plasmon excitations induces a remarkable current enhancement nonequilibrium electron distributions in the leads determine the transient current mainly by their thermalization process. The theoretical framework described above is used to analyze time-resolved conductance measurements of molecular junctions based on Ferrocene molecules.

[1] L. Wang and V. May, Phys.Chem.Chem.Phys. 13, 8755 (2011).
[2] Y. Zelinskyy and V. May, Nano Lett. 12, 446 (2012).
[3] Y. Zelinskyy, Y. Selzer and V. May, Phys. Rev. B (submitted)).

HL 104.9 Fri 11:45 H 0110

***Ab-initio* model of extended CNT-metal contact** — Artem Fediai[1,2,3], •Dmitry Ryndyk[1,2,3], and Gianaurelio Cuniberti[1,2,3] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — [2]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — [3]Dresden Center for Computational Materials Science (DCCMS), TU Dresden, 01062 Dresden, Germany

Relevant CNT-metal contacts belong to so-called extended type. Current flows from electrodes into CNT in a distributed manner, and contact resistance depends on the contact length. In such circumstances the standard *ab-initio* based transport techniques to calculate electron transport should be modified.

We have developed a special method which allows calculation of transport in the systems with metal-CNT contacts at *ab-initio* level. It takes into account both internal and external parts of the CNT-metal contact and requires simulation of the one principal and two auxiliary atomistic systems. Results of *ab-initio* calculations are then subjected to special treatment and being used in Green function formalism afterwards.

This method was applied to Al-CNT and Pd-CNT extended contacts. Results agree perfectly with existing experimental data being indeed obtained at a purely *ab-initio* level.

HL 104.10 Fri 12:00 H 0110

Hierarchical Quantum Master Equation Approach to Vibrationally Coupled Electron Transport in Single-Molecule Junctions — •Christian Schinabeck[1], Rainer Härtle[2], and Michael Thoss[1] — [1]Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany — [2]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 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 Markovian rate equations. Within the HQME framework, two different approaches are presented and compared, which describe the vibrational degrees of freedom as part of the system or the bath, respectively. The methodology is applied to a model molecular junction consisting of a molecular level coupled to fermionic leads as well as a vibrational mode. For this system, the accurate results of the hierarchical quantum master equation approach are compared with Markovian rate equation as well as fourth-order time-nonlocal master equation calculations in different parameter regimes. The convergence properties of the two HQME approaches are analyzed in detail.

[1] Y. Tanimura *et al.*, J. Phys. Soc. Jpn. 75, 082001 (2006).
[2] F. Jiang *et al.*, Phys. Rev. B 85, 245427 (2012).
[3] R. Härtle *et al.*, Phys. Rev. B 88, 235426 (2013).

HL 105: Transport: Majorana fermions (TT with DS/HL/MA/O)

Time: Friday 9:30–12:15 Location: H 0104

HL 105.1 Fri 9:30 H 0104

Majorana bound states in a Corbino geometry topological insulator Josephson junction — •Sunghun Park and Patrik Recher — Institute for Mathematical Physics, TU Braunschweig, Germany

An adiabatic exchange of Majorana bound states reveals their exotic anyonic nature. Here we propose an experimental setup consisting of a Corbino-geometry Josephson junction on the surface of a topological insulator, in which Majorana bound states can be created and transported. By solving the Bogoliubov-de Gennes equation, we show that two spatially separated Majorana bound states at zero excitation energy appear in the junction when two flux quanta are introduced, and that their positions can be moved by changing the superconducting phase difference across the junction. These features allow us to perform the exchange operation of the Majorana bound states if we vary the phase difference adiabatically.

HL 105.2 Fri 9:45 H 0104

Topological phases in magnetic adatom-chains on top of a Rashba superconducting surface — •Andreas Heimes, Daniel Mendler, and Panagiotis Kotetes — Institut für Theoretische Festkörperphysik, Karlsruher Institut für Technologie, 76131 Karlsruhe

We investigate a Majorana fermion (MF) platform consisting of a chain of magnetic adatoms placed on top of a conventional superconductor with Rashba spin-orbit coupling. By identifying the classical magnetic ground state of the adatom chain, we extract a phase diagram which exhibits ferromagnetic (FM), antiferromagnetic (AFM) as well as spiral orders. We determine the parameter regime for which the FM or AFM phases dominate over the spiral and perform a topological analysis of the low-energy electronic spectrum. To this end we derive an effective model relying on Shiba bound states. We find that for both magnetic patterns, FM and AFM, the hybrid system behaves as a topological superconductor which can harbor one or even two MFs per edge. We propose directions on how to experimentally access these different MF phases.

HL 105.3 Fri 10:00 H 0104

Localization length and non-adiabaticity - braiding errors in Majorana quantum wires — •Michael Sekania[1,3], Martin Greiter[1], Ronny Thomale[1], and Peter Schmitteckert[2] — [1]Institute for Theoretical Physics and Astrophysics, Julius-Maximilian University of Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, D-76344 Eggenstein-Leopoldshafen, Germany — [3]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany

Majorana fermions have been attracting substantial interest in recent years. Several experimental groups have already reported tentative observation of Majorana zero modes in quantum nanowires that are proximity-coupled to a bulk superconductor. The unambiguous detection of Majorana quasi-particles, however, has so far remained elusive. One of the ultimate experimental checks for the existence of Majorana zero modes would be a braiding experiment, that reveals the non-trivial braiding statistics of the Majorana fermions. We present numerical studies of the braiding of Majorana bound states (MBS) in presence of a quasi-particle background, and show braiding errors due to non-adiabaticity – which is a realistic scenario for experiments – and due to system sizes which are comparable to the localization length of the MBS. The latter seems to be the case for certain experimental realizations reported recently. We further address the influence of finite-range interactions on the braiding process.

HL 105.4 Fri 10:15 H 0104

Fractional Josephson Effect in HgTe based Josephson Junctions — •Jonas Wiedenmann[1], Erwann Bocquillon[1], Russel Deacon[2], Simon Hartinger[1], Luis Maier[1], Christopher Ames[1], Koji Ishibashi[2], Tarucha Seigo[3], Teun Klapwijk[4], Hartmut Buhmann[1], and Laurens Molenkamp[1] — [1]EP3, Physikalisches Institut, Universität Würzburg, Würzburg, Germany — [2]Advanced Device Laboratory, RIKEN, Japan — [3]Department of Applied Physics, Univeristy of Tokyo, Tokyo, Japan — [4]Kavli Institute of Technology, Delft University of Technology, Delft, The Netherlands

3D topological insulators are a new class of material in which electronic transport is governed by topological surface states while the bulk remains insulating. Due to the helical spin polarization of the surface states, the coupling to a conventional s-wave superconductor is predicted to lead to the emergence of zero-energy bound states at the S-TI interface. These gapless zero energy states (sometimes referred to as Majorana bound states) are topologically protected against scattering and thus give rise to a 4π periodic Josephson current.

We fabricated Josephson junctions based on the three dimensional topological insulator HgTe and study its response under external rf excitation. An unconventional A.C. Josephson effect is observed which leads us to the conclusion that a 4π contribution in the Josephson current is present. In addition to the observation of an unconventional excess current, this gives robust signatures of the presence of zero-energy states.

HL 105.5 Fri 10:30 H 0104

Josephson current and Majorana bound states through 2DEG with Spin-Orbit Interaction — •Pasquale Marra[1], Roberta Citro[1,2], and Alessandro Braggio[3] — [1]SPIN-CNR, I-84084 Fisciano (Salerno), Italy — [2]Dipartimento di Fisica "E. R. Caianiello", Universitá di Salerno, I-84084 Fisciano (Salerno), Italy — [3]SPIN-CNR, Via Dodecaneso 33, I-16146 Genova, Italy

We investigate the DC Josephson current in a two dimensional electron gas (2DEG) proximized with a s-wave superconductor, in the presence of spin-orbit interaction and magnetic field. Solving the Bogoliubov-De Gennes equations in the framework of a tight-binding Hamiltonian, we calculate the Andreev bound states, the Josephson current, and the Majorana polarization as a function of phase difference between the two superconductors. We therefore investigate the conditions under which Majorana bound states are localized at the system interfaces.

15 min. break.

HL 105.6 Fri 11:00 H 0104

Thermal conductance as a probe of the non-local order parameter for a topological superconductor with gauge fluctuations — •Fabian Hassler[1], Bernard van Heck[2], Emilio Cobanera[3], and Jascha Ulrch[1] — [1]JARA Institute for Quantum Information, RWTH Aachen University, 52056 Aachen, Germany —

[2]Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands — [3]Institute for Theoretical Physics, Leuvenlaan 4, 3584 CE Utrecht, The Netherlands

We investigate the effect of quantum phase slips on a helical quantum wire coupled to a superconductor by proximity. The effective low-energy description of the wire is that of a Majorana chain minimally coupled to a dynamical *2 gauge field. Hence the wire emulates a matter-coupled gauge theory, with fermion parity playing the role of the gauged global symmetry. Quantum phase slips lift the ground state degeneracy associated with unpaired Majorana edge modes at the ends of the chain, a change that can be understood as a transition between the confined and the Higgs-mechanism regimes of the gauge theory. We identify the quantization of thermal conductance at the transition as a robust experimental feature separating the two regimes. We explain this result by establishing a relation between thermal conductance and the Fredenhagen-Marcu string order-parameter for confinement in gauge theories. Our work indicates that thermal transport could serve as a measure of non-local order parameters for emergent or simulated topological quantum order.

HL 105.7 Fri 11:15 H 0104

Topological Kondo Effect in Transport through a Superconducting Wire with Multiple Majorana End States — •Oleksiy Kashuba and Carsten Timm — Institute für Theoretische Physik, Technische Universität Dresden

We investigate a system of multiple Majorana states at the end of a topological superconducting wire coupled to a normal lead. For a minimum of three Majorana fermions at the interface, we find nontrivial renormalization physics. Interface tunneling processes can be classified in terms of spin-1/2 and spin-3/2 irreducible representations of the SU(2) group. We show that the renormalization of the tunneling amplitudes belonging to different representations is completely different in that one type is suppressed, whereas the other is enhanced, depending on the sign of the interaction coupling. This results in distinct temperature dependencies of the tunneling current through the interface and different spin polarizations of this current.

HL 105.8 Fri 11:30 H 0104

Topological superconductivity in Rashba semiconductors without a Zeeman field — •Panagiotis Kotetes — Karlsruhe Institute of Technology

I propose new hybrid devices based on multichannel Rashba semiconductors, which harbor Majorana fermions (MFs) without a Zeeman field [1]. In contrast, magnetic fluxes, supercurrents or electric fields can be employed, yielding an enhanced device manipulability. The generic topological phase diagram exhibits features of quantum criticality and a rich interplay of phases with 0, 1 or 2 MFs per edge. The most prominent and experimentally feasible implementation, relies on the already existing platforms of InAs-2DEG on top of a Josephson junction. Appropriate design of the latter device, allows phases with 1 or 2 MFs, both detectable in zero-bias anomaly peaks with a single or double unit of conductance. The absence of the Zeeman field in these devices could be assisting for a Kondo-peak-free interpretation of the expected MF signatures.

[1] P. Kotetes, arXiv:1409.5264.

HL 105.9 Fri 11:45 H 0104

Majorana flat bands in anisotropic systems — •Daniel Mendler, Panagiotis Kotetes, and Gerd Schön — Institut für theoretische Festkörperphysik, Karlsruher Institut für Technologie

It has been recently proposed that topologically protected Majorana flat bands (MFBs) emerge in superconductors with nodal energy spectrum. In this work we introduce a new class of gapful superconductors, in which MFBs can occur due to strong anisotropy. The prototype system exhibiting this kind of behavior is the nematic $p_x + p_y$ spinless superconductor, which supports an edge MFB with controllable bandwidth. Our proposal can be for instance experimentally implemented in topological superconductors engineered from i. semiconductors with tunable spin-orbit coupling or ii. topological insulator surfaces with intrinsic magnetic order in proximity to a conventional SC. By investigating the topological properties of both setups, we show that their unique features render them feasible platforms for manipulating the Majorana fermion bandstructure and realizing MFBs.

HL 105.10 Fri 12:00 H 0104

Topological phases of interacting fermions in one-dimensional superconductor - normal metal geometry — Dganit Meidan[1,2], •Alessandro Romito[1], and Piet W. Brouwer[1] — [1]Department of Physics, Ben-Gurion University of the Negev, Beer-Sheva 84105, Israel — [2]Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany

One-dimensional superconductors can be in non-trivial topological phases harboring Majorana end-states, which possess non-abelian statistics. It has been recently established that in the presence of interactions the classification of topological superconducting phases can be significantly altered. Specifically, for one-dimensional superconductors possessing a time reversal symmetry (BDI class), interactions reduce the infinitely many non-interacting phases (Z topological index) to eight distinct ones (Z_8 topological index).

In this talk I will consider multi-mode superconducting wires in such BDI class when probed by an external contact, and discuss their low temperature and voltage bias transport properties. I will first show that the Andreev reflection component of the scattering matrix of the probing lead provides a topological index, r=-4, ..., 4, which distinguish the eight topological phases. The two topologically equivalent phases with r= 4,-4 support emergent many-body end states, which are identified to be a topologically protected Kondo-like resonance. The path in phase space that connects these equivalent phases crosses a non-fermi liquid fixed point where a multiple channel Kondo effect develops.

HL 106: Transport, magnetotransport and quantum Hall physics

Time: Friday 10:00–13:00 Location: EW 202

HL 106.1 Fri 10:00 EW 202

Fractional quantum Hall effect in monolayer and bilayer graphene: phase diagrams and edge excitations — •Maxim Kharitonov — Theoretische Physik IV, Universitaet Wuerzburg, 97074 Würzburg, Germany

We analytically investigate the fractional quantum Hall effect in monolayer and bilayer graphene at filling factors pertaining to the zero-energy Landau level, specifically concentrating on the order of the states in the valley-spin space. We obtain generic phase diagrams for the two-component states of arbitrary orbital structure, which turn out to be closely related to that of the $\nu = 0$ state. The transitions between different phases can in practice be realized by tilting the magnetic field and, in bilayer, by applying the perpendicular electric field. These transitions are accompanied by the transformations of the edge states, which could be detected in transport measurements.

HL 106.2 Fri 10:15 EW 202

Observation of quantum states bound by a magnetic field gradient — Bernd Schüler[1], Mihai Cerchez[1], •Thomas Heinzel[1], Dirk Reuter[2], Andreas Wieck[3], and Hengyi Xu[1] — [1]Inst. für Physik d. kondensierten Materie, HHU Düsseldorf — [2]Department Physik, Univ. Paderborn — [3]Angewandte Festkörperphysik, Ruhr-Universität Bochum

Resonant transmission through electronic quantum states that exist at the zero points of a magnetic field gradient inside a ballistic quantum wire is reported. Since the semiclassical motion along such a line of zero magnetic field takes place in form of unidirectional snake trajectories, these states have no classical equivalence. The existence of such quantum states has been predicted more than a decade ago by theoretical considerations.[1] We further show how their properties depend on the amplitude of the magnetic field profile as well as on the Fermi energy.[2]

[1]J. Reijniers et al., Europhys. Lett. 59, 749 (2002). [2] B. Schüler et al., Phys. Rev. B (Rapid Comm.), in print.

HL 106.3 Fri 10:30 EW 202

Snake orbit commensurability resonances in magneto-electric lateral superlattices — •Jakob Schluck[1], Stefan Fasbender[1], Thomas Heinzel[1], Dimitris Kazazis[2], Ulf Gennser[2], Klaus Pierz[3], and Hans Schumacher[3] — [1]Heinrich Heine Universität Düsseldorf — [2]CNRS-LPN, Marcoussis — [3]PTB Braunschweig

Hybrid lateral superlattices composed of a square array of antidots and a periodic magnetic modulation in one dimension are prepared in Ga[Al]As heterostructures. The two-dimensional electron gases exposed to these superlattices are characterized by magnetotransport experiments. The longitudinal magnetoresistivity ρ_{xx}, parallel to the magnetic modulation, shows pronounced resonances that originate from snake orbits that become commensurate with the antidot lattice for characteristic magnetic field amplitudes. The resistivity ρ_{yy} in the direction perpendicular to the magnetic modulation is governed by the magnetic barriers in series and shows weak antidot-induced modulations. Numerical simulations based on the classical Kubo model reproduce the most prominent features of the experimental data.

HL 106.4 Fri 10:45 EW 202

Spin polarization of composite fermions in the N=0 Landau Level — •Lina Bockhorn[1], Dieter Schuh[2], Christian Reichl[3], Werner Wegscheider[3], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover — [2]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93053 Regensburg — [3]Laboratorium für Festkörperphysik, ETH Zürich, CH-8093 Zürich

We study the fractional Quantum Hall effect (FQHE) in a high-mobility two-dimensional electron gas (2DEG) for different in-plane magnetic field components and by using a metallic topgate. Hall geometries are created by photolithography on a GaAs/GaAlAs quantum well containing a 2DEG. The high-mobility 2DEG has an electron density of $n_e = 3.2 \cdot 10^{11}\,cm^{-2}$ and a mobility of $\mu_e = 11.9 \cdot 10^6 cm^2/Vs$.

Around the filling factor ν=3/2 we observe spin transitions of several fractional filling factors ν=8/5, 11/7, 13/9, 10/7, 7/5, and 4/3 [1, 2]. The FQHE is understood in terms of weakly interacting composite fermions (CF). The CF theory provides an understanding of the spin physics of the FQHE. We also observe spin polarization of the fractions ν=6/5 and ν=9/7 which arise from interacting CF [3].

[1] R. G. Clark et al., Phys. Rev. Lett. 62, 1536 (1989).
[2] R. R. Du et al., Phys. Rev. Lett. 75, 3926 (1995).
[3] Y. Liu et al., Phys. Rev. B 90, 085301 (2014).

HL 106.5 Fri 11:00 EW 202

Voltage fluctuation to current converter with coupled quantum dots — •Pierre Pfeffer[1], Fabian Hartmann[1], Sven Höfling[1,2], Martin Kamp[1], and Lukas Worschech[1] — [1]Technische Physik, Physikalisches Institut, Universität Würzburg and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Am Hubland, D-97074 Würzburg, Germany — [2]SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, KY16 9SS, United Kingdom

Converting random fluctuations into useful energy is a major challenge in electronics and has triggered substantial experimental and theoretical work ranging from solid state to biological systems from the classical down to the quantum regime. Following recent proposals by Sothmann, Sanchez, Jordan and Büttiker [1,2], we realized a Coulomb-coupled quantum dot (QD) system and demonstrate a direct current in one part of the QD circuit due to charge fluctuations in the other part of the QD circuit. Both the direction and the amplitude of the current can be switched by an electric field superimposed on the open QD. No particle exchange between the two QD subsystems is involved and dependent on the noise amplitude, maximum output powers are found in the pW region.

[1] R. Sanchez and M. Büttiker, Phys. Rev. B 83, 085428 (2011).
[2] B. Sothmann, R. Sanchez, A. N. Jordan and M. Büttiker, Phys. Rev. B 85, 205301 (2012).

Coffee break

HL 106.6 Fri 11:30 EW 202

Polarized high power terahertz radiation induced oscillations of magnetoresistivity in GaAs heterostructures — •T. Herrmann[1], Z.D. Kvon[2], D.A. Kozlov[2], V.V. Bel'kov[3], B. Jentzsch[1], P. Olbrich[1], D. Weiss[1], and S.D. Ganichev[1] — [1]University of Regensburg, Regensburg, Germany — [2]Institute of Semiconductor Physics, Novosibirsk, Russia — [3]Ioffe Institute, St. Petersburg, Russia

We report on the study of terahertz (THz) high power laser radiation induced magnetoresistivity oscillations (TIRO) in a high density two-dimensional electron gas in GaAs quantum wells. TIRO were observed at He temperature in Corbino disc samples applying a magnetic field and nanosecond pulses of intense THz radiation of pulsed molecular laser operating in a frequency range from 0.6 to 2 THz [1]. The positions of oscillation maxima in magnetic field correspond to that of high harmonics of the cyclotron resonance (CR). Up to 9 harmonics are detected, having comparable amplitudes and yielding signals larger than that of the CR itself. Applying right- and left-handed polarized radiation we demonstrate that, while for a fixed magnetic field direction the CR is excited only for one light helicity the TIRO are insensitive to the radiation polarization state. Investigating TIRO for different power levels varying in the range from Watts to tens of kW we also show that the amplitude of the oscillations saturates with raising power.

[1] S.D. Ganichev and W. Prettl, Intense Terahertz Excitation of Semiconductors, Oxford University Press (2006)

HL 106.7 Fri 11:45 EW 202

Impurity induced phase transition in GaAs/AlGaAs two-dimensional electron gas — •Eddy P. Rugeramigabo, Lina Bockhorn, and Rolf J. Haug — Institute for Solid State Physics, Dep. Nanostructures, Leibniz Universität Hannover

A phase transition is observed at high magnetic fields in a two-dimensional electron gas (2DEG). The 2DEG is realized in a modulation Si-doped GaAs/AlGaAs quantum well (QW). Additionally, Si atoms were homogeneously incorporated in the GaAs QW layer. Here, they act as impurities. The 2DEG has an electron density of $n_e = 3.2{\cdot}10^{11}cm^{-2}$ and a mobility of $\mu_e = 1.2{\cdot}10^5 cm^2/Vs$.
We performed magnetotransport measurements between 30mK and 900mK. Magnetic field sweeps above 6.6T induce a phase transition at temperatures T<600mK. After the transition, we observe at low magnetic fields the formation of beating features in the Shubnikov-de Hass oscillations. At high magnetic fields, fractional filling factors between ν=2 and ν=1 become more developed.
The new phase has a metastable equilibrium at magnetic fields between 7T and 13T ($2<\nu<1$). Such a metastable state of the 2DEG was also reported by Kukushkin et al.[1], but for magnetic field range of $1<\nu<1/2$. We attribute our observations to a change in the scattering potential of the impurity states within the 2DEG. This can be e.g. frozen spin polarization caused by high magnetic fields at low temperatures.

[1] I. V. Kukushkin, et al., Phys. Rev. B **51**, 18045 (1995)

HL 106.8 Fri 12:00 EW 202

Electrical and THz magnetospectroscopy studies of InAs-based micro- and nanostructures — •Olivio Chiatti[1], Sven S. Buchholz[1], Christian Heyn[2], Wolfgang Hansen[2], Mehdi Pakmehr[3], Bruce D. McCombe[3], and Saskia F. Fischer[1] — [1]Neue Materialien, Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Institut für Angewandte Physik, Universität Hamburg, 20148 Hamburg, Germany — [3]Department of Physics, University at Buffalo, the State University of New York, Buffalo, NY 14260, USA

Nanostructures in narrow-gap semiconductors with strong spin-orbit interaction (SOI) offer the possibility to electrically manipulate spin-polarized currents. We present magnetotransport and THz magnetospectroscopy studies of Hall-bars from an InGaAs/InAlAs quantum well with an InAs-inserted channel. The two-dimensional electron gas is at 53 nm depth and has a carrier density of about $6 \cdot 10^{11}\,cm^{-2}$ and mobility of about $2 \cdot 10^5\,cm^2/Vs$. The measurements reveal an effective mass of $0.038m_0$ and an anisotropic g-factor of up to 20, larger than for bulk InAs. We demonstrate that quasi-one-dimensional channels (Q1D) can be successfully formed by micro-laser lithography and that the subband population is controlled by in-plane gates. Contrary to previous reports, asymmetric in-plane gate voltages applied to Q1D channels did not show signs of SOI-induced conductance anomalies [1].
[1] Chiatti *et al.*, arXiv:1410.8588v2 [cond-mat.mes-hall] (2014).

HL 106.9 Fri 12:15 EW 202

Mode-selected heat flow through a one-dimensional waveguide network — •Christian Riha[1], Philipp Miechowski[1], Sven S. Buchholz[1], Olivio Chiatti[1], Dirk Reuter[2], Andreas D. Wieck[3], and Saskia F. Fischer[1] — [1]Neue Materialien, Humboldt-

Universität zu Berlin, D-10099 Berlin — [2]Optoelektronische Materialien und Bauelemente, Universität Paderborn — [3]Angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum

Cross-correlated measurements of thermal noise are performed to determine the electron temperature in nanopatterned channels of a GaAs/AlGaAs heterostructure at 4.2 K. Two-dimensional (2D) electron reservoirs are connected via an extended one-dimensional (1D) electron waveguide network. Hot electrons produced by a current I_h in a source 2D reservoir are transmitted through the ballistic 1D waveguide and relax in a drain 2D reservoir. We find that the electron temperature increase ΔT_e in the drain is proportional to the square of the heating current I_h, as expected from Joule's law. We find that electron-phonon interaction is negligible for heat transport between 2D reservoirs at temperatures below 4.2 K. Furthermore, we demonstrate mode control of heat flow in the 1D electron waveguide by a top-gatevoltage [1].

[1] Riha *et al.*, arXiv:1410.2831

HL 106.10 Fri 12:30 EW 202

Influence of thiophene and pyridine containing fluorinated diketone-based passivation on the performance of ZnO TFTs — •Yulia Trostyanskaya, Marlis Ortel, Nataliya Kalinovich, Gerd-Volker Röschenthaler, and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Metal oxide TFTs are known to show unstable performance when the back channel is exposed to humid atmosphere. Therefore, ZnO TFTs deposited by spray pyrolysis were passivated by two different fluorine terminated diketones containing a pyridinyl- or a thienyl-group. All three groups are known to bind selectively to Zn-ions. XPS, AFM, UV-Vis and IV characterization of the passivated devices were conducted to distinguish between the effects of each bond type.

TFTs coated by thienyl-containing compounds showed a rise in mobility by 1,4 cm2/V and a shift of Von into negative direction. From XPS data, it was concluded that the diketo- and the thienyl-group bind to the back channel which indicates doping of the semiconductor due to the S-Zn bond. Samples passivated by pyridine-containing compound showed almost ideal Von of 0V, a small increase in mobility and only binding of the diketo-group to the surface. The tested materials stabilized the TFTs under negative and positive bias stress in ambient condition which indicates a successful passivation of active surface sites.

HL 106.11 Fri 12:45 EW 202

Current noises through a quantum dot in the presence of an oscillating gate voltage — •takafumi suzuki and takeo kato — Institute for Solid State Physics, University of Tokyo, Kashiwa, Chiba, Japan

We study photon-assisted transport in a quantum dot system under a periodically oscillating gate voltage. Photon-assisted current noises in the presence of the Coulomb interaction are calculated based on a gauge-invariant formulation of time-dependent transport. We derive an explicit expression of the vertex corrections within the self-consistent Hartree-Fock approximation in terms the Floquet-Green's functions. Moreover, we introduce an effective temperature to characterize nonequilibrium properties under the influence of the AC field. The vertex corrections are suppressed by the rise of the effective temperature, whereas characteristic resonant structures appear in the frequency spectra of the vertex corrections. The present result provides a useful viewpoint for understanding photon-assisted transport in interacting electron systems.

HL 107: Microcavities, polaritons and condensates

Time: Friday 10:15–13:00 Location: EW 015

HL 107.1 Fri 10:15 EW 015

Optical bistability in electrically driven polariton condensates — •Matthias Amthor[1], Timothy Liew[2], Christian Metzger[1], Sebastian Brodbeck[1], Martin Kamp[1], Ivan Shelykh[2,3], Alexey Kavokin[4,5], Christian Schneider[1], and Sven Höfling[1,6] — [1]Technische Physik and Wilhelm-Conrad-Röntgen-Research Center for Complex Material Systems, Universität Würzburg, D-97074 Würzburg, Am Hubland, Germany. — [2]Division of Physics and Applied Physics, Nanyang Technological University 637371, Singapore. — [3]Science Institute, University of Iceland, Dunhagi 3, IS-107, Reykjavik, Iceland. — [4]Spin Optics Laboratory, St-Petersburg State University, 1, Ulianovskaya, St.-Petersburg, 198504, Russia. — [5]Physics and Astronomy School, University of Southampton, Highfield, Southampton, SO171BJ, UK. — [6]School of Physics and Astronomy, University of St Andrews, St Andrews KY16 9SS, UK.

We observe a bistability in an electrically driven polariton condensate, which is manifested by a memory dependent threshold characteristic. In contrast to the polariton bistabilities previously observed, our effect occurs under non-resonant electric pumping and is triggered by the current injection scheme. We explain the origin of the bistability by a dependence of the electron-hole tunneling lifetime on the carrier density in the embedded QWs. The field screening effect creates a positive feedback loop, which yields the bistable behavior of the condensate. We develop a rate-equation based model which qualitatively explains the occurrence of the hysteresis, its reduction with increased magnetic field, and the absence of bistability under optical pumping.

HL 107.2 Fri 10:30 EW 015

Polariton condensates in textured microcavity potential landscapes — •Karol Winkler[1], Anne Schade[1], Julian Fischer[1], Robert Dall[3], Jonas Gessler[1], Elena A. Ostrovskaya[3], Martin Kamp[1], Christian Schneider[1], and Sven Höfling[1,2] — [1]Technische Physik and Wilhelm Conrad Röntgen Center for Complex Material Systems, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]SUPA, School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, United Kingdom — [3]Nonlinear Physics Centre and AMPL, Research School of Physics and Engineering, The Australian National University, Canberra, ACT 0200, Australia

Exciton-polaritons can be trapped in 0D quantum boxes by either trapping the excitonic or photonic part of these hybrid quasiparticles. Engineering the trapping potential then allows to tailor site-to-site evanescent coupling of the localised polariton mode wavefunctions in a periodic lattice. This leads to the formation of a tailorable polariton bandstructure which can be utilized to simulate complex many-body phenomena in the concept of quantum-simulators.

Here we report on recent measurements below and above bosonic condensation threshold on polariton lattices of different arrangement and dimensionality. The potential landscape in this structures is given by a versatile trapping technique that is based on local elongation of the $\lambda/2$-AlAs cavity layer in a high quality microcavity structure with embedded GaAs quantum wells.

HL 107.3 Fri 10:45 EW 015

The Structure of Polariton Macroscopic Quantum Phases in 2D Acoustic Lattices — •Jakov V. Buller[1], Edgar A. Cerda-Mendez[1], Raul E. Balderas-Navarro[1,2], Klaus Biermann[1], Dmitry N. Krizhanovskii[3], Maurice S. Skolnick[3], and Paulo V. Santos[1] — [1]Paul-Drude-Institut für Festkörperelektronik, 10117 Berlin, Germany — [2]Instituto de Investigación en Comunicación Óptica, 78000 San Luis Potosí, México — [3]University of Sheffield, Sheffield S37RH, United Kingdom

Exciton-polaritons are bosonic light-matter quasiparticles that result from the strong coupling of photon modes and quantum well excitons in a semiconductor microcavity. Due to their excitonic component, they show strong non-linear interactions, while their photonic component leads to very low effective masses and thus, formation of macroscopic quantum phases (MQPs) at kelvin temperatures. Also, their μm-long de Broglie wavelength allows modulation by micrometric acoustic potentials.

In this work, we present experimental results on the structure of polariton MQPs in tunable 2D acoustic lattices created by surface acoustic waves. The studies are carried out by a tomographic imaging technique, which gives energy-resolved information on the momentum- and real-space structure. The results show that MQPs with different symmetries, spatial distributions and coherence lengths coexist within the excitation laser spot. This work opens the way for the study of lattice vortex solitons and other polariton MQPs such as a Bose glass.

HL 107.4 Fri 11:00 EW 015

Analogy between optomechanical system and acoustic cavity — •Nicolas L. Naumann[1], Julia Kabuss[1], Andreas Knorr[1], and Weng W. Chow[2] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Berlin, Germany — [2]Sandia National Laboratories, Albuquerque, NM, USA

Quantum optomechanics recently developed into an important research area. The system dynamics is driven by radiation pressure.

We propose an acoustic cavity for exploring analogies to optomechanics. A reason for this comparative study is that the electron–phonon coupling is stronger than the coupling due to radiation pressure, which may enable easier implementation of devices. We give two examples to illustrate the similarities in their stationary and dynamical behavior: Both systems exhibit the nonlinear effect of bistability. Furthermore, the effective damping of the respective low frequency component (mechanical mode or phonon mode) can be enhanced or diminished by choosing the detuning of the cavity to the pump laser appropriately.

HL 107.5 Fri 11:15 EW 015

Nonlinear spectroscopy of exciton-polaritons in a GaAs-based microcavity — •Johannes Schmutzler[1], Marc Aßmann[1], Thomas Czerniuk[1], Martin Kamp[2], Christian Schneider[2], Sven Höfling[2,3], 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 — [3]SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, KY16 9SS, United Kingdom

We present a systematic investigation of two-photon excitation processes in a GaAs-based microcavity in the strong-coupling regime. Second harmonic generation resonant to the upper and lower polariton level is observed, which exhibits a strong dependence on the photonic fraction of the corresponding polariton. In addition we have performed two-photon excitation spectroscopy to identify $2p$ exciton states which are crucial for the operation as a terahertz lasing device, which was suggested recently [1]. However, no distinct signatures of a $2p$ exciton state could be identified, which indicates a low two-photon pumping efficiency [2].

[1] A. V. Kavokin et al., Phys. Rev. Lett. 108, 197401 (2012)
[2] J. Schmutzler et al., Phys. Rev. B 90, 075103 (2014)

Coffee break

HL 107.6 Fri 11:45 EW 015

Excition-polariton relaxation in a ZnO-based microresonator — •Oliver Herrfurth, Tom Michalsky, Helena Franke, Chris Sturm, Rüdiger Schmidt-Grund, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstraße 5, 04103 Leipzig

We report on time-resolved photoluminescence (PL) measurements of the lower polariton branch (LPB) in a microresonator (MR) with a wedge-shaped cavity revealing the impact of longitudinal optical (LO) phonons on the polariton relaxation at low temperatures. The MR was fabricated by pulsed laser deposition. The wedge-shaped cavity enables access to different detunings between the uncoupled exciton and photon mode by probing different positions on the sample surface. If the LPB ground state is in the spectral vicinity of a LO phonon replica of the exciton-like polariton reservoir, then the polariton system can scatter efficiently with LO phonons. In particular, for such detuning PL spectra show maximal intensity and time-resolved PL measurements detect the slowest decay of the polariton ensemble. For these measurements only a small interval in k-space around the LPB ground state was chosen and resolved in time with a streak camera.

HL 107.7 Fri 12:00 EW 015

Strong light-matter interaction in ZnO nanowires concentrically coated with Bragg reflectors — •Tom Michalsky, Helena Franke, Rüdiger Schmidt-Grund, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstraße 5, 04103 Leipzig

In this work we present the investigation of the optical and structural properties of ZnO nanowires concentrically coated with distributed Bragg reflectors. The whole structure was grown by pulsed laser deposition. Scanning electron microscope images reveal excellent structural and interface quality. Angularly and spatially resolved microphotoluminescence (PL) and reflectivity spectra prove lateral confinement and strong exciton-photon coupling even at room temperature. With increasing PL excitation density we observe a controlled transition from the strong to the weak coupling regime as evidenced by stimulated emission out of the uncoupled resonator modes.

HL 107.8 Fri 12:15 EW 015

Ultrafast all-optical switching of a single micropillar cavity — Henri Thyrrestrup[1], Emre Yüce[1], •Georgios Ctistis[1,2], Julien Claudon[3,4], Jean-Michel Gérard[3,4], and Willem L. Vos[1] — [1]Complex Photonic Systems (COPS), MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands — [2]Nano-Bio Interfaces, Saxion University of Applied Sciences, Enschede, The Netherlands — [3]CEA/INAC/SP2M, Nanophysics and Semiconductor Laboratory, Grenoble, France — [4]University Grenoble Alpes, INAC-SP2M, Nanophysics and Semiconductors Lab, F-38000 Grenoble, France

Micropillar cavities are versatile nanophotonic structures for locally enhancing light-matter interaction due to their high quality factors, low mode volumes, and clean free-space optical interface. These qualities have facilitated the successful application of micropillars as efficient single photon sources, for cavity QED strong coupling, and diode lasers. We present here frequency- and time-resolved pump-probe experiments of a single GaAs/AlAs micropillar cavity with a diameter of 6 μm studying the dynamics of the cavity resonance. All-optical switching is achieved by excitation of free carriers. We observe a simultaneous shift of two different transverse modes in the micropillar. The high-resolution frequency time traces of the resonances show a strongly non-exponential relaxation dynamics [1]. We interpret this with a second-order mechanism including the radiative recombination of electron and holes and a slow free carrier trapping time.

[1] H. Thyrrestrup et al, Appl. Phys. Lett. 105, 111115 (2014)

HL 107.9 Fri 12:30 EW 015

Dynamics of light and matter in ultrafast-switched semiconductor microcavities — •Georgios Ctistis[1,2], Emre Yüce[1], Henri Thyrrestrup[1], Julien Claudon[3,4], Allard P. Mosk[1], Jean-Michel Gérard[3,4], and Willem L. Vos[1] — [1]Complex Photonic Systems (COPS), MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands — [2]Nano-Bio Interfaces, Saxion University of Applied Sciences, Enschede, The Netherlands — [3]CEA/INAC/SP2M, Nanophysics and Semiconductor Laboratory, Grenoble, France — [4]University Grenoble Alpes, INAC-SP2M, Nanophysics and Semiconductors Lab, F-38000 Grenoble, France

The interest in all-optical switching of photonic nanostructures is rapidly increasing due to the inherent speed of the process. Achieving all-optical switching on ultrafast timescales promises both new developments in information technology and a novel control in cavity QED. A very popular switching mechnism is thereby the excitation of free carriers. The dynamics of this process is usually explained by the recombination dynamics of the excited carriers using a single population model. Here, we present time dependent differential reflectivity measurements of a GaAs/AlAs planar microcavity over a broad frequency range. We observe that the switching dynamics shows a spectral dependence. To accurately describe and understand this behavior we propose a model beyond the existing single population model.

HL 107.10 Fri 12:45 EW 015

The role of the local density of optical states in the frequency conversion of light in a microcavity — Emre Yüce[1], Henri Thyrrestrup[1], •Georgios Ctistis[1,2], Julien Claudon[3,4], Jean-Michel Gérard[3,4], and Willem L. Vos[1] — [1]Complex Photonic Systems (COPS), MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands — [2]Nano-Bio Interfaces, Saxion University of Applied Sciences, Enschede, The Netherlands — [3]CEA/INAC/SP2M, Nanophysics and Semiconductor Laboratory, Grenoble, France — [4]4 University Grenoble Alpes, INAC-SP2M, Nanophysics and Semiconductors Lab, F-38000 Grenoble, France

Converting light to a controllable frequency is well-known in traditional non-linear optics. In modern nanophotonics one frequency converts light which is trapped in a cavity or waveguide. Supposedly, the physics of frequency conversion differs between traditional non-linear optics and modern nanophotonics, regarding the rate of change and output spectrum. Here, we unify these disparate views. To this end, we consider a nanophotonic system, a planar microcavity, sustaining

both a cavity resonance and a flat continuum of modes. We study the frequency conversion that occurs when the cavity is switched in an ultrafast way via the electronic Kerr effect [1]. We thereby observe either a red- or a blue-shift of the confined light, depending on the timing of the pulses in the pump-probe experiment. We study color-conversion for different quality factors, which allows us to identify the role of the local density of optical states available to the generated light.

[1] E. Yüce et al., arXiv:1406.3586 (2014)

HL 108: Graphene: Intercalation (O with HL/TT)

Time: Friday 10:30–12:45 Location: MA 041

HL 108.1 Fri 10:30 MA 041

Keeping Argon under a Graphene Lid - Argon intercalation between Graphene and Ni(111) — •Florian Späth, Karin Gotterbarm, Christoph Gleichweit, Max Amende, Udo Bauer, Oliver Höfert, Hans-Peter Steinrück, and Christian Papp — Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstraße 3, 91058 Erlangen, Germany

Graphene with its thickness of only one single atomic layer can be considered as the thinnest membrane or gas barrier. We present a spectroscopic investigation of related properties under well-defined ultra-high vacuum conditions in a surface science experiment: We implant argon into a Ni(111) crystal by sputtering prior to the growth of graphene. Subsequently, when growing graphene on Ni(111), argon diffuses out of the bulk and is caught underneath graphene. We investigate the system with high-resolution in-situ X-ray photoelectron spectroscopy. From the growth behavior of these intercalated argon bubbles during graphene preparation and from temperature programmed XP spectra we are able to deduce a model of the intercalation system (G/Ar/Ni) and estimate the pressure for argon under graphene. Furthermore, we find an increased thermal stability of graphene due to a decoupling of graphene from the Ni(111) substrate. This work was supported by SFB 953 "Synthetic Carbon Allotropes"

HL 108.2 Fri 10:45 MA 041

Intercalation of Gadolinium underneath graphene on SiC(0001) — •Stefan Link, Stiven Forti, Alexander Stöhr, and Ulrich Starke — Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany

Investigating the properties of graphene in a highly doped state, such that the Fermi level reaches a saddle point of it's electronic bands is an on-going field. Superconductivity could be one potential effect in this regime. Functionalization with highly reactive species such as alkali and/or earth alkali atoms has been pursued for strong doping effects. However, such systems are prone to fast degradation by environmental influences which needs to be circumvented for any kind of application.

Here, we present a method of doping graphene to such levels and simultaneously making the system stable to temperatures higher than 1000°C as well as to air exposure. This was achieved by the intercalation of Gadolinium atoms underneath the so-called buffer layer on SiC(0001), i.e., the carbon rich $(6\sqrt{3}\times6\sqrt{3})$R30° reconstruction of this surface. Significant hybridization effects of the graphene π-bands with the adatom states are observed in the ARPES data. In addition, evidence for strong electron-phonon scattering is visible. Spectroscopic weight appears in the measurements completely interlinking two Dirac cones through the $\overline{\text{M}}$-point, thus indicating the presence of an electronic topological transition (ETT).

HL 108.3 Fri 11:00 MA 041

Nitrogen Intercalation and Nitrogen-based Molecular Doping of Epitaxial Graphene on 6H-SiC(0001) — •Nuala Mai Caffrey, Rickard Armiento, Rositsa Yakimova, and Igor Abrikosov — Department of Physics, Chemistry and Biology (IFM), Linköping University, Linköping, Sweden

The thermal decomposition of silicon carbide (SiC) is one of the most promising methods to produce high-quality epitaxial graphene on a wafer scale. Sufficient control has even been achieved to selectively grow monolayer, bilayer and few-layer graphene, rendering it a indispensable technique for the manufacture of graphene-based electronics. A disadvantage of this method is that the first carbon layer is covalently bonded to the surface Si atoms, with only subsequent layers displaying the characteristic electronic features of graphene. Several methods have been proposed to electronically decouple this buffer layer, as well as to reduce the high substrate-induced doping, including intercalation and chemical doping. Understanding such chemical functionalisations is a fundamental first step towards engineering the properties of graphene on SiC. It is clear that the graphene layer, as well as the interface between it and the SiC surface, can be significantly influenced by the growth environment. We consider how common environmental dopants can affect the electronic structure of mono- and bilayer graphene grown on a 6H-SiC(0001) substrate. We show, using first-principles calculations, how nitrogen intercalation and nitrogen-based molecular dopants, such as NO2 and NH3, present a promising route to tailor the properties of this system.

HL 108.4 Fri 11:15 MA 041

Investigation of the electrostatic changes induced by metal islands on graphene/SiC(0001) using field-emission resonance spectroscopy with STM — •Anastasia Sokolova[1], Alexander Stöhr[2], Stiven Forti[2], Ulrich Starke[1,2], and M.Alexander Schneider[1] — [1]Solid State Physics, Friedrich-Alexander-University Erlangen-Nuremberg, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

Using the Scanning Tunneling Microscope in field-emission resonance spectroscopy mode (FRS-STM) it is possible to map changes of the electrostatic potential in front of the graphene surface at the nanoscale [1]. We investigated the properties of 10 nm-sized metal islands on top of epitaxial graphene on SiC(0001) as well as islands intercalated underneath the graphene layer.

For cobalt and palladium islands on top of graphene we observe a spatially localized shift of the 1st field-emission resonance to higher energy strictly occurring at the topographical step. This is consistent with larger work functions of the metals with respect to that of graphene. In the case of intercalated cobalt islands FRS-STM shows a rise of the 1st field-emission resonance energy of only 150 meV and a spatially delocalized transition. Considering the properties of graphene flakes on an extended Co(0001) surface [2] this suggests negative charge of the capping graphene layer and a positive charge on the cobalt island.

[1] S. Bose *et al* 2010 *New Journal of Physics* **12** 023028
[2] D. Eom *et al* 2009 *Nano Letters* **9** 2844-2848

HL 108.5 Fri 11:30 MA 041

Oxygen orders differently under graphene: new superstructures on Ir(111) — •Antonio J. Martínez-Galera[1], Felix Huttmann[1], Ulrike Schröder[1], Fabian Craes[1], Carsten Busse[1], Vasile Caciuc[2], Nicolae Atodiresei[2], Stefan Blügel[2], and Thomas Michely[1] — [1]Universität zu Köln, II. Physikalisches Institut, Germany — [2]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany

Modifying the properties of graphene (Gr) by intercalation of atoms or molecules at the Gr/substrate interface has been proven to be a straightforward and versatile concept. However, the effect of the Gr layer on the ordering of the intercalated material remains much less studied. We present evidence that indeed the Gr cover has a substantial influence on the resulting superstructures of oxygen chemisorbed on Ir(111). As a function of exposure to molecular oxygen and temperature the oxygen adsorbate superstructures on Ir(111) are identified by scanning tunneling microscopy (STM). They are compared to the ones formed by intercalation in between graphene and Ir(111). For bare Ir(111) we observe O-(2x2) and O-(2x1) structures, thereby clarifying a long-standing debate on the existence of these structures and the role of defects for their stability. For Gr/O/Ir(111) with increasing exposure O-(2x2), O-(R3xR3)-R30, O-(2x1) and O-(2R3x2R3)-R30 superstructures referred to Ir(111) are observed. The (R3xR3)-R30 and (2R3x2R3)-R30 structures were not yet reported and they exist only under Gr. Based on density functional theory (DFT) we discuss the origin of the new adsorbate superstructures under graphene.

HL 108.6 Fri 11:45 MA 041

Oxidation of sulfuric acid intercalated graphite: the role of sulfuric acid and permanganate ions — •Steffen Seiler and

Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

Wet-chemical exfoliation of graphite via Hummers' method [1,2] is a promising route for large-scale graphene production. This solution-based process is carried out in concentrated sulfuric acid and involves several steps: first, graphite is converted into a sulfuric acid–graphite intercalation compound (GIC), then the GIC is transformed into oxidized graphite, graphene oxide (GO) layers are separated in solution by hydrolysis reactions, and finally the GO layers are reduced to graphene [3].
To obtain atomistic insights into the mechanisms of the chemical reactions in liquid sulfuric acid within the confined space between graphene layers we performed Car-Parrinello molecular dynamics (CP-MD) simulations. By changing the coverage of hydroxy and epoxy groups their stabilizing effect on the attack of sulfuric acid (solvent) and $KMnO_4$ (oxidizing agent) molecules was investigated. Furthermore, different carbon atoms on the partly oxidized graphene sheets were attacked to elucidate the most reactive sites.

[1] W. S. Hummers, *J. Am. Chem. Soc.* **80**, 1339 (1958).
[2] D. C. Marcano et al., *ACS Nano* **4**, 4806 (2010).
[3] A. M. Dimiev and J. M. Tour, *ACS Nano* **8**, 3060 (2014).

HL 108.7 Fri 12:00 MA 041

Approaching ideal graphene: The structure of hydrogen- and germanium-intercalated graphene on 6H-SiC(0001) — •F.C. Bocquet[1,2], J. Sforzini[1,2], T. Denig[3], A. Stöhr[3], T.-L. Lee[4], S. Subach[1,2], U. Starke[3], and F.S. Tautz[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA), Fundamentals of Future Information Technology, 52425 Jülich, Germany — [3]Max Planck Institute for Solid State Research, Heisenbergstraße, 70569 Stuttgart, Germany — [4]Diamond Light Source Ltd, Didcot, OX11ODE, Oxfordshire, United Kingdom

We investigated Quasi-Free-standing Monolayer Graphene epitaxially grown on 6H-SiC(0001) obtained by decoupling the buffer-layer from the Si-terminated surface by hydrogen intercalation (1) or by intercalating one or two monolayers of germanium (2). All three samples show a clear linear dispersion around the K-point, confirming their Quasi-Free-standing character. We used the X-ray standing wave (XSW) technique, combining dynamical diffraction and X-ray photoelectron spectroscopy, to detect the coherent distribution of the chemically different species (Si, C and Ge) at the interface. Based on the lattice parameter of bulk SiC, we accurately determine the vertical height differences between each chemical species. Comparing the overlaps of van der Waals radii between the graphene layer and the topmost intercalating atoms, we conclude on the degree of decoupling of the graphene layers.

HL 108.8 Fri 12:15 MA 041

Bismuth Intercalated Graphene on Iridium Probed by STM and ARPES — •Jonas Warmuth[1], Matteo Michardi[2], Torben Hänke[1], Marco Bianchi[2], Jens Wiebe[1], Roland Wiesendanger[1], Philip Hofmann[2], and Alexander Khajetoorians[3] — [1]Department of Applied Physics, University of Hamburg, Germany — [2]Department of Physics and Astronomy, University of Aarhus, Denmark — [3]Institute for Materials and Molecules, Radboud University, Nijmegen, Netherlands

We report on the investigation of bismuth intercalated graphene grown on Ir(111) by means of STM and ARPES. The STM measurements reveal a complex periodic structure upon Bi intercalation which we attribute to the formation of a $\sqrt{3}$ Bi surface alloy. We characterize the changes to the band structure using ARPES, including the doping effects and the modification to the Dirac dispersion.

HL 108.9 Fri 12:30 MA 041

Enhancement of many-body effects observed on epitaxial monolayer graphene/Au/SiC(0001) — •Stiven Forti[1], Stefan Link[1], Alexander Stöhr[1], Yuran Niu[2], Alexei Zakharov[2], and Ulrich Starke[1] — [1]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart,Germany — [2]Max-Lab, Lund University, Box 118, Lund, S-22100, Sweden

The interaction of graphene with gold atoms has gained high relevance for a series of reasons, from electrical contacts to plasmonics. Here we present the realization of n-type epitaxial monolayer graphene on SiC(0001) via the intercalation of a layer of Au atoms at the heterointerface between the graphene and the SiC substrate. Such a phase exhibits enhanced many-body effects, as observed by ARPES. The plasmaron band is observed and its dispersion is well discernible from the hole-Dirac cone. The effective dielectric constant extracted from the ARPES data is about five times smaller than what is reported in the literature so far. The effectiveness of the intercalation is corroborated by μLEED measurements, which clearly indicate a suppression of the diffraction spots on the $(6\sqrt{3}\times 6\sqrt{3})$R30° grid, except for spots arising from multiple diffraction. CLPES measurements indicate the presence of a single gold component, namely assigned to gold silicides. The quality of the epitaxial graphene grown on SiC(0001) in Ar atmosphere, together with the aforementioned preparation, makes possible to observe bands of unprecedent sharpness for this system. Dispersive states arising from the 5d orbitals of the interfacial gold are observed as well, as predicted by theory.

HL 109: Quantum dots and wires: Quantum communication and quantum information science

Time: Friday 11:15–13:15 Location: ER 164

HL 109.1 Fri 11:15 ER 164

Optical Tomography of Electron Spins in (In,Ga)As Quantum Dots — •Janina Schindler[1], Steffen Varwig[1], Alexandre René[1], Sophia Economou[2], Alex Greilich[1], Dmitri Yakovlev[1,3], Dirk Reuter[4], Andreas Wieck[4], Thomas Reinecke[2], and Manfred Bayer[1] — [1]Experimentelle Physik II, TU Dortmund, D-44221 Dortmund, Germany — [2]Naval Research Laboratory, Washington D.C. 20375, USA — [3]Ioffe Physical Technical Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia — [4]Angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Electron spins in quantum dots are considered as a promising candidate for implementing quantum bits in semiconductors. As already has been shown in preceding experiments, their control, manipulation and read-out can be achieved purely optical. For the implementation of quantum gates, two interacting qubits are required. There has already been evidence for interaction between two qubits, which are realized by electron spin ensembles of self-assembled (In,Ga)As quantum dots. To scrutinise the interaction between these ensembles, we perform optical time-resolved pump-probe ellipticity measurements on the spin polarisation. More precisely, we study the time evolution of a spin component along the magnetic field based on optically induced spin rotations to read out all spin-vector components.

HL 109.2 Fri 11:30 ER 164

Properties of excitonic V-shaped quantum dot systems for optical switches — •Yves Alexander Leier[1], Dirk Mantei[1], Jens Förstner[1], Simon Gordon[1], Dirk Reuter[1], Andreas D. Wieck[2], and Artur Zrenner[1] — [1]Center for Optoelectronics and Photonics Paderborn (CeOPP), Universität Paderborn, Warburger Straße 100, 33098 Paderborn, Germany — [2]Ruhr-Universität Bochum, Universitätsstraße 150, Gebäude NB, 44780 Bochum, Germany

For the optical manipulation of a single quantum system, diverse approaches such as Rabi Oscillations and the Adiabatic Rapid Passage are well established techniques. To achieve an inversion as complete as possible we present a new possibility by examining a single quantum system with V-type three level scheme, a common ground state and two distinguishable and separately excitable transitions. Their sequential, pulsed excitation allows for the preparation of a robust, fault-tolerant and phase-insensitive inversion. In our contribution we demonstrate this concept, which is based on the polarization-selective excitation of a fine structure split exciton ground state in a single InGaAs quantum dot. We further propose a scheme for a robust optical switch, which is based on a related approach. A first horizontally polarized pi-pulse excites completely one of the fss-transitions of a quantum dot ensemble. Because of Pauli blocking a second pulse with orthogonal polarization can therefore not change the occupation of the quantum dot and passes the quantum dot without absorption.

HL 109.3 Fri 11:45 ER 164

Resonance Fluorescence from Quantum Dots embedded in GaAs/AlGaAs Ridge Waveguide Structures — •Mario Schwartz, Ulrich Rengstl, Matthias Paul, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Allmandring 3, 70569 Stuttgart, Germany

The implementation of a logical quantum CNOT gate on-chip is one of the major goals in quantum information science. Requirements for such a gate are the generation, guiding and detection of indistinguishable single-photons on-chip. Due to photons from a QD have the best coherence properties under resonant excitation, this excitation method is a requirement for highly indistinguishable single-photons.

Here, we demonstrate resonance fluorescence (RF) of InAs QDs embedded in a GaAs/AlGaAs ridge waveguide (WG). Low propagation losses along the WG exhibit the suitability of the QD/WG system. The additional use of a weak off-resonant laser, acting as an optical gate for the RF is documented.

HL 109.4 Fri 12:00 ER 164

Ultra-bright emission of indistinguishable photons from deterministic quantum-dot microlenses — •Alexander Thoma, Peter Schnauber, Manuel Gschrey, Marc Seifried, Ronny Schmidt, Jan-Hindrik Schulze, Tobias Heindel, Sven Rodt, André Strittmatter, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, D-10623, Germany

Non-classical light sources emitting single indistinguishable photons at high flux rates are key components for concepts in the field of quantum information technology such as the quantum repeater. Single self-organized semiconductor quantum dots (QDs) integrated into microcavity systems are promising candidates to realize such sources. In recent years significant progress has been achieved in this field, however, most of the realized devices are based on spatially and spectrally random quantum emitters. In this work we report on a versatile device concept that is based on deterministically fabricated single QD microlenses using in-situ electron beam lithography. These quantum light sources can be realized with very high process yield $> 90\%$ and allow for ultrabright emission on demand. We observe photon extraction efficiencies of up to $(23.3 \pm 3.0)\%$ in combination with a strong suppression of multi-photon emission events $g^{(2)}(0) < 0.01$. A Hong-Ou-Mandel-type two-photon interference experiment reveals a visibility of $V = (43 \pm 4)\%$ even in saturation of the active QD.

HL 109.5 Fri 12:15 ER 164

A quantum dot single-photon source with on-the-fly all-optical polarization control — •Dirk Heinze, Dominik Breddermann, Artur Zrenner, and Stefan Schumacher — Physics Department and Center for Optoelectronics and Photonics Paderborn (CeOPP), University of Paderborn, Warburger Strasse 100, 33098 Paderborn, Germany

Semiconductor quantum dots have been highlighted as efficient on demand sources for single photons. In contrast to the usual cascaded biexciton-exciton emission, here we study the direct two-photon emission from the biexciton. We show that emission through this higher-order transition is a promising and in certain ways superior alternative to generate a single photon. In the scheme we propose, the two-photon emission from the biexciton is enabled by a laser field (or laser pulse) driving the system into a virtual state inside the band gap. From this intermediate virtual state, the single photon of interest is then spontaneously emitted as the quantum dot relaxes to its electronic ground state. The big advantage of this scheme lies in the fact that the properties of the emitted photon (such as polarization state, time of emission, frequency) can be controlled all-optically by the classical laser field enabling the emission. This gives our scheme great potential to be used in the next generation of flexible semiconductor single-photon sources.

HL 109.6 Fri 12:30 ER 164

Coherent photocurrent spectroscopy of single InAs quantum dots at 1500 nm — •Simon Gordon[1], Matusala Yacob[2], Yves Alexander Leier[1], Mohamed Benyoucef[2], Johann Peter Reithmaier[2], and Artur Zrenner[1] — [1]CeOPP, Universität Paderborn, Paderborn, Germany — [2]INA, Universität Kassel, Kassel, Germany

For long distance quantum communication it is essential to use flying qubits in the telecom wavelength bands. Quantum emitters or detectors in this wavelength regime can be realized with InAs quantum dots on InP substrate. In this work, such InAs quantum dots are investigated by low-temperature photocurrent spectroscopy. Suitable p-i-n diode structures with self-assembled quantum dots have been grown by molecular beam epitaxy on InP(100) substrates. The layer sequence of the diodes consists of an n-InP back contact, an intrinsic region of lattice-matched InAlGaAs, which contains the quantum dots, and a p-InP front contact. The quantum dots are coherently excited by an optical parametric oscillator. By changing the applied reverse voltage the resonance energy of the quantum dot is tuned by the quantum confined Stark effect to the energy of the light pulse. Increasing the power of the excitation light pulses leads to a nonlinear response of the photocurrent. We observe a clear signature of Rabi oscillations. By measuring the photocurrent it is also possible to determine the occupancy of the two level quantum system after coherent excitation.

HL 109.7 Fri 12:45 ER 164

Toward long-lived excitonic qubits in deterministic quantum-dot microlenses — •Tobias Heindel[1], Alexander Thoma[1], Emma Schmidgall[2], Liron Gantz[2], Ido Schwartz[2], Manuel Gschrey[1], Peter Schnauber[1], Jan-Hindrik Schulze[1], André Strittmatter[1], Sven Rodt[1], David Gershoni[2], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, D-10623, Germany — [2]Department of Physics, Technion, Haifa 32000, Israel

In recent years the coherent properties of bright exciton (BE) states in self-assembled semiconductor quantum dots (QD) have been explored [1]. However, the use of BEs for quantum information processing tasks is limited due to their relatively short lifetime - set by its radiative recombination rate. On the other hand, dark exciton states have already proven to constitute an extremly long-lived qubit which is optically accesible via specific biexcitonic states [2].

In this work we report on the exploration of such biexcitonic triplet states in single QDs integrated deterministically into microlenses with enhanced photon-extraction efficiency. In contrast to the common spin-singlet biexciton state, the triplet states are constituted of two s-shell electrons and two holes having parallel spins - thus one hole must be located in the p-shell due to Pauli exclusion principle. A detailed analysis of the dynamics of these spin-blockaded biexciton states is presented via polarization resolved photon-crosscorrelation measurements.

[1] Kodriano et al., Semicond. Sci. Technol. 29, 053001 (2014)
[2] Poem et al., Nature Physics 6, 993 (2010)

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Fiber-coupled quantum dot based single-photon sources operated by a Stirling cryocooler — •Alexander Schlehahn, Esra Tauscher, Thomay Megas, Manuel Gschrey, Jan-Hindrik Schulze, André Strittmatter, Sven Rodt, Tobias Heindel, and Stephan Reitzenstein — Technische Universität Berlin, Institut für Festkörperphysik, 10623 Berlin, Germany

Easy-to-operate single-photon sources are one of the key components in quantum communication. Up till now such non-classical light sources have been operated almost exclusively in shielded lab-environments and practical concepts appeared elusive. Here we report on the application of a compact and user-friendly Stirling cryocooler in the field of nanophotonics. It is capable of operating single-photon emitters at a base temperature well below 30 K with high purity ($g^{(2)}(0) = 0.04$), while offering cost efficiency and independence from liquid helium supply. A method for direct fiber coupling of single quantum emitters inside the Stirling cryostat is introduced. Sample alignment is obtained by an innovative two-step deep-etching process for GaAs. It allows us to deterministically position single quantum dot structures within a few tens of micrometers precision on a 2.5 mm diameter, racket-shaped sample. Mounting sample and fiber into standard ceramic fiber sleeves with sub-micrometer diameter deviation achieves excellent alignment of fiber core and mesa. Laser excitation and quantum dot emission are guided via the same optical fiber, leading to a drift- and vibration-unaffected signal. This demonstration paves the way towards user-friendly and high-quality table-top non-classical light sources.