Semiconductor Physics Division
Fachverband Halbleiterphysik (HL)

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Overview of Invited Talks and Sessions

(Lecture Rooms: Pot 6, Pot 51, Pot 81, Pot 112, Pot 151, and Pot 251; Posters: P1 (Zelt), P2 (HSZ))

Invited Talks

HL 1.1	Sun	16:00–16:35	HSZ 403	**Von Lithium zu Lithium-Ionen-Batterien und zurück** — •Martin Winter
HL 1.2	Sun	16:35–17:10	HSZ 403	**Magnetic materials for green energy applications** — •Oliver Gutfleisch
HL 1.3	Sun	17:20–17:55	HSZ 403	**Recent developments of dye sensitized and mesoscopic solar cells** — •Toby Meyer
HL 1.4	Sun	17:55–18:30	HSZ 403	**Perspectives of an artificial leaf based on inorganic semiconductors for water splitting: Device structure, interface engineering, catalytic demands** — •Wolfram Jaegermann
HL 3.1	Mon	9:30–10:00	POT 081	**Parameterfree calculations of excitations and spectra: Fiction or reality for semiconductors?** — •Friedhelm Bechstedt
HL 9.1	Mon	10:00–10:30	POT 081	**Ultrathin Nanowires: Multiplex Templating Synthesis, Macroscopic Assemblies, and Applications** — •Shu-Hong Yu
HL 14.1	Mon	11:45–12:15	POT 151	**Vertical-cavity surface-emitting lasers (VCSELs) for optical interconnects** — •James A. Lott
HL 17.1	Mon	15:00–15:30	POT 081	**Low-temperature scanning probe investigations of nanostructures at high and low magnetic fields** — Nikola Pascher, •Thomas Ihn, Aleksey Kozikov, Richard Steinacher, Clemens Rössler, Klaus Ensslin, Christian Reichl, Werner Wegscheider
HL 22.1	Mon	15:30–16:00	POT 006	**Unveiling the origin of resistive switching in organic electronic devices** — •Emil J.W. List-Kratochvil
HL 34.1	Tue	9:30–10:00	POT 081	**Influence of molecular structure, conformation and morphology on the performance of polymer solar cells** — •Elizabeth von Hauff
HL 36.1	Tue	12:30–13:00	POT 081	**Organic-inorganic perovskite solar cells: The new generation of PV** — •Gary Hodes
HL 51.1	Tue	14:00–14:30	POT 112	**Advanced optical properties of (In,Ga)As nanowire heterostructures** — •Gregor Koblmueller
HL 56.1	Wed	9:30–10:00	POT 006	**Ab initio many-body perturbation theory for organic photovoltaics** — •Xavier Blase
HL 63.1	Wed	12:00–12:30	POT 006	**Exciton-phonon coupling in nitride-based nanostructures** — G. Callsen, G. Hönig, S. Kalinowski, J. Settke, C. Kindel, J. Brunnmeier, T. Markurt, M. Albrecht, S. Kako, A. Schliwa, Y. Arakawa, •A. Hoffmann
HL 87.1	Thu	9:30–10:00	POT 081	**Time-resolved optical spectroscopy of 2D dichalcogenides** — •Tobias Korn, Gerd Plechinger, Philipp Nagler, Christian Schüller
HL 94.1	Thu	11:00–11:30	POT 006	**Template-realized three-dimensional functional nanostructures of semiconductors for high-performance device applications** — •Yong Lei

HL 96.1	Thu	15:00–15:30	POT 051	**An Electrically Driven Polariton Laser** — •Arash Rahimi-Iman
HL 110.1	Fri	9:30–10:00	POT 051	**Quantum dynamics of exciton migration and dissociation in functional organic polymer materials** — •Irene Burghardt
HL 119.1	Fri	11:00–11:30	POT 006	**A 3D topological insulator quantum dot for optically controlled quantum memory and quantum computing** — Hari P. Paudel, •Michael N. Leuenberger

Invited Talks in Focus Sessions

HL 4.1	Mon	9:30–10:00	POT 151	**Impact of topology on physical properties of quantum rings** — •Vladimir M. Fomin
HL 4.2	Mon	10:00–10:30	POT 151	**Fabrication of ordered quantum rings** — •Zhiming Wang
HL 4.3	Mon	10:45–11:15	POT 151	**Self-organized formation and XSTM characterization of GaSb/GaAs quantum rings** — •Andrea Lenz
HL 16.1	Mon	15:00–15:30	POT 051	**Single Charge Relaxation in a Silicon Double Quantum Dot** — •Jason Petta
HL 16.4	Mon	16:00–16:30	POT 051	**Spin Qubits in Silicon** — •Andrew Dzurak
HL 16.7	Mon	17:15–17:45	POT 051	**Spin Hot Spots in Quantum Dots** — •Peter Stano
HL 38.1	Tue	9:30–10:00	POT 251	**Nonclassical light from semiconductor quantum dots** — •Gregor Weihs, Tobias Huber, Harishankar Jayakumar, Thomas Kauten, Ana Predojević
HL 38.5	Tue	10:45–11:15	POT 251	**Taming single photons emitted by solid state systems** — •Stephan Götzinger
HL 54.1	Tue	14:00–14:30	POT 251	**Quantum network challenges for solid-state spins and photons** — •Mete Atature
HL 58.1	Wed	9:30–10:00	POT 081	**Computational design of oxide semiconductors** — •Stephan Lany
HL 58.7	Wed	11:30–12:00	POT 081	**Beta-Ga2O3: Single crystal growth and semiconductor applications** — •Encarnacion G. Villora, Daisuke Inomata, Stelian Arjoca, Kazuo Aoki, Kiyoshi Shimamura
HL 58.9	Wed	12:15–12:45	POT 081	**Combinatorial approach to group-III sesquioxides** — •Holger von Wenckstern
HL 69.1	Wed	15:00–15:30	POT 081	**Electronic properties of the transparent semiconducting oxides Ga2O3 and In2O3** — •Recardo Manzke
HL 69.7	Wed	17:00–17:30	POT 081	**Surface properties of In_2O_3 and other semiconducting metal oxides** — •Ulrike Diebold
HL 89.1	Thu	9:30–10:00	POT 251	**Metamorphic III-V-on-IV structures and its application to optoelectronic devices** — Yoshiaki Nakano, •Masakazu Sugiyama, Takuo Tanemura
HL 89.2	Thu	10:00–10:30	POT 251	**Two types of buffer layer for the growth of GaN on highly lattice mismatched substrates and their impact on the development of sustainable systems** — Tadashi Mitsunari, Koji Okuno, Yoshio Honda, Shigeyasu Tanaka, •Hiroshi Amano
HL 89.6	Thu	11:30–12:00	POT 251	**Development of High Performance Semipolar GaN-based Blue and Green Lasers: Control of Stress Relaxation** — •James Speck
HL 100.1	Thu	15:00–15:30	POT 251	**Integration of cubic III/V semiconductors on silicon (001)** — •Kerstin Volz

Invited talks of the joint symposium SYMO

See SYMO for the full program of the symposium.

SYMO 1.1	Mon	9:30–10:00	HSZ 02	**Molecular quantum spintronics with single-molecule magnets** — •Wolfgang Wernsdorfer
SYMO 1.2	Mon	10:00–10:30	HSZ 02	**EPR Studies of Rare-Earth Molecular Nanomagnets** — •Stephen Hill, Sanhita Ghosh, Dorsa Komijani, Salvador Cardona-Serra, Jose-Jaime Baldovi, Yan Duan, Alejandro Gaita-Arino, Eugenio Coronado
SYMO 1.3	Mon	10:45–11:15	HSZ 02	**On-surface magnetochemistry of spin-bearing metalorganic molecules** — •Peter M. Oppeneer, Kartick Tarafder, Ehesan Ali, Nirmalya Ballav, Christian Wäckerlin, Thomas A. Jung

SYMO 1.4	Mon	11:15–11:45	HSZ 02	**Interfacing single-molecule magnets with metals** — •Andrea Cornia, Valeria Lanzilotto, Luigi Malavolti, Matteo Mannini, Mauro Perfetti, Luca Rigamonti, Roberta Sessoli
SYMO 1.5	Mon	11:45–12:15	HSZ 02	**Linking magnetic molecules to themselves, to others and to surfaces** — •Richard Winpenny

Invited talks of the joint symposium SYSG

See SYSG for the full program of the symposium.

SYSG 1.1	Tue	9:30–10:00	HSZ 02	**Intrinsic magnetism in graphene** — •Irina Grigorieva
SYSG 1.2	Tue	10:00–10:30	HSZ 02	**Defect Induced Magnetic Moments in Graphene** — •Roland Kawakami
SYSG 1.3	Tue	10:30–11:00	HSZ 02	**Role of MgO barriers for spin and charge transport in Co/MgO/graphene spin-valve devices** — •Bernd Beschoten
SYSG 1.4	Tue	11:15–11:45	HSZ 02	**Defect-Mediated Spin Relaxation and Dephasing in Graphene** — Mark Lundeberg, Silvia Folk, •Joshua Folk
SYSG 1.5	Tue	11:45–12:15	HSZ 02	**Electron spin relaxation in graphene: resonant scattering off local magnetic moments** — •Jaroslav Fabian, Denis Kochan, Martin Gmitra

Invited talks of the joint symposium SYOM

See SYOM for the full program of the symposium.

SYOM 1.1	Fri	9:30–10:10	HSZ 02	**Atomic-scale dopant wires for quantum computer architectures** — •Michelle Y Simmons
SYOM 1.2	Fri	10:10–10:50	HSZ 02	**$1+\delta$: Tuning the Dimensionality of Organic Conductors** — •Martin Dressel
SYOM 1.3	Fri	11:10–11:50	HSZ 02	**Spectral and transport properties of one-dimensional correlated electrons** — •Volker Meden
SYOM 1.4	Fri	11:50–12:30	HSZ 02	**Atomic nanowires on surfaces: Spectroscopic reality versus theoretical fiction** — •Ralph Claessen

Sessions

HL 1.1–1.4	Sun	16:00–18:35	HSZ 403	**Tutorial: Energy materials**
HL 2.1–2.11	Mon	9:30–12:30	POT 051	**Topological insulators: mostly structure and electronic structure (with MA/O/TT)**
HL 3.1–3.1	Mon	9:30–10:00	POT 081	**Invited Talk Friedhelm Bechstedt**
HL 4.1–4.4	Mon	9:30–11:30	POT 151	**Physics of quantum rings (Focus session with TT)**
HL 5.1–5.6	Mon	9:30–11:00	POT 251	**Nitrides: mostly transport properties and recombination processes**
HL 6.1–6.5	Mon	9:30–12:15	HSZ 02	**Symposium SYMO: Magnetic/organic interfaces and molecular magnetism**
HL 7.1–7.9	Mon	9:30–12:15	ZEU 222	**Organic electronics and photovoltaics I (organized by CPP)**
HL 8.1–8.14	Mon	9:30–13:15	BEY 81	**Transport: Quantum dots, quantum wires, point contacts I (organized by TT)**
HL 9.1–9.1	Mon	10:00–10:30	POT 081	**Invited Talk Shu-Hong Yu**
HL 10.1–10.5	Mon	10:15–11:30	IFW A	**Functional materials I - Energy storage (organized by MM)**
HL 11.1–11.8	Mon	10:30–13:15	TRE Ma	**Frontiers of electronic structure theory - Non-equilibrium phenomena at the nano-scale I (organized by O)**
HL 12.1–12.7	Mon	10:45–12:30	POT 081	**Energy materials: Water splitting, batteries, and supercapacitors (with CPP/MM)**
HL 13.1–13.6	Mon	11:15–12:45	POT 251	**Nitrides: Optical characterization**
HL 14.1–14.1	Mon	11:45–12:15	POT 151	**Invited Talk James Lott**
HL 15.1–15.1	Mon	13:15–13:45	HSZ 02	**Semicrystalline polymers (organized by CPP)**
HL 16.1–16.11	Mon	15:00–18:45	POT 051	**Electron spin qubits in semiconductor quantum dots (Focus session with TT)**

HL 17.1–17.1	Mon	15:00–15:30	POT 081	**Invited Talk Thomas Ihn**
HL 18.1–18.7	Mon	15:00–16:45	POT 112	**Carbon: Diamond, nanotubes and Buckyballs**
HL 19.1–19.9	Mon	15:00–17:15	POT 151	**Nitrides: Devices**
HL 20.1–20.5	Mon	15:00–17:45	HSZ 02	**Symposium SYCM: Crystallography in materials science**
HL 21.1–21.10	Mon	15:00–18:00	ZEU 222	**Organic electronics and photovoltaics II (organized by CPP)**
HL 22.1–22.1	Mon	15:30–16:00	POT 006	**Invited Talk Emil List-Kratochvil**
HL 23.1–23.7	Mon	16:00–17:45	POT 006	**Quantum wires: Transport properties (with TT)**
HL 24.1–24.8	Mon	15:45–17:45	POT 081	**Topological insulators: mostly interaction with magnetic fields (with MA/TT)**
HL 25.1–25.9	Mon	16:00–18:30	HSZ 204	**Transport: Quantum dots, quantum wires, point contacts II (organized by TT)**
HL 26.1–26.12	Mon	16:00–19:00	WIL C107	**Graphene: Structural properties (organized by O)**
HL 27.1–27.10	Mon	16:00–18:45	TRE Ma	**Frontiers of electronic structure theory - Non-equilibrium phenomena at the nano-scale II (organized by O)**
HL 28.1–28.7	Mon	18:00–19:45	CHE 91	**Organic electronics and photovoltaics I (organized by DS)**
HL 29.1–29.11	Mon	17:00–20:00	P2	**Poster: Organic semiconductors and hybrid organic-inorganic heterostructures / Organic photovoltaics**
HL 30.1–30.27	Mon	17:00–20:00	P2	**Poster: Quantum dots and wires: Preparation, characterization, optical properties and transport**
HL 31.1–31.13	Mon	17:00–20:00	P2	**Poster: Nitrides**
HL 32.1–32.11	Mon	17:00–20:00	P2	**Poster: ZnO and its relatives**
HL 33.1–33.6	Tue	9:30–11:00	POT 006	**Optical properties I**
HL 34.1–34.1	Tue	9:30–10:00	POT 081	**Invited Talk Elizabeth von Hauff**
HL 35.1–35.9	Tue	10:00–12:30	POT 081	**Organic semiconductors: Photovoltaics (with CPP/DS/O)**
HL 36.1–36.1	Tue	12:30–13:00	POT 081	**Invited Talk Gary Hodes**
HL 37.1–37.4	Tue	9:30–10:30	POT 151	**Preparation and characterization**
HL 38.1–38.5	Tue	9:30–11:15	POT 251	**Quantum light sources based on solid state systems: Status and visions I (Focus session with TT)**
HL 39.1–39.5	Tue	9:30–12:15	HSZ 02	**Symposium SYSG: Spin properties of graphene**
HL 40.1–40.4	Tue	9:30–10:30	BEY 81	**Transport: Spintronics and magnetotransport (organized by TT)**
HL 41.1–41.13	Tue	9:30–13:15	WIL C107	**Transport: Graphene (organized by TT)**
HL 42.1–42.11	Tue	10:30–13:15	GER 38	**Topological insulators (organized by O)**
HL 43.1–43.9	Tue	10:30–13:15	TRE Ma	**Frontiers of electronic structure theory - Non-equilibrium phenomena at the nano-scale III (organized by O)**
HL 44.1–44.8	Tue	10:45–12:45	POT 151	**ZnO and its relatives: Devices**
HL 45.1–45.5	Tue	11:15–12:30	POT 006	**Optical properties II**
HL 46.1–46.4	Tue	11:45–12:45	POT 051	**Nitrides: mostly structural characterization**
HL 47.1–47.9	Tue	13:45–16:00	HSZ 401	**Spintronics (organized by MA)**
HL 48.1–48.8	Tue	14:00–16:00	POT 006	**Transport**
HL 49.1–49.8	Tue	14:00–16:00	POT 051	**Energy materials: Thermoelectrics**
HL 50.1–50.7	Tue	14:00–15:45	POT 081	**Organic semiconductors: Transistors and OLEDs (with CPP/DS)**
HL 51.1–51.1	Tue	14:00–14:30	POT 112	**Invited Talk Gregor Koblmüller**
HL 52.1–52.7	Tue	14:30–16:15	POT 112	**Quantum wires: Optical properties (with TT)**
HL 53.1–53.9	Tue	14:00–16:15	POT 151	**Nitrides: Preparation of nonpolar and semipolar orientations**
HL 54.1–54.6	Tue	14:00–15:45	POT 251	**Quantum light sources based on solid state systems: Status and visions II (Focus session with TT)**
HL 55.1–55.8	Tue	14:00–16:00	HSZ 304	**Transport: Topological insulators I (organized by TT)**
HL 56.1–56.1	Wed	9:30–10:00	POT 006	**Invited Talk Xavier Blase**
HL 57.1–57.10	Wed	9:30–12:15	POT 051	**Graphene: Transport (with MA/O/TT)**
HL 58.1–58.10	Wed	9:30–13:00	POT 081	**Emerging oxide semiconductors I (Focus session with DS)**
HL 59.1–59.7	Wed	9:30–11:15	POT 151	**Topological insulators: Theory (with MA/O/TT)**
HL 60.1–60.7	Wed	9:30–11:15	POT 251	**Quantum dots: Optical properties I (with TT)**
HL 61.1–61.12	Wed	9:30–12:45	ZEU 260	**Organic electronics and photovoltaics III (organized by CPP)**
HL 62.1–62.7	Wed	10:15–12:00	POT 006	**Spintronics I (with MA/O/TT)**
HL 63.1–63.1	Wed	12:00–12:30	POT 006	**Invited Talk Axel Hoffmann**

HL 64.1–64.10	Wed	10:30–13:15	TRE Ma	**Frontiers of electronic structure theory - Non-equilibrium phenomena at the nano-scale IV (organized by O)**
HL 65.1–65.7	Wed	11:30–13:15	POT 151	**Devices**
HL 66.1–66.6	Wed	11:30–13:00	POT 251	**Quantum dots: Optical properties II (with TT)**
HL 67.1–67.6	Wed	15:00–16:30	POT 006	**Quantum information systems I (with MA/TT)**
HL 68.1–68.8	Wed	15:00–17:00	POT 051	**Heterostructures and interfaces**
HL 69.1–69.12	Wed	15:00–18:45	POT 081	**Emerging oxide semiconductors II (Focus session with DS)**
HL 70.1–70.9	Wed	15:00–17:15	POT 112	**Semiconductor laser I: VECSEL and cascade lasers**
HL 71.1–71.9	Wed	15:00–17:15	POT 151	**Energy materials: Silicon-based photovoltaics**
HL 72.1–72.5	Wed	15:00–16:15	POT 251	**Quantum dots: Transport properties**
HL 73.1–73.12	Wed	15:00–18:15	ZEU 260	**Organic electronics and photovoltaics IV (organized by CPP)**
HL 74.1–74.1	Wed	15:00–15:45	GER 37	**Invited Talk: Heidemarie Schmidt (organized by DF)**
HL 75.1–75.10	Wed	15:00–18:00	HSZ 03	**Transport: Majorana fermions (organized by TT)**
HL 76.1–76.13	Wed	16:00–19:15	WIL C107	**Graphene: Electronic properties (organized by O)**
HL 77.1–77.11	Wed	16:00–19:15	TRE Ma	**Frontiers of electronic structure theory - Non-equilibrium phenomena at the nano-scale V (organized by O)**
HL 78.1–78.9	Wed	16:30–18:45	POT 251	**Quantum dots: Preparation and characterization**
HL 79.1–79.8	Wed	16:30–18:30	HSZ 204	**Transport: Topological insulators II (organized by TT)**
HL 80.1–80.8	Wed	16:30–18:30	HSZ 304	**Transport: Carbon nanotubes (organized by TT)**
HL 81.1–81.17	Wed	17:00–20:00	P1	**Poster: Energy materials incl. photovoltaics**
HL 82.1–82.5	Wed	17:00–20:00	P1	**Poster: Surfaces, interfaces and heterostructures (with O)**
HL 83.1–83.12	Wed	17:00–20:00	P1	**Poster: Graphene (with MA/O)**
HL 84.1–84.22	Wed	17:00–20:00	P1	**Poster: Electronic structure theory / Carbon (other than graphene) / Si, Ge, and SiC / III-V semiconductors (other than nitrides)**
HL 85.1–85.5	Thu	9:30–10:45	POT 006	**Organic light emission**
HL 86.1–86.7	Thu	9:30–11:15	POT 051	**Photonic crystals and cavities**
HL 87.1–87.1	Thu	9:30–10:00	POT 081	**Invited Talk Tobias Korn (with TT)**
HL 88.1–88.9	Thu	10:00–12:30	POT 081	**Graphene-like materials: Silicene, MoS_2 and relatives (with DY/MA/O/TT)**
HL 89.1–89.10	Thu	9:30–13:00	POT 251	**Metamorphic structures: Bringing together incompatible materials I (Focus session with DF)**
HL 90.1–90.13	Thu	9:30–13:15	HSZ 204	**Low-dimensional systems: Topological order (organized by TT)**
HL 91.1–91.6	Thu	9:30–12:45	CHE 91	**Sustainable photovoltaics with earth-abundant materials I (organized by DS)**
HL 92.1–92.9	Thu	10:00–12:15	POT 151	**Spintronics II (with MA/O/TT)**
HL 93.1–93.10	Thu	10:30–13:15	TRE Ma	**Frontiers of electronic structure theory - Non-equilibrium phenomena at the nano-scale VI (organized by O)**
HL 94.1–94.1	Thu	11:00–11:30	POT 006	**Invited Talk Yong Lei**
HL 95.1–95.6	Thu	11:30–13:00	POT 051	**Polaritons**
HL 96.1–96.1	Thu	15:00–15:30	POT 051	**Invited Talk Arash Rahimi-Iman**
HL 97.1–97.7	Thu	15:30–17:15	POT 051	**Semiconductor laser II: Microcavities and quantum-dot laser**
HL 98.1–98.11	Thu	15:00–18:00	POT 081	**Graphene: Spintronics, transistors, and sensors (with DY/MA/O/TT)**
HL 99.1–99.8	Thu	15:00–17:00	POT 151	**Electronic structure theory**
HL 100.1–100.5	Thu	15:00–16:30	POT 251	**Metamorphic structures: Bringing together incompatible materials II (Focus session with DF)**
HL 101.1–101.7	Thu	15:00–18:25	HSZ 03	**Theoretical advances in interacting topological phases (organized by TT)**
HL 102.1–102.10	Thu	15:00–17:30	CHE 91	**Sustainable photovoltaics with earth-abundant materials II (organized by DS)**
HL 103.1–103.11	Thu	16:00–18:45	WIL C107	**Graphene: Adsorption, intercalation, doping (organized by O)**
HL 104.1–104.8	Thu	17:45–19:45	CHE 91	**Organic electronics and photovoltaics II (organized by DS)**
HL 105.1–105.12	Thu	17:00–20:00	P1	**Poster: Topological insulators (with MA/O)**
HL 106.1–106.7	Thu	17:00–20:00	P1	**Poster: Spintronics (with MA/O)**
HL 107.1–107.21	Thu	17:00–20:00	P1	**Poster: Emerging oxide semiconductors / Oxides other than ZnO and its relatives**

HL 108.1–108.31	Thu	17:00–20:00	P1	**Poster: Ultra-fast phenomena / Optical properties / Semiconductor laser / Devices and device concepts**
HL 109.1–109.5	Fri	9:30–10:45	POT 006	**Ultra-fast phenomena I**
HL 110.1–110.1	Fri	9:30–10:00	POT 051	**Invited Talk Irene Burghardt**
HL 111.1–111.6	Fri	9:30–11:00	POT 081	**Graphene: Bi- and multi-layers (with MA/O/TT)**
HL 112.1–112.11	Fri	9:30–12:30	POT 112	**Energy materials: CIGS and related photovoltaics**
HL 113.1–113.5	Fri	9:30–10:45	POT 151	**Quantum information systems II (with TT)**
HL 114.1–114.12	Fri	9:30–12:45	POT 251	**Oxides: Bulk, films and interfaces**
HL 115.1–115.4	Fri	9:30–12:30	HSZ 02	**Symposium SYOM: One-dimensional metals - Reality or fiction?**
HL 116.1–116.9	Fri	9:30–12:00	HSZ 04	**Topological insulators (organized by MA)**
HL 117.1–117.9	Fri	10:15–12:30	POT 051	**Organic semiconductors: Material properties (with CPP/DS)**
HL 118.1–118.7	Fri	11:15–13:00	POT 081	**Graphene: Interaction with the substrate (with DY/MA/O/TT)**
HL 119.1–119.1	Fri	11:00–11:30	POT 006	**Invited Talk Michael Leuenberger**
HL 120.1–120.5	Fri	11:30–12:45	POT 006	**Ultra-fast phenomena II**
HL 121.1–121.7	Fri	11:30–13:15	CHE 89	**Graphene (organized by DS)**

Annual General Meeting of the Semiconductor Physics Division

Thursday 18:30–19:30 POT 006

HL 1: Tutorial: Energy materials

This tutorial introduces basic physical concepts underlying the microscopic working principles of a broad and diverse range of energy materials ranging from organic solar cells to strong magnets for wind turbines. Leading scientists from various different disciplines – both from academia and industry – will give an exciting overview of the state-of-the art in their specific field of expertise. The topics to be covered include: Electrochemical energy storage and battery research, superstrong magnets and magnetocalorics, dye-sensitized solar cells from the Graetzel cell to hybrid inorganic-organic perovskites, and solar water splitting. We also refer to the parallelly running tutorial on thermoelectricity. All talks are specifically prepared for a broad audience.

Organized by Erich Runge, TU Ilmenau, and Christoph Lienau, Carl von Ossietzky Universität Oldenburg, on behalf of the Semiconductor Physics Division jointly with the Magnetism Division.

Time: Sunday 16:00–18:35 Location: HSZ 403

Invited Talk HL 1.1 Sun 16:00 HSZ 403
Von Lithium zu Lithium-Ionen-Batterien und zurück — •Martin Winter — WWU Münster, Deutschland

Invited Talk HL 1.2 Sun 16:35 HSZ 403
Magnetic materials for green energy applications — •Oliver Gutfleisch — TU Darmstadt, Material Science, Functional Materials — Fraunhofer Project Group Materials Recycling and Resource Strategy IWKS

Due to their ubiquity, magnetic materials play an important role in improving the efficiency and performance of devices in electric power generation, conversion and transportation 1. Permanent magnets are essential components in motors and generators of hybrid and electric cars, wind turbines, etc. Magnetocaloric materials could be the basis for a solid state energy efficient cooling technique alternative to compressor based refrigeration. Any improvements in magnetic materials will have a significant impact in these areas, on par with many *hot* energy materials efforts (e.g. hydrogen storage, batteries, thermoelectrics, etc.).

The talk focuses on rare earth and rare earth free permanent magnet and magnetocaloric materials with an emphasis on their optimization for energy and resource efficiency in terms of the usage of critical elements. The synthesis, characterization, and property evaluation of the materials will be examined briefly having in mind their critical micromagnetic length scales and phase transition characteristics.

Coffee break (10 min.)

Invited Talk HL 1.3 Sun 17:20 HSZ 403
Recent developments of dye sensitized and mesoscopic solar cells — •Toby Meyer — Solaronix SA, Aubonne, Switzerland

The latest results on the Dye Sensitized Solar Cell developments at Solaronix are presented in the international context, both scientifically and economically. Examples include the first application in a 250 m^2 vertical façade at the Swisstech Convention Center (EPFL, Lausanne). Furthermore, we discuss the rapid progress in perovskite-based photovoltaics and show results on Solaronix's novel "perovskite" solid-state mesoscopic solar cells.

Invited Talk HL 1.4 Sun 17:55 HSZ 403
Perspectives of an artificial leaf based on inorganic semiconductors for water splitting: Device structure, interface engineering, catalytic demands — •Wolfram Jaegermann — TU Darmstadt, Instiute of Materials Science, Jovanka-Bontschits-Str. 2, D-64287 Darmstadt

For an effective conversion of solar energy to a chemical fuel a number of elementary processes as well as their coupling to each other must be optimized without severe losses in the number and the chemical potential of the originally generated electron-hole pairs. Light absorption coupled to efficient charge carrier generation and separation may be realized by thin film semiconductor devices - preferentially tandem cells - which may provide broad band quantum efficiencies close to 1. Alternatively, Janus type photocatalysts may be chosen which favour vectorial electron-hole pair transport into opposite directions. Subsequently, H2 (or HC-fuels) and O2 from H2O (and CO2) must be formed by electron and hole transfer reactions with minimized loss of chemical potential. This will only be possible if the involved charge transfer steps are coupled to selective multi electron transfer catalysts. Technologically feasible solutions seem to be possible for water splitting and H2-generation, as we will show with a number of investigations performed recently combining electrochemical investigations with surface science approaches.

Closing remarks

HL 2: Topological insulators: mostly structure and electronic structure (with MA/O/TT)

Time: Monday 9:30–12:30 Location: POT 051

HL 2.1 Mon 9:30 POT 051
InAs/GaSb compound quantum wells for electrically tunable topological insulator devices — •Georg Knebl[1], Matthias Dallner[1], Robert Weih[1], Sven Höfling[1,2], and Martin Kamp[1] — [1]Universität Würzburg, Deutschland — [2]University of St Andrews, Scotland

InAs/GaSb compound quantum wells (CQW) sandwiched between two AlSb layers and a front/back gate were proposed by Liu et al. [1] to show a topological insulator phase. The advantage of this structure is the possibility to tune the phase transition from a normal to a topological insulator via the front and back gate voltage. In addition, this material combination allows the use of established III/V semiconductor technology for epitaxy and device processing.

We present results on the growth of InAs/GaSb CQWs via molecular beam epitaxy on GaSb and GaAs substrates using different buffers. Furthermore, we will discuss device fabrication on InAs/GaSb layer structures, which requires special care since oxidation or process induced damage can lead to the formation of conducting surface channels. Electrical characterization of Hall bars and the tunability of the transport properties via gates will be reported.

[1] C. Liu, et al., Phys. Rev. Lett. 100, pp. 1-4, (2008)

HL 2.2 Mon 9:45 POT 051
Resolving the linear dispersion relation of topological insulator nanowires — •Johannes Gooth, Bacel Hamdou, August Dorn, Robert Zierold, and Kornelius Nielsch — Institute of Applied Physics, Universität Hamburg, Hamburg, Germany

Due to the linear dispersion relation, charge carriers in the surface states of a topological insulator (TI) behave like relativistic particles described by the Dirac equation for spin-1/2 particles leading to exotic new physics and applications. In bulk topological insulators the linear dispersion relation at the surface has been resolved by angle-resolved photoemission spectroscopy (ARPES). On nanostructures ARPES measurements have not been successful, due to the limited sample size. Instead magnetoelectrical transport measurements became the most common way to indicate the existance of surface states in nanomaterials. However, the linear dispersion relation has not been directly resolved in nanostructures to date.

Here, we show that the linear dispersion relation on the surface of a Bi_2Te_3 nanowire can directly be deduced from gate dependend magnetotot ransport measurements. Further carrier concentration, mobility and effective mass of the dirac fermions are determined as a function of gate voltage. It can be shown that at 2K the transport in the surface states is dominated by electron-electron interaction.

HL 2.3 Mon 10:00 POT 051

Temperature-dependent surface band gap of Dirac fermions observed at the (111) surface of the crystalline topological insulator Pb-Sn-Se — •Partha S. Mandal[1], Gunther Springholz[2], Günther Bauer[2], Valentine V. Volobuev[2], Andrei Varykhalov[1], Oliver Rader[1], and Jaime Sánchez-Barriga[1] — [1]Helmholtz-Zentrum Berlin — [2]Johannes-Kepler-Universität Linz

Using angle-resolved photoemission, we studied (111)-oriented epitaxial films of Pb-Sn-Se grown by molecular beam epitaxy. The topological-to-trivial-insulator phase transition [1] is monitored probing the bulk valence band as a function of Sn concentration and temperature between 30 K and room temperature. In the topological phase, the topological surface state opens a band gap indicating a mass aquisition that is not caused by broken time reversal symmetry. We discuss this phenomenon in comparison to conventional topological insulators [2] protected by time-reversal symmetry.

[1] P. Dziawa, B. J. Kowalski, K. Dybko, R. Buczko, A. Szczerbakow, M. Szot, E. Łusakowska, T. Balasubramanian, B. M. Wojek, M. H. Berntsen, O. Tjernberg, T. Story, Nature Mat. 11, 1023 (2012).

[2] T. Sato, K. Segawa, K. Kosaka, S. Souma, K. Nakayama, K. Eto, T. Minami, Y. Ando, and T. Takahashi, Nature Phys. 7, 840 (2011).

HL 2.4 Mon 10:15 POT 051

Surface-Dominated Transport on a Bulk Topological Insulator — •Lisa Kühnemund[1], Lucas Barreto[2], Frederik Edler[1], Christoph Tegenkamp[1], Jianli Mi[3], Martin Bremholm[3], Bo Brummerstedt Iversen[3], Christian Frydendahl[2], Marco Bianchi[2], and Philip Hofmann[2] — [1]Leibniz Universität Hannover, Inst. f. Festkörperphysik — [2]Aarhus University, Dep. of Physics and Astronomy, iNANO — [3]Aarhus University, Center for Materials Crystallography, iNANO

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 so-far 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. Here we present a direct measurement of surface-dominated conduction on an atomically clean surface of Bi_2Te_2Se. Using nano-scale four point setups with variable contact distance, we show that the transport at 30 K is two-dimensional rather than three-dimensional and by combining these measurements with angle-resolved photoemission results from the same crystals, we find a surface state mobility of 390(30) $cm^2V^{-1}s^{-1}$ at 30 K at a carrier concentration of $8.71(7)\times10^{12}$ cm^{-2}.

HL 2.5 Mon 10:30 POT 051

Room temperature high frequency transport of Dirac fermions in MBE grown Sb_2Te_3 based topological insulators — •T. Herrmann[1], P. Olbrich[1], S.N. Danilov[1], Ch. Weyrich[3], J. Kampmeier[3], G. Mussler[3], D. Grützmacher[3], L. Plucinski[3], C.M. Schneider[3], M. Eschbach[3], L.E. Golub[2], V.V. Bel'kov[2], and S.D. Ganichev[1] — [1]University of Regensburg, Regensburg, Germany — [2]Ioffe Institute, St. Petersburg, Russia — [3]Peter Grünberg Institute (PGI) & Jülich Aachen Research Alliance (JARA-FIT), Research Center Jülich, Jülich, Germany

We report on the observation of terahertz (THz) laser radiation induced currents in epitaxially grown Sb_2Te_3 based topological insulators (TI) [1]. We demonstrate that the excitation of the sample with linearly polarized THz radiation results in a photoresponse solely stemming from the surface states of the 3D TI. Our analysis shows that the photocurrent is caused by the photogalvanic effect [2], which emerges in the surface states but is forbidden in the centrosymmetric bulk material. As an important result our measurements demonstrate that the high frequency transport can be obtained in the Dirac fermion system even at room temperature.

[1] Plucinski et al.; J. Appl. Phys. **113**, 053706 (2013)

[2] Weber et al.; Phys. Rev. B **77**, 245304 (2008)

HL 2.6 Mon 10:45 POT 051

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

Topological insulators (TIs) are a new state of quantum matter which insulates in the bulk and conducts on the surface. The study of bulk TIs has been hindered by high conductivity in the bulk, arising from crystalline defects. Such problems can be tackled through compositional engineering or the synthesis of TI nanomaterials. We combined both approaches in a systematic study of various growth parameters to achieve uniform, high purity nanowires with high substrate coverage.

The highlight of this study is the development of a new growth route for nanowires, based on a TiO_2 catalyst rather than the conventional Au. Comparative studies demonstrate that Au significantly contaminates the nanowires, whereas TiO_2 stays well separated. Details of the Au and TiO_2-catalysed growth mechanism were investigated. For Au it was found that the growth mechanism is vapour-liquid-solid. For TiO_2 nanoparticles, in contrast, the growth mechanism can be described in the vapour-solid scheme.

Nanowires of the doped compound $(Bi_{0.78}Sb_{0.22})_2Se_3$ were studied using synchrotron radiation. It was discovered that the material mainly adopts an orthorhombic phase known from Sb_2Se_3. The Raman spectrum is reported and matched with the structural information for the first time. Furthermore, a method to control the length and diameter of Bi_2Se_3 nanowires through laser-cutting was developed.

Coffee break (15 min.)

HL 2.7 Mon 11:15 POT 051

Optoelectronic flow trajectories in topological insulators — •Paul Seifert[1], Christoph Kastl[1], Tong Guan[2], Kehui Wu[2], X. Y. He[2], Yongqing Li[2], and Alexander W. Holleitner[1] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München — [2]Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

We report on the optoelectronic properties of thin films of the topological insulator $(Bi_xSb_{1-x})_2Te_3$ grown by molecular beam epitaxy. In spatially resolved experiments, we observe photocurrent patterns with positive and negative amplitude [1]. We interpret the patterns to originate from a local photocurrent generation due to potential fluctuations [1]. Exploiting the local photocurrent generation in combination with a sub 100-nm lithography, we visualize the current flow in nanoscale circuits based on topological insulators [2].

[1] C. Kastl, T. Guan, X. Y. He, K. H. Wu, Y. Q. Li, and A. W. Holleitner, Appl. Phys. Lett. 101, 251110 (2012). [2] C. Kastl et al., (2014).

We gratefully acknowledge financial support from the DFG-project HO3324/8 within the SPP 1666 on topological insulators.

HL 2.8 Mon 11:30 POT 051

Polarization-controlled picosecond spin currents in topological insulators — •Christoph Kastl[1], Christoph Karnetzky[1], Helmut Karl[2], and Alexander W. Holleitner[1] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München, 85748 Garching, Germany — [2]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Controlling spin currents in topological insulators may lead to applications in future spintronic devices [1]. Here, we show that surface currents in Bi2Se3 can be controlled by circularly polarized light on a time-scale of a picosecond with a fidelity near unity even at room temperature. We reveal the temporal interplay of such ultrafast spin currents with photo-induced thermoelectric and drift currents in optoelectronic circuits [2].

[1] C. Kastl, T. Guan, X. Y. He, K. H. Wu, Y. Q. Li, and A. W. Holleitner, Appl. Phys. Lett. 101, 251110 (2012).

[2] C. Kastl et al., (2014).

We gratefully acknowledge financial support from the DFG-project HO3324/8 within the SPP 1666 on topological insulators.

HL 2.9 Mon 11:45 POT 051

Scanning Tunneling Microscopy of Ultrathin Topological Insulator Sb_2Te_3 Films on Si(111) grown by Molecular Beam Epitaxy — •Martin Lanius, Jörn Kampmeier, Gregor Mussler, and Detlev Grützmacher — Peter Grünberg Institut, Forschungszentrum Jülich, Germany

Topological insulators (TIs) are a class of materials in the field of condensed matter physics. In addition to the fascinating electronic properties, the Van der Waals growth mode of TIs, i.e. the TI epilayer is only weakly bonded to the substrate, which allows the use of substrates with high lattice mismatch, is of high interest. In this case we have studied the nucleation and growth process of the TI Sb_2Te_3 on Si(111) substrates by STM (Scanning Tunneling Microscopy) and AFM (Atomic Force Microscopy). The thin films from several nanometers thickness down to one quintuple layer thickness have been grown by molecular beam epitaxy. To determine the thickness and composition of the films we used x-ray reflectivity and x-ray diffraction. Further investigations of $Ge_2Sb_2Te_3$, which is a phase-changing material and a topological insulator, and the comparison to the growth mode of Sb_2Te_3 will be presented.

HL 2.10 Mon 12:00 POT 051

Transport of Dirac fermions in the presence of spin-orbit impurities — •Pierre Adroguer[1], Dimitri Culcer[2], and Ewelina Hankiewicz[1] — [1]Institute for Theoretical Physics and Astronomy, Würzburg University, Würzburg, Germany — [2]School of Physics, University of New South Wales, Sidney, Australia

The recent exprimental realizations of three dimensional topological insulators (3DTI) have provided a new tool to investigate Dirac physics.

Indeed, these materials exhibit an insulating bulk and a single metallic surface state described by Dirac fermion physics.

In the regime of weak scalar disorder, Dirac fermions do not backscatter because of time-reversal symmetry. Further, this absence of backscattering leads to a weak antilocalization correction (an increase in conductivity in the absence of magnetic field, due to quantum interference of conjugated paths) [1,2].

In this presentation, we will review these phenomena, and show how these features are modified when there are spin-orbit impurities in the Dirac fermion systems.

We acknowledge financial support via grant HA 5893/4-1 within SPP 1666.

[1] G. Tkachov and E. M. Hankiewicz, Phys. Rev. B 84, 035444 (2011)

[2] P. Adroguer, D. Carpentier, J. Cayssol, and E. Orignac, New Journal of Physics 14, 103027 (2012)

HL 2.11 Mon 12:15 POT 051

Oscillatory surface dichroism of the insulating topological insulator Bi_2Te_2Se — •Susmita Basak[1], Madhab Neupane[2], Hsin Lin[1], N. Alidoust[2], S.-Y. Xu[2], Chang Liu[2], I. Belopolski[2], G. Bian[2], J. Xiong[2], H. Ji[3], S. Jia[3], S.-K. Mo[4], M. Bissen[5], M. Severson[5], N. P. Ong[2], T. Durakiewicz[6], R. J. Cava[3], A. Bansil[1], and M. Z. Hasan[2] — [1]Department of Physics, Northeastern University, Boston, Massachusetts, USA — [2]Joseph Henry Laboratory and Department of Physics, Princeton University, Princeton, New Jersey, USA — [3]Department of Chemistry, Princeton University, Princeton, New Jersey, USA — [4]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California, USA — [5]Synchrotron Radiation Center, Stoughton, Wisconsin, USA — [6]Condensed Matter and Magnet Science Group, Los Alamos National Laboratory, Los Alamos, New Mexico, USA

We present a study of the effect of angular momentum transfer between polarized photons and topological surface states of the insulating topological insulator Bi_2Te_2Se using circular dichroism-angle resolved photoemission spectroscopy. The photoelectron dichroism demonstrate a dramatic sign flip with the change of photon frequency and we show that this is a consequence of a strong coupling between the photon field and the spin-orbit nature of the initial Dirac states on the surface. Our studies reveal the intrinsic dichroic behavior of topological surface states and point toward the potential utility of bulk insulating topological insulators in opto-spintronics device applications.

HL 3: Invited Talk Friedhelm Bechstedt

Time: Monday 9:30–10:00 Location: POT 081

Invited Talk HL 3.1 Mon 9:30 POT 081

Parameterfree calculations of excitations and spectra: Fiction or reality for semiconductors? — •Friedhelm Bechstedt — Friedrich-Schiller-Universitaet, Jena, Germany

The dream of theorists annd computational physicists is to have predictive power for important material properties and physical effects. Its realization requires ab initio calculations without experimental input parameters but accounting fully for the many-body interactions. The status of realization is examined for electronic excitations and related spectra. The basic approaches - density functional theory and many-body perturbation theory (quasiparticle and excitonic effects) - are introduced. Progress, accuracy problems, and applications are discussed for three classes of properties: (i) atomic equilibrium geometries, (ii) energies of electronic quasiparticles, and (iii) optical spectra including electron-hole pair excitations. Results are exemplarily presented for band structures and photoemission/X-ray/optical spectra of semiconductors such as Si, nitrides and oxides. The outlook concerns free carriers, defects, and nanostructures.

HL 4: Physics of quantum rings (Focus session with TT)

Innovative recent findings in both experimental and theoretical physics of quantum rings and ring-like atom systems based on the most advanced state-of-the-art fabrication and characterization techniques as well as theoretical methods will be discussed. The experimental efforts allow for obtaining new classes of semiconductor quantum rings and quantum-ring-based metamaterials. An adequate characterization of quantum rings is realized using scanning tunneling microscopy methods. Dedicated theoretical models allow for interpretation of the novel topology-driven physical properties of quantum rings.

Organizer: Axel Lorke, Universität Duisburg-Essen.

Time: Monday 9:30–11:30 Location: POT 151

Topical Talk HL 4.1 Mon 9:30 POT 151

Impact of topology on physical properties of quantum rings — •Vladimir M. Fomin — Institute for Integrative Nanosciences, IFW-Dresden, Helmholtzstraße 20, 01069 Dresden, Germany

Advanced micro- and nanostructure fabrication techniques can be exploited to generate non-trivially shaped objects possessing man-designed topological features, such as doubly-connectedness (quantum rings) and one-sidedness (Möbius strips) [1]. Even though self-assembled semiconductor quantum rings ('quantum volcanos') are singly-connected and anisotropic, they exhibit the Aharonov-Bohm effect on the persistent current because the electron wave functions are exponentially decaying towards the center and are topologically identical to those in doubly-connected quantum rings. Theoretically predicted Aharonov-Bohm effect in 'quantum volcanos' was experimentally detected by torsion magnetometry. Symbiosis of a geometric potential and an inhomogeneous twist renders an observation of the topology effect on the electron ground-state energy in microscale Möbius strips into the realm of experimental verification. A 'delocalization-to-localization' transition for the electron ground state is unveiled in inhomogeneous Möbius strips [2]. This transition can be quantified through the Aharonov-Bohm effect on the persistent current. Recent findings

suggest perspectives of topological control over electronic, spin, optical, magnetic and transport properties of micro- and nanostructures.

[1] V. M. Fomin (Ed.), Physics of Quantum Rings, Springer, Berlin–Heidelberg, 2014, 487 p. [2] V. M. Fomin, S. Kiravittaya, O. G. Schmidt, Phys. Rev. B 86, 195421 (2012).

Topical Talk HL 4.2 Mon 10:00 POT 151

Fabrication of ordered quantum rings — •Zhiming Wang — School of Microelectronics and Solid-State Electronics, University of Electronic Science and Technology of China, Chengdu, 610054 , P. R. China

Quantum rings possess unique properties and have attracted extensive theoretical and experimental attention. Up to now, various effects have been devoted to fabrication of quantum rings via both top-down techniques and self-assembly. Epitaxy has been demonstrated as an effective method to fabricate self-assembled quantum rings. Despite the well-controlled morphology of self-assembled quantum rings produced by using both Stranski-Krastanov growth and droplet epitaxy, the lateral ordering of quantum rings remains challenging[1]. In this presentation, both vertically and laterally aligned quantum rings are described. The fabrication of laterally aligned quantum rings is based on the transformation of ordered quantum dots using the self-organized anisotropic strain engineering technique. The vertically aligned quantum rings are fabricated by multi-step droplet epitaxy. The growth mechanisms of both vertically aligned and laterally ordered quantum rings are discussed. Fabrication of ordered quantum rings is of high priority for practical applications, in particular, as photovoltaic devices and photodetectors.

References

[1] J. Wu and Z. Wang, in: V. M. Fomin (Ed.), Physics of Quantum Rings, Springer, Berlin-Heidelberg, 2014, pp. 143-159.

Coffee break (15 min.)

Topical Talk HL 4.3 Mon 10:45 POT 151

Self-organized formation and XSTM characterization of GaSb/GaAs quantum rings — •Andrea Lenz — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

In the GaSb/GaAs material system, quantum rings (QRs) can occur already after the material deposition on GaAs(001), sometimes even without capping. Upon capping almost all quantum dots are transformed into QRs [1].

This presentation gives an overview of the structural parameters and the formation process of the GaSb/GaAs QRs using cross-sectional scanning tunneling microscopy (XSTM). Furthermore, information on the electronic structure of the QRs is shown, which is gained using scanning tunneling spectroscopy mode (XSTS). XSTS reveals the type-II alignment for GaSb/GaAs QRs [2], which makes them very promising for charge storage devices and in photovoltaics. Furthermore, the GaSb/GaAs system exhibits a strong Aharonov-Bohm effect since the central opening of the QRs is much more pronounced as compared with other material systems, like e.g. the InGaAs/GaP system, for which QRs have been observed quite recently [3].

This work was supported by the EC through the SANDiE NoE and by projects Da 408/13 and Sfb 787 of the DFG.

[1] A. Lenz and H. Eisele, in: V. M. Fomin (Ed.), Physics of Quantum Rings, Springer, Berlin-Heidelberg, 2014, pp. 123-142. [2] R. Timm et al., Nano Lett. 10, 3972 (2010). [3] C. Prohl et al., Appl. Phys. Lett. 102, 123102 (2013).

HL 4.4 Mon 11:15 POT 151

Current-induced spin dynamics in ring-like atom clusters on surfaces — •Benjamin Baxevanis, Christoph Hübner, Lars-Hendrik Frahm, and Daniela Pfannkuche — I. Institut für Theoretische Physik, Universität Hamburg, Germany

Recently, much attention has been devoted to artificially assembled magnetic structures made of iron atoms on non-magnetic substrates using a scanning tunneling microscope [1,2,3]. Some of these structures show unique dynamics and switching of magnetism under the influence of a spin-polarized current and the interaction with the substrate [2,3]. We theoretically consider the spin dynamics in a ring-like cluster of Fe atoms on a substrate tunnel-coupled to a magnetic tip. Employing a master equation approach, the effects of the spin-polarized current, anisotropy field and symmetry of the ring-like cluster [4] on the spin dynamics are studied.

[1] A. A. Khajetoorians, J. Wiebe et al., Nature Physics 8, 497 (2012)
[2] S. Loth, S. Baumann, C. P. Lutz et al., Science 335, 196 (2012)
[3] A. A. Khajetoorians, B. Baxevanis et al., Science 339, 55 (2013)
[4] B. Baxevanis and D. Pfannkuche, in: V. M. Fomin (Ed.), Physics of Quantum Rings, Springer, Berlin-Heidelberg, 2014, pp. 381-408.

HL 5: Nitrides: mostly transport properties and recombination processes

Time: Monday 9:30–11:00 Location: POT 251

HL 5.1 Mon 9:30 POT 251

Non-radiative recombination mechanisms in GaN by first-principles total energy calculations — •Ying Cui, Christoph Freysoldt, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40627 Düsseldorf

Non-radiative recombination limits the efficiency of GaN based LEDs. However, the chemical nature and atomic geometry of the recombination centers and their recombination cross-sections are generally not known. Employing a Shockley-Read-Hall model, we propose a one-dimensional (1-D) model to locate the transition state in the capture process using the defect level occupation as a natural reaction coordinate. The calculations are based on density functional theory with hybrid functional (HSE). Employing this approach, we obtain the electron (hole) capture cross-sections, which can be directly compared with experimental results, such as deep-level transient spectroscopy(DLTS). Among all the defects in our study, nitrogen vacancies show the largest potential to be effective non-radiative recombination centers. Their calculated activation energy and electron capture cross-sections agree well with experimental data reported in literature.

HL 5.2 Mon 9:45 POT 251

Recombination rates in GaInN/GaN quantum wells: Beyond the ABC model — •Torsten Langer[1], Alexey Chernikov[2], Dimitri Kalincev[2], Marina Gerhard[2], Heiko Bremers[1], Uwe Rossow[1], Martin Koch[2], and Andreas Hangleiter[1] — [1]Institute of Applied Physics, Technische Universität Braunschweig — [2]Faculty of Physics and Materials Science Center, Philipps-Universität Marburg

We report on an excitonic enhancement of recombination processes in GaInN/GaN single quantum wells being evident from temperature and density dependent time-resolved photoluminescence spectroscopy over a wide range of excitation densities. The proposed method allows for a determination of the radiative and nonradiative recombination times as a function of the excess carrier density (rather than a function of the generation rate) free of any a priori assumptions on the dynamics of the recombination processes. Excitonic radiative recombination is evidenced by density independent radiative lifetimes in the high injection regime, i.e. excess densities are larger than the background density. The transition from low to high injection is calibrated via the observed increase of Shockley-Read-Hall lifetimes in the intermediate regime. At high densities, a weak temperature dependence of nonradiative lifetimes that are proportional to the inverse of the density imply an excitonic, threshold-less Auger process. The density dependence of both radiative and nonradiative lifetimes thus differs strongly from the predictions of simple free-carrier ABC models.

HL 5.3 Mon 10:00 POT 251

Reduced electron accumulation at InN(0001) surfaces via saturation of surface states by donor- or acceptor-type adsorbates — •Stephanie Reiss, Anja Eisenhardt, Stefan Krischok, and Marcel Himmerlich — Institut für Physik and Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, PF 100565, 98684 Ilmenau, Germany

We investigate the impact of selected donor- and acceptor-type adsorbates (potassium and oxygen) on the electronic properties of InN(0001) surfaces implementing in-situ photoelectron spectroscopy. Potassium adsorption leads to a strong decrease in the work function Φ from initially 4.4 to 1.6 eV indicating electron transfer from K adatoms to-

wards the InN surface. In parallel, a reduction of the surface downward band bending V_{bb} by 0.2 eV and the formation of potassium induced electron states close to the valence band maximum are observed. The interaction of oxygen induces an increase of Φ up to 5.2 eV due to an opposite charge transfer towards the adsorbate and a reduction of V_{bb} by 0.4 eV. The depletion of the surface electron accumulation layer in both cases can be explained by adsorbate-induced saturation of free dangling bonds at the InN surface resulting in the disappearance of surface states, which initially pin the Fermi level and induce downward band bending. The results prove that the electronic structure can be modified by adlayers resulting in a possible pathway for compensation of the surface electron accumulation.

HL 5.4 Mon 10:15 POT 251

Formation of Schottky contacts on n-type GaN bulk crystals grown by hydride vapor phase epitaxy (HVPE) — •Ronald Stübner[1], Vladimir Kolkovsky[1], Jörg Weber[1], Gunnar Leibiger[2], and Frank Habel[2] — [1]Technische Universität Dresden, 01062 Dresden, Germany — [2]Freiberger Compound Materials GmbH, 09599 Freiberg, Germany

In the present study we investigate the formation of Schottky contacts on GaN grown by hydride vapor phase epitaxy (HVPE). Evaporated silver exhibits good rectifying contacts with leakage currents of about 10^{-5} A cm^{-2} and a rectification ratio of about 2000 on as-grown n-type GaN for small growth ratios between N and Ga. Contacts have no rectifying behavior in samples grown at a higher ratio of N/Ga. We correlate these observations with the presence of negatively charged gallium vacancies in our samples. They compensate the positively charged donors and lead to a significant increase in series resistance. Deep level transient spectroscopy studies reveal two deep level defects E250 and E610 in our samples. The results are consistent with the previous assignment of E250 to a defect containing a gallium-vacancy [1] and E610, which was attributed to the nitrogen antisite [2]. [1] Z.-Q. Fang *et al.* Appl. Phys. Lett. **78**, 332 (2001). [2] P. Hacke *et al.*, J. Appl. Phys. **76**, 304 (1994).

HL 5.5 Mon 10:30 POT 251

Electrical properties of Si-doped AlGaN layers with high aluminum mole fraction — •Harald Pingel[1], Frank Mehnke[1], Eberhard Richter[2], Frank Brunner[2], Tim Wernicke[1], Christian Kuhn[1], Viola Kueller[2], Arne Knauer[2], Michael Lapeyrade[2], Markus Weyers[2], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Germany — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Berlin, Germany

The electrical properties of Si-doped $Al_xGa_{1-x}N$ layers with $x > 0.8$ were studied by temperature-dependent resistance and Hall measurements. $Al_xGa_{1-x}N$:Si layers with a thickness of 1.2 μm – 1.6 μm were grown by metal organic vapor phase epitaxy using TMAl, TMGa, NH_3 as precursors and SiH_4 and H_2 as dopant source and carrier gas, respectively. A set of samples with different aluminum content and SiH_4/III-ratios was investigated. At room temperature the resistivity strongly depends on the aluminum content as well as the SiH_4/III-ratio. With increasing aluminium content the resistivity increases from 0.07 Ωcm ($x = 0.82$) to 4.3 Ωcm ($x = 0.95$) at a constant SiH_4/III-ratio of 2×10^{-5}. A distinct minimum in the resitivity was found for a series of SiH_4/III-ratios. In order to investigate the cause of this behavior, the charge carrier density, the resistivity and the mobility were measured between 300 K and 720 K. From this, the donor densities and the activation energies were determined. The increase in resistivity for increasing aluminum content could be attributed to an increase in the donor activation energy.

HL 5.6 Mon 10:45 POT 251

Field-dependent photoluminescence of InAlN/GaN based HEMT structures — •Christoph Koch[1], Martin Feneberg[1], Rüdiger Goldhahn[1], María Fátima Romero[2], Fernando Calle[2], Zhan Gao[2], María Ángeles Pampillón[3], Enrique San Andrés[3], Pedro C. Feijoo[3], and Pavel Y. Bokov[4] — [1]Otto-von-Guericke Universität, Magdeburg, Germany — [2]Universidad Politécnica de Madrid, Madrid, Spain. — [3]Universidad Complutense de Madrid, Madrid, Spain — [4]Moscow State University, Moscow, Russia

The optical properties of InAlN/GaN based HEMT structures were examined by field-dependent photoluminescence spectroscopy as a function of temperature.

Samples grown on Si subtrate were investigated. On top of a thick GaN buffer layer, an InAlN barrier of 10 nm causes a two-dimensional electron gas (2DEG), which dominates PL spectra at low temperatures at energies slightly below the donor-bound exciton. Semi-transparent metal contacts were processed either directly on top of the structures or seperated by an additional high-k dielectric, serving as Schottky or MIS diodes, respectively. Free exciton recombinations of the GaN buffer were observed for higher temperatures and allow determination of the strain in the GaN layer. Due to sample structure PL measurements exhibit mostly GaN related features.

PL spectra with varying voltages and thus modified band diagrams were systematically studied. Consequently, a voltage-dependent shift of 2DEG related luminescence is observed, corroborating the assignment of this band to a 2DEG to free-hole transition.

HL 6: Symposium SYMO: Magnetic/organic interfaces and molecular magnetism

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

Invited Talk HL 6.1 Mon 9:30 HSZ 02

Molecular quantum spintronics with single-molecule magnets — •Wolfgang Wernsdorfer — Institut Néel, CNRS, BP 166, 38042 Grenoble, France

We will address the field called molecular quantum spintronics, combining the concepts of spintronics, molecular electronics and quantum computing. Various research groups are currently developing low-temperature scanning tunnelling microscopes to manipulate spins in single molecules, while others are working on molecular devices (such as molecular spin-transistors, spin valves and filters, and carbon-nanotube-based devices) to read and manipulate the spin state and perform basic quantum operations. For ex., we have built a novel spin-valve device in which a non-magnetic molecular quantum dot, consisting of a Single-Wall Carbon Nanotube, is laterally coupled to a TbPc2 molecular magnet. The localized magnetic moment of the SMM led to a magnetic field-dependent modulation of the conductance in the nanotube with magnetoresistance ratios of up to 300%. Using a molecular spin-transistor, we achieved the electronic read-out of the nuclear spin of an individual metal atom embedded in a single-molecule magnet (SMM). We could show very long spin lifetimes (several tens of seconds). Using the hyperfine Stark effect, which transforms electric fields into local effective magnetic fields, we could not only tune the resonant frequency by several MHz, but we also performed coherent quantum manipulations on a single nuclear qubit by means of electrical fields only.

Invited Talk HL 6.2 Mon 10:00 HSZ 02

EPR Studies of Rare-Earth Molecular Nanomagnets — •Stephen Hill[1], Sanhita Ghosh[1], Dorsa Komijani[1], Salvador Cardona-Serra[2], Jose-Jaime Baldovi[2], Yan Duan[2], Alejandro Gaita-Arino[2], and Eugenio Coronado[2] — [1]Department of Physics and NHMFL, Florida State University, Tallahassee, FL 32310, USA — [2]ICM, Universidad de Valencia, 46980 Paterna, Spain

I will discuss the application of multi-frequency EPR to study the static and dynamic properties of a family of mononuclear Ln(III) (Ln = Ho or Tb) nanomagnets encapsulated in polyoxometallate (POM) cages. The encapsulation offers the potential for spintronics applications on surfaces or in devices, as it preserves the intrinsic properties of the nanomagnet outside of a crystal. A large magnetic anisotropy arises due to a splitting of the Hund's coupled angular momentum ($J = L+S$) ground state in the POM ligand field. High-frequency EPR studies for the Ho(III) compound ($J = 8$) reveal an anisotropic eight line spectrum corresponding to transitions within the lowest $m_J = \pm 4$ doublet, split by a hyperfine interaction with the $I = 7/2$ Ho nucleus. Meanwhile, X-band studies reveal the presence of a large tunneling gap ($\Delta \sim 9$ GHz) within the $m_J = \pm 4$ doublet. Spin-echo measurements allow studies of the coherent spin dynamics, including Rabi oscillations. Remarkably long T_2 times are found, even for the most concentrated samples. It is postulated that this is due to the large gap, Δ, which provides an optimal operating point for coherent manipulations at X-band such that the quantum dynamics are relatively insensitive to dipolar fields.

15 min. break

Invited Talk HL 6.3 Mon 10:45 HSZ 02

On-surface magnetochemistry of spin-bearing metalorganic molecules — •Peter M. Oppeneer[1], Kartick Tarafder[1], Ehesan Ali[1], Nirmalya Ballav[2], Christian Wäckerlin[3], and Thomas A. Jung[3] — [1]Uppsala University, Uppsala, Sweden — [2]IISER, Pune, India — [3]PSI, Villigen, Switzerland

Planar spin-bearing metalorganic molecules such as metal-porphyrins and -phthalocyanines are paramagnetic in the gas phase, however an interface exchange coupling develops when these molecules are assembled on magnetic surfaces, which induces spontaneous molecular magnetic order at room temperature. To unveil fundamental origins of the exchange interaction leading to the metalorganic molecule/substrate spin-interface we use ab-initio DFT+U calculations with dispersion corrections added. Our calculations provide detailed, orbitally-resolved insight in the molecule-surface exchange interactions as well as the spin-switching induced by additional ligation in the free ligand position of the metal ion by small molecules such as NO and NH_3. We find that on-surface coordination chemistry of planar metalorganic complexes gives rise to novel magnetochemical effects, which challenge the notions of classical coordination chemistry. A key to these magnetochemical effects is the weak bonding to the surface, i.e. a "surface" trans effect. Our calculations further reveal that certain systems, as e.g. Cu-phthalocyanine on Co, are liable to formation of novel spin-polarized interface states that are expected to be particularly suited for spin-polarized electron injection in metalorganic layers.

Invited Talk HL 6.4 Mon 11:15 HSZ 02

Interfacing single-molecule magnets with metals — •Andrea Cornia[1], Valeria Lanzilotto[2], Luigi Malavolti[2], Matteo Mannini[2], Mauro Perfetti[2], Luca Rigamonti[1], and Roberta Sessoli[2] — [1]Dip. di Scienze Chimiche e Geologiche, Univ. di Modena e Reggio Emilia & INSTM, Modena, Italy — [2]Dip. di Chimica U. Schiff, Univ. di Firenze & INSTM, Sesto Fiorentino (FI), Italy

Encoding and manipulating information through the spin degrees of freedom of individual molecules are central challenges in molecular scale electronics. With their large magnetic moment and long spin relaxation time, single molecule magnets (SMMs) are of special importance in this field. The electrical addressing of individual SMMs is now well within reach using scanning probe methods, which require organizing molecules on electrically conductive surfaces [1,2]. Herein we present the latest achievements in the deposition of SMMs on metal substrates, like ultraflat surfaces [3] and nanoparticles [4]. Special emphasis is placed on the design of molecular structures that withstand processing by solution [3,4] or vapour-phase [5,6] methods as well as on chemical strategies for controlling molecular orientation. Rewardingly, these efforts have shown that the distinctive property of SMMs, i.e. slow spin relaxation, can persist in metal-wired molecules [3,4].

[1] S. Loth, et al. Science 2012, 335, 196. [2] A. A. Khajetoorians, et al. Science 2013, 339, 55. [3] M. Mannini, et al. Nature 2010, 468, 417. [4] M. Perfetti, et al. Small 2013, DOI: 10.1002/smll.201301617. [5] L. Rigamonti, et al. Inorg. Chem. 2013, 52, 5897. [6] L. Malavolti, et al. Chem. Commun. 2013, 49, 11506.

Invited Talk HL 6.5 Mon 11:45 HSZ 02

Linking magnetic molecules to themselves, to others and to surfaces — •Richard Winpenny — University of Manchester, United Kingdom

We are learning how to link together polymetallic compounds to give complex structures [1]. During this presentation recent work will be discussed in two distinct approaches. Firstly, we will describe recent work creating new hybrid inorganic-organic rotaxanes [2] and in the second approach we will discuss functionalising polymetallic rings so that they can act as ligands for other metal complexes and surfaces [3,4]. We will also describe the use of pulsed EPR spectroscopy to measure weak interactions between these molecular magnets.

1.G. A. Timco, T. B. Faust, F. Tuna and R. E. P. Winpenny, Chem. Soc. Rev., 2011, 40, 3067-3075. 2.C.- F. Lee, D. A. Leigh, R. G. Pritchard, D. Schultz, S. J. Teat, G. A. Timco and R. E. P. Winpenny, Nature, 2009, 458, 314-318. 3.G. A. Timco, S. Carretta, F. Troiani, F. Tuna, R. G. Pritchard, E. J. L. McInnes, A. Ghirri, A. Candini, P. Santini, G. Amoretti, M. Affronte and R. E. P. Winpenny, Nature Nanotechnology, 2009, 4, 173-178. 4 G. F. S. Whitehead, F. Moro, G. A. Timco, W. Wernsdorfer, S. J. Teat and R. E. P. Winpenny, Angew. Chem. Int. Ed., 2013, 52, 9932-9935.

HL 7: Organic electronics and photovoltaics I (organized by CPP)

small molecules, hybrid materials

Time: Monday 9:30–12:15 Location: ZEU 222

Invited Talk HL 7.1 Mon 9:30 ZEU 222

Structure-property relations in perylene bisimids: Charge mobility, exiton diffusion and singlet exciton fission — •Ferdinand Grozema — Delft University of Technology, Department of Chemical Engineering, Delft, The Netherlands

Perylene diimides (PDIs) represent a class of materials that is promising for application as the active layer in field effect transistors and as an electron accepting material in organic photovoltaic cells. The electronic properties of PDI-based materials strongly depend on the supramolecular order in the material. Therefore, a thorough understanding of the relation between the electronic properties and the organization on the molecular scale can result in design rules for the synthesis of new π-conjugated organic molecules .

To achieve this we have performed a combined experimental and theoretical study of the electronic properties of a large library of PDI derivatives that differ in the side chains, resulting in subtle differences in the crystal structure. By time-resolved microwave conductivity measurements we show a strong correlation between the supramolecular organization and the charge carrier mobility, with a maximum mobility of 0.41 cm2/Vs. Singlet exciton fission, a process in which a singlet excited state is efficiently converted into two triplets, is also found to be strongly dependent on the supramolecular organization.

This comprehensive study shows that the engineering of the supramolcular organization in PDIs and conjugated molecules in general is viable approach to tailor a variety of electronic properties of such materials over a wide range.

HL 7.2 Mon 10:00 ZEU 222

Influence of morphology on organic solar cell performance comparing crystalline diindenoperylene (DIP) and its amorphous derivative tetraphenyldibenzoperiflanthene (DBP) — •Stefan Grob, Mark Gruber, Ulrich Hörmann, Theresa Linderl, and Wolfgang Brütting — University of Augsburg, Germany

The DIP molecule, consisting of seven benzene and two cyclopentadiene rings, forms the backbone of the DBP molecule, which has two further benzene rings and four additional, rotatable phenyl groups. Compared to the planar arrangement of DIP, these phenyl groups give DBP a more three-dimensional shape, changing the growth behavior in thin films completely. While we observe crystalline domains of almost upright standing DIP, layers of DBP exhibit an amorphous character and therefore a relatively small exciton diffusion length, being about ten times shorter than that of its crystalline counterpart. However, the drawback of the upright standing arrangement of DIP molecules is the unfavorable orientation of the transition dipole moment resulting in a low absorption coefficient and thus a smaller short-circuit current density. The difference in morphology also leads to different coupling between donor and acceptor molecules at the interface. As a consequence there is an appreciable distinction in the recombination processes occurring within the solar cell. We investigate this phenomenon by temperature-dependent j-V-measurements, electroluminescence and photothermal deflection spectroscopy. Based on these results, we discuss the influence of different film structure and morphology on electrical transport and device performance.

HL 7.3 Mon 10:15 ZEU 222

Spray deposition of zinc oxide nanostructured films for applications in dye-sensitized solar cells — •Kuhu Sarkar[1], Erik V. Braden[1], Stefan Pogorzalek[1], Shun Yu[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching —

[2]DESY, Notkestr. 85, 22607 Hamburg

Zinc oxide (ZnO) has emerged as a suitable alternative to titania (TiO2) in the recent years in the field of dye-sensitized solar cells (DSSCs). The inorganic metal oxide films for DSSCs are highly desirable to have an increased surface for enhanced adsorption of a photosensitizer. Hence, nanostructured films of ZnO are synthesized from a solution based approach. Different deposition techniques are investigated to have a significant film thickness for a considerable amount of light absorption. In this respect, spray deposition is shown to be a highly efficient and scalable technique to produce films matching the above-mentioned criteria. Surface as well as bulk morphology of the films have been studied using SEM and GISAXS. These ZnO films are successfully shown to provide good performance in a dye-sensitized solar cell with the highest short circuit current density reported so far.

HL 7.4 Mon 10:30 ZEU 222

Extremely Thin Absorber Solar Cells based on Sb_2S_3 — •Eugen Zimmermann, Jonas Weickert, Thomas Pfadler, James Dorman, and Lukas Schmidt-Mende — Universität Konstanz

The introduction of nanostructured metal oxides as electron acceptor resulted in the concept of extremely thin absorber solar cells. Thus, low cost fabricated inorganic semiconductors like Sb_2S_3 can be utilized as sensitizer, which typically possess promising properties, such as a tunable band gap and high extinction coefficient. However, optimization of the fabrication process and a detailed characterization of intrinsic properties is unavoidable in order to find the best device architecture and suitable material combinations for highly efficient solar cells. For this purpose, chemical bath deposition conditions and parameters have been examined and resulted in a detailed recipe for fabrication of high quality Sb_2S_3 coatings. In combination with optimized layer thicknesses of P3HT, efficiencies of up to 3.2% could be achieved in flat heterojunction architecrue. In order to identify intrinsic limitations, comparative measurements with P3HT:PCBM cells have been, revealing monomolecular recombination processes of excitons, a potential dependency of charge separation, and long charge carrier pathways as main loss mechanisms of fabricated flat heterojunction cells. In addition, investigation of several hole transport materials (HTM) revealed a disadvantageous influence on charge generation due to the parasitic absorption of light by the HTM. Based on these results, the use of nanostructured metal oxides in combination with transparent HTMs is proposed to possibly overcome some of the found limitations.

HL 7.5 Mon 10:45 ZEU 222

Towards low-temperature synthesis of polymer/titania hybrid films for application in photovoltaics — Martin A. Niedermeier[1], Monika Rawolle[1], Erik V. Braden[1], Kuhu Sarkar[1], Eva M. Herzig[2], Volker Körstgens[1], and •Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]TU München, Munich School of Engineering, James-Franck-Str. 1, 85748 Garching

In a hybrid solar cell an inorganic matrix, such as titania, is combined with a hole-conducting polymer to form a so-called bulk heterojunction. The functionality of such a system depends strongly on the quality of the polymer/semiconductor interface. A very common approach to fabricate that interface is the so-called backfilling of the existing inorganic matrix with the conducting polymer. This approach is generally a two-step process, as the fabrication of the inorganic matrix usually involves high temperatures, which destroy all organic material present in the system. To date the subsequent backfilling of that matrix remains challenging, since a lot of problems have to be overcome. A workaround to these problems is promised by a low-temperature sol-gel process, in which the polymer and the inorganic semiconductor network are fabricated simultaneously. Approaches towards such low-temperature synthesis of polymer/titania hybrid films for application in photovoltaics are presented. These novel routes make use of special tailored block copolymers as structure directing agent. Film morphology and device function are investigated.

15 min break

HL 7.6 Mon 11:15 ZEU 222

Photoinduced charge transfer in $CuInS_2$ nanocrystal/polymer composites — •Rany Miranti[1], Yuliar Firdaus[2], Christopher Krause[1], Mark van der Auweraer[2], Holger Borchert[1], and Jürgen Parisi[1] — [1]Univ. of Oldenburg, Dept. of Physics, Energy and Semiconductor Research Laboratory, 26129 Oldenburg, Germany — [2]Lab. for Photochemistry & Spectroscopy, Div. of Mol. Imaging & Photonics, Chemistry Dept., Katholieke Universiteit Leuven, Celestijnenlaan 200 F B-3001 Heverlee, Belgium.

The photoinduced excited states and the effects properties of charge transfer in $CuInS_2$ (CIS) nanocrystal/polymer composites were studied by applying quasi steady-state photoinduced absorption (PIA) and steady state photoluminescense as well as time-resolved photoluminescense. The time-resolved properties and excited state dynamics of our systems were studied using the time-correlated single photon counting (TCSPC) technique. We used two different systems of composites with two different kind of polymer, i.e. poly(3-hexylthiophene) (P3HT) and poly[2,6-(4,4-bis-(2-ethylhexyl)-4H-cyclopenta[2,1-b;3,4-b']dithiophene)-alt-4,7-(2,1,3-benzothiadiazole)] (PCPDTBT). Optical absorption and emission spectra of thin films of CIS nanocrystal/polymer composites exhibit several interesting features such as luminescence quenching and polaronic photoinduced absorption (PIA) indicating photoinduced charge transfer. The effect of different organic ligands surrounding the CIS nanocrystals on the charge separation process in CIS nanocrystal/ polymer composites will be presented as well.

HL 7.7 Mon 11:30 ZEU 222

Structured growth of ZnO for light trapping enhancement in organic solar cells — •Nivedita Yumnam and Veit Wagner — Jacobs University, 28759 Bremen, Germany

Organic photovoltaic cells are promising candidates for large-area and low-cost production of solar cells. However, their performance is limited due to the short diffusion length of excitons and low absorption in the active semiconductor layer. The absorption of light can be enhanced by incorporating ZnO nanostructures, which act as scattering centres and hence, they increase the optical path length of light. Our work focuses on the investigation of light trapping mechanism of solar cells based on electrochemically grown ZnO nanorod and active layer of conjugated polymer P3HT and PCBM. The size and the structure of the ZnO nanorods are varied by changing the parameters of electrochemical deposition. Angle resolved scattering measurements are employed to investigate the amount of light scattered by the nanorods. These results are correlated to the performance of the solar cell determined from electrical measurements.

HL 7.8 Mon 11:45 ZEU 222

Temperature-dependent molecular orientation of the organic semiconductor PTCDI-C_8: Optical and structural properties — •Sebastian Bommel[1,2], Linus Pithan[2], Christopher Weber[2], Anton Zykov[2], Gonzalo Santoro[1], Stephan V. Roth[1], Jörg Megow[2], and Stefan Kowarik[2] — [1]Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, D-22607 Hamburg, Germany — [2]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, D-12489 Berlin, Germany

Optical and structural properties of molecular materials are not only essential for the rational design of opto-electrical devices, but also for the understanding of intermolecular interactions. Here, we report on the structural and optical properties of the organic semiconductor PTCDI-C_8 investigated by temperature-dependent Grazing Incidence X-ray Diffraction (GIXD) and photoluminescence (PL) measurements. Our *in situ* studies yield a large impact of temperature on unit cell parameters and optical transitions. The energy of the optical transition E_{10}-E_{01} in the PL spectra shifts from 1.80 eV for 273 K to 1.85 eV for 413 K. Furthermore, a rearrangement of the molecular ensemble was found, indicated by a large change of the beta-angle of the PTCDI-C8 unit cell from 107° (273 K) to 102° (413 K). The influence of these structural changes, which are an indication for a change of molecular orientation with temperature, on the optical properties will be discussed in detail. Additionally, the structural and optical properties are supported by temperature-dependent molecular dynamics (MD) simulation based calculations.

HL 7.9 Mon 12:00 ZEU 222

Highly Efficient Silicon/Polythiophene Hybrid Solar Cell Devices — •Matthias Zellmeier[1], Johannes Frisch[2], Silvia Janietz[3], Norbert Koch[2], Jörg Rappich[1], and Norbert Nickel[1] — [1]Helmholtz-Zentrum Berlin, Institut für Silizium Photovoltaik, Kekulèstr. 5, D-12489 Berlin — [2]Humboldt-Universität zu Berlin, Institut für Physik, Brook-Taylor-Str. 6,D-12489 Berlin — [3]Fraunhofer-Institut für Angewandte Polymerforschung IAP, Abteilung Polymere und Elektronik, Geiselbergstr. 9, D-14476 Potsdam

Highly efficient hybrid solar cell devices based on crystalline silicon with three different solution processed polymer emitter layers are realized. The inorganic part of the device is optimized with a hole-selective back contact (BSF) and a low defect density hot water oxide (D_{it}=2×10^{-12} $eV^{-1}cm^{-2}$), which provides the necessary wetting properties for the solution processed emitter layers. The applied polymer materials, e.g. poly(3-hexylthiophene-2,5-diyl) (P3HT), poly(3-[3,6-dioxaheptyl]-thiophene) (P3DOT), and poly(3-[2,5,8-trioxanonyl]-thiophene) (P3TOT), differ mainly in the oxygen content in the side groups. Substituting the alkyl chains attached to the thiophene rings with ether groups leads to a modified layer formation during spin coating. The results of the optical, electrical and structural characterization of the polymer layers is correlated to the key figures in the final devices. The open circuit voltage V_{OC} increases from 0.3 V to 0.5 V and the short circuit current j_{SC} increases from 15.2 mA cm^{-2} up to 28.3 mA cm^{-2} in the sequence P3HT, P3DOT, P3TOT and results in a power conversion efficiency close to 10 % for a planar Si/P3TOT device.

HL 8: Transport: Quantum dots, quantum wires, point contacts I (organized by TT)

Time: Monday 9:30–13:15 Location: BEY 81

HL 8.1 Mon 9:30 BEY 81

Transport through nanostructures: Finite time vs. finite size — •Peter Schmitteckert[1], Sam Carr[2], and Hubert Saleur[3,4] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany — [2]School of Physical Sciences, University of Kent, Canterbury CT2 7NH, UK — [3]Institut de Physique Théorique, CEA, IPhT and CNRS, URA2306, 91191 Gif Sur Yvette, France — [4]Department of Physics, University of Southern California, Los Angeles, CA 90089-0484

Numerical simulations and experiments on nanostructures out of equilibrium usually exhibit strong finite size and finite measuring time $t_{\rm m}$ effects. We discuss how these affect the determination of the full counting statistics for a general quantum impurity problem [1]. We find that, while there are many methods available to improve upon finite-size effects, any real-time simulation or experiment will still be subject to finite time effects: in short **size matters**, but **time is limiting**. We show that the leading correction to the cumulant generating function (CGF) at zero temperature for single-channel quantum impurity problems goes as $\ln t_{\rm m}$ and is universally related to the steady state CGF itself for non-interacting systems. We then give detailed numerical evidence for the case of the self-dual interacting resonant level model that this relation survives the addition of interactions. This allows the extrapolation of finite measuring time in our numerics to the long-time limit, to excellent agreement with Bethe-ansatz results.
[1] P. Schmitteckert, S. C. Carr, H. Saleur, arXiv:1307.7506

HL 8.2 Mon 9:45 BEY 81

Towards steady state currents on finite systems — •Tim Collet[1] and Peter Schmitteckert[2] — [1]Theoretical Condensed Matter physics, KIT — [2]Institute for Nanotechnology, KIT

The determination of transport properties of strongly correlated quantum systems by quenches in the charge imbalance is a well established technique. However, the achievable time scales are limited by the system size inducing a finite transit time. Here we present a technique in the spirit of absorbing boundary conditions. This allows to obtain steady states on a finite system and to overcome said limitation from finite transit times. We discuss the application of this concept in the context of transport through quantum impurities.

HL 8.3 Mon 10:00 BEY 81

Kwant - a software package for quantum transport — •Michael Wimmer[1], Christoph Groth[2], Anton Akhmerov[1], and Xavier Waintal[2] — [1]TU Delft, The Netherlands — [2]CEA Grenoble, France

Computing transport properties numerically is a problem that appears in many different areas of physics. I will present a wave-function based approach to computing transport properties in non-interacting tight-binding systems that scales more favourably than standard algorithms such as the recursive Green's function algorithm.

We have implemented this method in an open-source software package Kwant based on the python language. It allows for an easy definition of arbitrary tight-binding problems using intuitive concepts ("like writing the problem on the blackboard"), and allows to compute transport properties such as the conductance, but also local properties such as electron densities. The software package itself together with extensive documentation, tutorials and examples of research where Kwant has already been used can be found at www.kwant-project.org.
[1] C. W. Groth, M. Wimmer, A. R. Akhmerov, X. Waintal. arXiv:1309.2926 (2013)

HL 8.4 Mon 10:15 BEY 81

Non perturbative approach to transport through Anderson quantum dot: the influence of charge fluctuations — •Davide Mantelli and Milena Grifoni — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Deutschland

Transport through a strongly interacting Anderson quantum dot is analyzed for tunneling couplings Γ comparable or larger than the thermal energy $k_{\rm B}T$. In this regime the commonly used sequential tunneling approximation, where tunneling rates are calculated to the lowest order in Γ, breaks down. By accounting for charge fluctuations accompanying the transfer of one electron onto the dot, "dressed" tunneling rates and the associated current across the dot can be calculated [1]. The difference between the standard lowest order theory and the "dressed" one is carefully analyzed in the weak ($\Gamma \ll k_{\rm B}T$), intermediate ($\Gamma \simeq k_{\rm B}T$) and strong ($\Gamma \gg k_{\rm B}T$) coupling regimes. At low temperatures features typical of the Kondo resonance are recovered.
[1] J. Kern and M. Grifoni, Eur. Phys. J. B **86**, (2013) 384

HL 8.5 Mon 10:30 BEY 81

Energy current cotunnelling features for the Anderson quantum dot — •Niklas M. Gergs[1], Christoph B. M. Hörig[1], Dirk Schuricht[1], and Maarten R. Wegewijs[2,3,4] — [1]Institute for Theoretical Physics, Utrecht University, Netherlands — [2]Institute for Theory of Statistical Physics, RWTH Aachen University, Germany — [3]JARA–Fundamentals of Future Information Technology — [4]Peter Grünberg Institut, Forschungszentrum Jülich, Germany

We discuss the particle and energy current through an Anderson quantum dot with a strong Coulomb interaction U subject to both voltage and temperature bias. A diagrammatic perturbation theory up to second order in the tunnel rates Γ is set up in Liouville space. We find that pair tunnelling features show up in the particle and energy current, while pure inelastic cotunnelling spinflip features are absent in the energy current. The latter cotunnelling processes do appear however when assisted by sequential tunnelling (COSET). Therefore, the energy current contains more distinctive features than the particle current. Thus one can use the energy current for enhanced spectroscopy of quantum dot systems.

HL 8.6 Mon 10:45 BEY 81

Non-equilibrium transport through a Josephson quantum dot — •Jan Frederik Rentrop[1,2], Severin Jakobs[1,2], and Volker Meden[1,2] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University, Germany — [2]JARA Fundamentals of Future Information Technology, 52056 Aachen, Germany

We investigate a quantum dot featuring Hubbard interaction coupled to superconducting leads. Applying a bias voltage across the system leads to a time-dependent periodic Hamiltonian. This implies that the observable, namely the current through the system, aquires a periodic time-dependence (AC Josephson effect). The non-equilibrium feature of so called Multiple Andreev Reflections (MAR), known from the non-interacting case, is observed in the static component of the current.

The self-energy on the dot is calculated with the functional renormalization group method. The derived first and second order truncation schemes allow for a "quasi-static" (i.e. allowing for the periodic time-dependence but not more) approximation of the self-energy. Model and method allow for asymmetric choices of the super-conducting gaps, the lead temperatures, the lead-dot couplings, tuning of the Hubbard interaction, shifting of on-site energy and applying a magnetic field. Numerical results are presented for symmetric choices at zero magnetic field and zero temperature, while lead-dot coupling, on-site energy and

Hubbard interaction are tuned. Also, first order self-consistent perturbation theory results are presented as a benchmark.

We discuss limitations that the MAR physics impose on any perturbative scheme that expands in small orders of the interaction.

HL 8.7 Mon 11:00 BEY 81

Magneto-electric spectroscopy of Andreev bound states in Josephson quantum dots — •Nils Wentzell[1], Tobias Meng[2], Volker Meden[3], Sabine Andergassen[1], and Serge Florens[4] — [1]University of Vienna — [2]University of Basel — [3]RWTH Aachen University — [4]CNRS Grenoble

We theoretically investigate the behavior of Andreev levels in a single-orbital interacting quantum dot in contact to superconducting leads, focusing on the effect of electrostatic gating and applied magnetic field, as relevant for recent experimental spectroscopic studies. In order to account reliably for spin-polarization effects in presence of strong correlations, we further extend here two simple and complementary approaches that are tailored to capture effective Andreev levels: the static functional renormalization group and the self-consistent Andreev bound states theory. We provide a systematic analysis of the Andreev level spectroscopy for the full electric and magnetic tuning available in quantum dot devices.

15 min. break.

HL 8.8 Mon 11:30 BEY 81

In gap and out of gap features in the cotunneling spectroscopy of a superconductor coupled quantum dot — •Sascha Ratz and Milena Grifoni — Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

We present a nonequilibrium real-time diagrammatic theory for the systematic investigation of low temperature quantum transport properties of a superconductor contacted quantum dot in an individual single wall carbon nanotube. In the low temperature regime particle transport is dominated by cotunneling and Andreev reflection processes. As recent experiments show, elastic/inelastic cotunneling features are clearly visible inside the Coulomb blockade regime, sharpened by the superconducting leads. The proximity induced higher order Andreev reflection processes result in subgap features, however. Temperature dependent measurements show in addition rich features inside the superconducting gap which can be attribute to thermally excited quasiparticles. More detailed experimental investigations and theoretical calculations are in progress to understand the experimental findings.

HL 8.9 Mon 11:45 BEY 81

Unconventional superconductivity in quantum dot systems — Björn Sothmann[1], •Stephan Weiss[2], Michele Governale[3], and Jürgen König[1] — [1]Departement de Physique Theorique, Universite de Geneve, Switzerland — [2]Theoretische Physik, Universität Duisburg-Essen and CENIDE, Germany — [3]School of Chemical and Physical Sciences, Victoria University of Wellington, New Zealand

Conventional superconductivity of electrons is well described in terms of the BCS theory. Fermi statistics dictates the overall symmetry of e.g. the order parameter. The single ingredients could take either symmetric or antisymmetric properties, hence spin as well as spatial degrees of freedom and time might independently change sign and unconventional pairing amplitudes emerge [1]. We show how quantum dot setups may be used to create unconventional pairing between electrons. Brought into proximity to a conventional SC, Cooper pairs tunnel into the double (quadrupel)-quantum dot (DQD/QDD) system [2,3]. Locally, manipulations of the electronic state is possible by tuning electric and/or magnetic fields. An inhomogeneous magnetic field between the dots breaks the SU(2) symmetry of the spin. This results in nonzero unconventional order parameters. We study the emergence and decay of even/odd singlet and triplet order parameters in different geometries. For DQD and QDD setups spectroscopic properties and signatures of unconventional correlations in the Andreev current are studied.

[1] F. S. Bergeret, et al., Rev. Mod. Phys. 77, 1321 (2005).
[2] M. Governale, et al., Phys. Rev. B 77, 134513 (2008).
[3] J. Eldridge, et al., Phys. Rev. B 82, 184507 (2010).

HL 8.10 Mon 12:00 BEY 81

The interplay of the proximity and Kondo effects in spin-resolved transport through quantum dots — •Krzysztof P. Wójcik and Ireneusz Weymann — Faculty of Physics, Adam Mickiewicz University, Umultowska 85, 61-614 Poznań, Poland

Transport properties of hybrid quantum dots coupled to ferromagnetic (FM) and superconducting (SC) leads are studied by means of the numerical renormalization group method [1,2]. By constructing the full density matrix of the system [3], the linear conductance and respective spectral functions are calculated. Aiming to emphasize the role of Andreev processes in transport, we model the quantum dot coupled to the superconductor by an effective Hamiltonian in the limit of large superconducting gap [4]. First, a three-terminal setup is considered, for which we study the proximity effect on the spin-dependent current flowing between the two FM leads. Then, the transport properties in a two-terminal setup, with one FM and one SC lead, are analyzed. In this case we focus on the interplay of the exchange field induced by FM lead, the Kondo effect and the Andreev processes. We show that the conductance generally depends on the ratio of these three quantities, leading to nontrivial transport behavior.

[1] K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975).
[2] We use the open-access Budapest NRG code, O. Legeza, C. P. Moca, A. I. Toth, I. Weymann, G. Zarand, arXiv:0809.3143 (2008).
[3] A. Weichselbaum, J. von Delft, Phys. Rev. Lett. **99**, 076402 (2007).
[4] Y. Tanaka, N. Kawakami, A. Oguri, J. Phys. Soc. Jap. **76**, 074701 (2007).

HL 8.11 Mon 12:15 BEY 81

The electroluminescence of the transmission line driven by a biased quantum point contact — •Jinshuang Jin[1,2,3], Michael Marthaler[2,4], Andreas Heimes[2,4], and Gerd Schön[2,4] — [1]Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology, Karlsruhe, Germany — [2]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology(KIT), Karlsruhe, Germany — [3]Department of Physics, Hangzhou Normal University, Hangzhou, China — [4]DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, Karlsruhe, Germany

A transmission line resonator driven by a biased quantum point contact is investigated. The quantum point contact (QPC) is not only an efficient detector but also a light emission device. We find that the excited photon number in the resonator is monotonically increased with the bias voltage for $eV > \hbar\omega_r$ with V the applied bias voltage and $\hbar\omega_r$ the frequency of the resonator. The linewidth and the height of the emission spectrum are sensitive to the parameters of the QPC, such as the tunneling rate, the applied bias voltage, and the coupling strength between the QPC and resonator. Moreover, we demonstrate that the noise spectrum of the current through QPC has characteristic features showing peak and dip, which is closely related to the excited photon dynamics of the resonator.

HL 8.12 Mon 12:30 BEY 81

Accumulation of spin anisotropy in a nanoparticle in the mesoscopic Stoner regime — •Philipp Stegmann[1], Björn Sothmann[2], and Jürgen König[1] — [1]Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany — [2]Département de Physique Théorique, Université de Genève, CH-1211 Genève 4, Switzerland

We theoretically discuss the accumulation of spin-quadrupole moment [1, 2] in an isotropic system giving rise to a large spin anisotropy although the spin-dipole moment remains strongly suppressed. Our system is a nanoparticle weakly tunnel coupled to two ferromagnetic leads. For such system, it has been demonstrated that the spin fluctuations give rise to enhanced shot noise [3]. Here, large positive spin-quadrupole moments are generated by abruptly switching off the bias voltage for parallel leads‘ polarizations. Moreover, applying an oscillating bias voltage results in large negative spin-quadrupole moments for parallel or antiparallel polarizations.

[1] B. Sothmann, and J. König, Phys. Rev. B **82**, 245319 (2010).
[2] M. M. E. Baumgärtel, M. Hell, S. Das, and M. R. Wegewijs, Phys. Rev. Lett **107**, 087202 (2011).
[3] B. Sothmann, J. König, and Y. Gefen, Phys. Rev. Lett. **108**, 166603 (2012).

HL 8.13 Mon 12:45 BEY 81

Overhauser effect in spin blockaded double quantum dots-the case of dual hysteresis — •Bhaskaran Muralidharan and Siddharth Buddhiraju — Electrical Engineering Department, Indian Institute of Technology Bombay, Mumbai, India

In the spin blockade transport regime through GaAs double quantum dots (DQD), experiments [1] revealed that the hyperfine interaction with host nuclei can have profound consequences on the electron-spin dynamics. One of which, is the observation of bistablity and flat-topped behavior in the current versus applied DC magnetic-field characteristics. In this talk, we will first explain the essence of this flat-topped hysteretic behavior using a simple six-state model that captures the multiple-feedback mechanisms that are involved. We will then consider a more detailed model that elucidates the role of the physical parameter space of the DQD set up and a feedback mechanism involving the difference Overhauser field caused by the two separate nuclear spin baths of the DQD set up.
[1] K. Ono and S. Tarucha, Phys Rev Lett., 92, 256803 (2004).

HL 8.14 Mon 13:00 BEY 81

Fixing the Energy Scale in Scanning Tunneling Microscopy on Semiconductor Surfaces — Gerhard Münnich[1], •Andrea Donarini[2], Jascha Repp[1], and Martin Wenderoth[3] — [1]Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany — [2]Institute of Theoretical Physics, University of Regensburg, 93053 Regensburg, Germany — [3]IV. Physikalisches Institut der Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

In scanning tunneling experiments on semiconductor surfaces, the energy scale within the tunneling junction is usually unknown due to tip-induced band bending. Here, we experimentally recover the zero point of the energy scale by combining scanning tunneling microscopy with Kelvin probe force spectroscopy. With this technique, we revisit shallow acceptors buried in GaAs [1]. Enhanced acceptor-related conductance is observed in negative, zero, and positive band-bending regimes. An Anderson-Hubbard model is used to rationalize our findings, capturing the crossover between the acceptor state being part of an impurity band for zero band bending and the acceptor state being split off and localized for strong negative or positive band bending, respectively.
[1] G. Münnich, A. Donarini, J. Repp, and M. Wenderoth, Phys. Rev. Lett. 111, 216802 (2013)

HL 9: Invited Talk Shu-Hong Yu

Time: Monday 10:00–10:30 Location: POT 081

Invited Talk HL 9.1 Mon 10:00 POT 081

Ultrathin Nanowires: Multiplex Templating Synthesis, Macroscopic Assemblies, and Applications — •Shu-Hong Yu — Hefei National Laboratory for Physical Sciences at Microscale, University of Science and Technology of China, Hefei 230026, P. R. China

In this lecture, we propose a multiplex templating process for controlled synthesis of a huge family of functional ultrathin nanowires and their macroscopic assemblies, and applications. We first introduce ultrathin Te nanowires (Te NWs) and their advantages as a templating material. A family of 1D nanostructures including semiconductors, noble metals, carbon, polymers, their binary and multiple hybrids can be prepared through this multiplex templating process. The reactivity and stability of ultrathin Te nanowires will be discussed. In addition, a series of macroscopic assemblies of nanowires, including free-standing membranes, films, hydrogels, and aerogels can be fabricated, which exhibit enormous potential for attractive applications, such as electronic devices, transparent electrodes, elastomeric conductors, electrocatalysis, liquid filtration and separation, super adsorbent, and polymer-based nanocomposites. The versatility of this templating process, scalable assembling process as well as the large-scale synthesis can together enhance the application reliability of these functional 1D nanostructures.

HL 10: Functional materials I - Energy storage (organized by MM)

Time: Monday 10:15–11:30 Location: IFW A

HL 10.1 Mon 10:15 IFW A

Graphene-based supercapacitors for energy storage under extreme temperature conditions — •Ranjith Vellacheri, Ahmed Al-Haddad, Wenxin Wang, Huaping Zhao, Chengliang Wang, Zhijie Wang, and Yong Lei — Ilmenau University of Technology, Institute of Physics & IMN MacroNano (ZIK) 98693 Ilmenau (Germany)

Graphene-based supercapacitors have been fabricated for energy storage in a very wide range of temperatures. The optimized supercapacitors showed good charge storage capabilities from -24 °C to 50 °C. Specific capacitance of the electrode obtained from charge/discharge measurements was 91 F/g at room temperature (RT) and no considerable change when tested at different temperatures (e.g. 73 F/g and 100 F/g at -24 °C and 50 °C, respectively). Our samples also exhibited outstanding capacitance retention and cyclic stability at different operating temperatures. Extremely low equivalence series resistance (ESR) and charge transfer resistance were confirmed by electrochemical Impedance measurements. Especially, the low ESR could also result in high power density even at low operating temperatures. We believe that our results highlight the great prospective of the graphene-based supercapacitors for the efficient energy storage at extreme environments with a wide range of temperature difference

HL 10.2 Mon 10:30 IFW A

Nano-Engineered Three-Dimensional Core/Shell Nanotube Arrays for Realizing High Performance Asymmetric Supercapacitors — •Fabian Grote, Liaoyong Wen, Huaping Zhao, and Yong Lei — Ilmenau University of Technology, Institute of Physics & IMN MacroNano (ZIK) Prof. Schmidt-Str. 26, 98693 Ilmenau

The ongoing technological advances in areas such as electric mobility, consumer electronics, and energy harvesting set new demands for energy storage systems. The next generation of high performance devices requires a strongly enhanced electrochemical performance as well as operating safety, limited environmental impact, and economic viability. In order to fulfill these aims a crucial role is addressed to supercapacitors. Today, the main challenge is to increase the specific energy of supercapacitors without sacrificing specific power. Thereby the development of novel functional nanostructures for energy storage is a key challenge. Hence we nano-engineered a complex 3D electrode material based on free-standing open-ended core/shell nanotube arrays with tailored functions, using anodic aluminum oxide nano-templates and atomic layer deposition. The core provides a well electron transport through the entire electrode matrix and the thin shell guarantees a well utilization of the active electrode material. Importantly, we designed and nanostructured both the negative and positive electrode materials individually, using an innovative material combination of polypyrrole and manganese oxide. It is shown that the asymmetric electrode nature of the prepared supercapacitor device enabled us to increase the cell voltage to 1.7 V, which is a major leap to increase the specific energy.

HL 10.3 Mon 10:45 IFW A

Temperature induced modifications of hydrides in Gd(0001) thin films — •Sara Wanjelik, Samuel Königshofen, and Mathias Getzlaff — Institute of Applied Physics, University of Düsseldorf

Hydrogen in metals has been of great interest in research for the past few decades. But only few investigations are carried out by imaging techniques with a lateral resolution on the nm-scale. Even less research deals with the inital stage of hydride formation. Here we present STM measurements on thin Gadolinium films grown on a W(110) surface concentrating on the inital steps of hydrogen absorption. Absorption of hydrogen at room temperature results in hydride formation. We observe plastic deformations due to the larger volume of the hydrides. On the one hand, disk-like islands with a diameter of approximately 3 nm and a height of 0.3 nm occur, while on the other hand there are con-

nected areas formed by ramps. The islands arrange in chains. It has also been observed that a new feature, a triangular shaped structure appears together with the islands. Maps of the differential conductivity prove that it has a different electronic structure. The origin of the island and the other structure is not fully understood and yet a field of open research. Additionally, we will present modifications of these structures induced by increasing temperature up to that point which they vanish at.

HL 10.4 Mon 11:00 IFW A

Hydrophobicity patterning of gas diffusion media for polymer electrolyte fuel cells — •Indro Biswas[1], Pawel Gazdzicki[1], Martin Tomaš[2], and Mathias Schulze[1] — [1]German Aerospace Center (DLR), Insitute of Technical Thermodynamics, Pfaffenwaldring 38-40, 70569 Stuttgart, Germany — [2]University of West Bohemia, New Technologies Research Centre, Univerzitní 8, 306 14 Plzeň, Czech Republic

Polymer electrolyte fuel cells with their high gravimetric energy density face a water balance problem especially under variable loads, e.g. in automotive conditions: The excess product water needs to be removed from the fuel cell while maintaining a humidified membrane.

The gas diffusion layer, which also provides contact to the electrochemically active components, has to achieve the passive management of the water balance. Heterogeneously hydrophobic gas diffusion media have already shown to be more capable of balancing these opposing requirements than conventional materials. Various methods of patterning gradients of hydrophobicity are applied, like microperforation and laser, focused X-Ray and ion beam irradiation. The modifications are analysed with photoemission and infrared spectroscopy and compared for their performance, applicability and scalability.

The research leading to these results has received funding from the European Union's Seventh Framework Programme (FP7/2007-2013) for Fuel Cell and Hydrogen Joint Technology Initiative under Grant No. 303446 (Impala).

HL 10.5 Mon 11:15 IFW A

NMR Investigations of the Aluminium Substituted Barium Clathrate Ba_8Si_{46} — •Matej Bobnar, Iryna Antonyshyn, Michael Wedel, Duong Nguyen, Ulrich Burkhardt, Yurii Prots, Bodo Böhme, Liudmila Muzica, Raul Cardoso, Walter Schnelle, Igor Veremchuk, Michael Baitinger, and Juri Grin — Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden

Clathrates are interesting for their thermoelectric properties, due to their heigh electric and low thermal conductivity. $Ba_{8-x}Si_{46}$ is a type I clathrate obtained at 800 °C and at high pressure of 2-5 GPa. The covalently bonded Si atoms form a framework of small, 20 atom, and large, 24 atom, cages that are fully or partially filled by Ba atoms. Some of the Si atoms may be substituted by a number of other atoms, including Al. $Ba_8Al_xSi_{46-x}$ is reported with a homogeneity range of $8 \leq x \leq 15$. Our investigations, however, begin with a clathrate of even lower Al content, $Ba_8Al_{6.8}Si_{39}$ and continue towards the Al-rich phases. We try to determine, which Si atoms are substituted by Al and how a disorder increases or decreases with a growing Al content. Since Al and Si stand next to each other in the periodic table of elements, they are very difficult to discern by X-ray. For this reason, the NMR was employed, which observes local environments of each nucleus separately and gives some hints about the intrinsic properties of the samples. In this work, we present a model for Al and Si distribution in the clathrate I framework based on ^{29}Si and ^{27}Al NMR results.

HL 11: Frontiers of electronic structure theory - Non-equilibrium phenomena at the nano-scale I (organized by O)

Non-equilibrium processes such as charge and heat transport are central to electronic and thermoelectric applications. Understanding these phenomena at the nanoscale challenges both theory and experiment. Basic theoretical issues are related to the role of quantum mechanics, the interplay of ballistic, diffusion and hopping processes, the importance of dissipation, the effect of electronic correlation, and the signatures of unusual quantum states. On the experimental side devising measurements to unravel these phenomena in a controlled way poses severe difficulties. In this regard, optical lattices of cold atoms are emerging as a powerful laboratory to test theoretical models and discover unforeseen phenomena.

This symposium will cover current issues in the field by bringing together scientists working in different specific areas with the aim of fostering interdisciplinary discussion, assessing current theoretical understanding, and indicating future goals with emphasis on electronic structure theory.

Organizers: Roberto Car (Princeton), Kristian S. Thygesen (Lyngby) and Matthias Scheffler (Berlin)

Time: Monday 10:30–13:15 Location: TRE Ma

Topical Talk HL 11.1 Mon 10:30 TRE Ma

Molecular junction transport: some theoretical and computational considerations — •Mark Ratner[1] and Matthew Reuter[2] — [1]Chemistry, Northwestern University, Evanston Illinois 60208 USA — [2]Chemistry, Northwestern University, Evanston Illinois 60208 USA

Following the development of break junction techniques, and very elegant measurements by many labs worldwide, the understanding of the community for single molecule transport junctions on the experimental side has been very nicely unified. While there are still challenges, interpretations of the transport (and indeed of some second-order response properties) is now quite sophisticated.

There have been major advances in the computational approaches also, and in many cases, computations and measurements can be compared quantitatively. But there are some remaining difficulties in the computational and theoretical approaches, and this talk will discuss a few of them.

The topics addressed will be: single molecule aspects, histograms and their usage, time-dependence of the transport, and ghost transmission and computational accuracy.

HL 11.2 Mon 11:00 TRE Ma

On the description of biased nanocontacts from ab initio — •Steven Achilles[1], Jürgen Henk[1], Michael Czerner[2], Christian Heiliger[2], and Ingrid Mertig[1] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, D-06099 Halle, Germany — [2]I. Physikalisches Institut, Justus Liebig University, D-35392 Giessen, Germany

A suitable description of arbitrary shaped and biased nanocontacts is very important for investigating and predicting physical effects of materials on the nanometer scale. In particular, the electronic transport properties under finite bias voltages are of great interest.

To account for systems under finite bias we extended our Korringa-Kohn-Rostoker Green's function method [1] to the Keldysh formalism [2]. The method was developed for different types of geometries, i.e. planar junctions [3] and embedded real-space clusters [4]. Both implementations include a self-consistent treatment of the electronic structure under external bias using the nonequilibrium density.

We present ab initio results of voltage drops, the charge relaxation under finite bias voltage and current-voltage characteristics for different types of geometries.

[1] R. Zeller, P.H. Dederichs, B. Ujfalussy, L. Szunyogh, and P. Weinberger, Phys. Rev. B 52, 8807 (1995).; P. Zahn, I. Mertig, R. Zeller, and P.H. Dederichs, Mat. Res. Soc. Symp. Proc. 475, 525 (1997).
[2] L.V. Keldysh, Sov. Phys. JETP 20 (4), 1018-1026 (1965).
[3] S. Achilles et al., Phys. Rev. B 88 (12), 125411 (2013).
[4] S. Achilles et al., to be published

HL 11.3 Mon 11:15 TRE Ma

Elasticity changes in molecular junctions under bias: an ab-initio study — •Clotilde S. Cucinotta[1], Meilin Bai[1,2], Ivan Rungger[1], Shmin Hou[2], and Stefano Sanvito[1] — [1]School of Physics and CRANN, Trinity College Dublin, College Green, Dublin 2, Ireland — [2]2Key Laboratory for the Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, Beijing 100871, China

Non-conservative current induced forces are at the origin of a rich variety of dynamical processes, including vibrations, rotations, phonon energy flow, desorption and reactions. The ability to simulate these phenomena paves the way for crucial advances in interface physics and in molecular electronics. New insights into how the presence of non-conservative forces can affect the vibrational spectrum of prototypic Au-H2-Au nano-junctions are obtained by the Non Equilibrium Green Functions approach combined with Density Functional Theory as implemented in the Smeagol code [1]. The modification of the phonon spectrum of the junction in the presence of an external bias is for the first time analysed, in terms of charge redistribution caused by the electron flow, potential drop and differences in an average distance collective variable. Phonon modes changes are related to a change in bias of some of the elastic constants.The importance of electric field vs. current effects is compared. The elasticity changes of the molecular junction with bias are interpreted in terms of the current flowing through the system. [1] http://www.smeagol.tcd.ie/SmeagolDownloads.htm.

HL 11.4 Mon 11:30 TRE Ma

Carbon nanotubes decorated with magnetic clusters: magnetism, electron transport and gas sensing — •Zeila Zanolli[1] and Jean-Christophe Charlier[2] — [1]Forschungszentrum Juelich, PGI and IAS, Juelich, Germany — [2]IMCN, Université catholique de Louvain (UCL), Belgium

In this work, first-principles techniques and non-equilibrium Green's function approaches are used to investigate magnetism and spin-polarized quantum transport in carbon nanotubes (CNTs) decorated with transition metal magnetic nanoclusters (NC).

For small cluster sizes (< 1 nm), *ab initio* calculations predict a considerable local magnetic moment that induces spin polarization in the host CNT due to a strong mutual interaction with the magnetic NC. Such a huge local magnetic perturbation can be tailored by molecular adsorption on the metallic NC, thus modifying both the magnetization and the spin-dependent conductance of the hybrid CNT-NC system. The adsorption of benzene on Ni- or Pt-decorated metallic CNTs has been investigated as a test case. The ab initio simulations demonstrate that the magnetization change due to the absorption of a single C_6H_6 molecule should be large enough to be detected experimentally using either magnetic-AFM or SQUID magnetometer. Consequently, the present research suggests a novel approach for single molecule gas detection, based on local magnetic moment measurements in CNT-NC hybrid systems [1].

[1] Z. Zanolli, J.-C. Charlier, ACSnano **6** (2012) 10786-10791.

15 min. break

Topical Talk HL 11.5 Mon 12:00 TRE Ma

Insight into Charge Transport in Molecular Junctions from Ab Initio Theories of Level Alignment — •Jeffrey B. Neaton — Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA, USA — Department of Physics, University of California, Berkeley, Berkeley, CA — Kavli Energy Nanosciences Institute, Berkeley, CA

Recent scanning tunneling microscope-based break-junction experiments of molecular junctions – devices formed by trapping organic molecules between macroscopic metallic electrodes – have reported robust conductance, thermopower, switching behavior, quantum interference effects, spin-filtering phenomena, and even nonlinear effects such as rectification, establishing such junctions as unique and revealing windows into the physics of charge transport at the molecular scale. In this talk, I will summarize a predictive approach to compute and understand the transport properties of molecular junctions with good accuracy. Our approach includes important exchange and correlation effects missing in standard DFT Kohn-Sham junction level alignment, building on self-energy corrections within a GW approximation. Advantages and limitations of our approach will be discussed quantitatively in the context of a direct comparison with recent photoemission and transport measurements. I will also describe applications of this approach to select junctions exhibiting novel trends in conductance, thermopower, and nonlinear IV characteristics, where new physical insight is obtained by relating computed transport phenomena to junction structure and chemistry.

HL 11.6 Mon 12:30 TRE Ma

Towards First-Principles Modeling of Solvent Effects in Photo-Catalytic Water Splitting — •Stefan Ringe, Harald Oberhofer, Sebastian Matera, and Karsten Reuter — Technische Universität München, Germany

In the context of solar energy conversion the search for new materials for photo-catalytic water splitting has received new impetus. While in general powerful, computational screening approaches are struggling with the complexity of the underlying physical processes at the solid-liquid interface. Recent work points in particular at the necessity to include at least an efficient description of solvent screening effects to compute meaningful descriptors even in simple computational hydrogen electrode approaches. To this end, we present an implementation of the modified Poisson-Boltzmann (MPB) implicit solvation model in the highly parallel and numerically efficient all-electron DFT code FHI-aims. Optimally integrating into this code environment, we solve the MPB equation in a novel approach based on an expansion of the electrostatic potential in the localized basis functions of FHI-aims. In contrast to common numerical multi-grid solvers this approach can directly make use of the optimized integration schemes used to reach self-consistency and removes the need for numerical interpolation between different grids. We demonstrate the approach and its efficiency for a range of molecular test systems, and show first results for catalytic water splitting on gold nano-clusters.

HL 11.7 Mon 12:45 TRE Ma

Towards a combined QM/MM and implicit solvent description of photoelectrochemical processes — •Markus Sinstein[1], Daniel Berger[1], Ran Jia[2], Volker Blum[3], Harald Oberhofer[1], and Karsten Reuter[1] — [1]Technische Universität München, Germany — [2]Jilin University, P.R. China — [3]Duke University, USA

Photoelectrochemical systems are widely explored to drive energy-relevant redox reactions like water splitting or CO_2 reduction. The detailed analysis of the involved elementary processes via first-principles calculations is challenged by the necessity to simultaneously account for the extended semiconductor photocatalyst and the liquid electrolyte. Especially for charge (proton and/or electron) transfer steps traditionally employed periodic boundary condition approaches involve charged supercells with difficult to control finite size errors. To this end, we present a solid state QM/MM embedding approach, in which only a finite cluster model of the photocatalyst surface is treated quantum mechanically and the correct Madelung potential of the periodic system is obtained by embedding into a charge field. For the efficient modeling of photoelectrochemical processes we combine this approach with an implicit solvation scheme within the DFT package FHI-aims. Finally, we also show early test results of the combined QM/MM implicit solvent model.

HL 11.8 Mon 13:00 TRE Ma

Ab-initio Simulation of Molecular Networks on the Surface of Water — •Ralph Koitz, Marcella Iannuzzi, Ari P Seitsonen, and Jürg Hutter — University of Zurich, Zurich, Switzerland

Molecules adsorbed on surfaces play an important role in catalysis, surface science, and nanotechnology. Traditionally, research has focused on various adsorbates atop metals and metal oxides using computational and surface-science techniques. More recently, however, it was demonstrated that ordered monolayer networks can also be formed on the surface of liquid water by using metal ions to bind together multidentate precursor molecules. As these assemblies are difficult to characterize, computational methods can provide valuable insight into their formation and structure.

In this contribution we present large-scale DFT-based molecular dynamics simulations of the formation of a network of *tris*-terpyridine-derived molecules (TTPB) on a water slab. In particular, we focus on the structure of the molecule on the surface, the mechanism of Zn^{2+} ion insertion from the solution and the subsequent linking of molecules into aggregates. We employ the metadynamics method to quantify the free energy surface of the involved processes. Our results provide detailed insight into on-surface and subsurface diffusion in this system and chemical reactions of TTPB on the surface of water.

HL 12: Energy materials: Water splitting, batteries, and supercapacitors (with CPP/MM)

Time: Monday 10:45–12:30 Location: POT 081

HL 12.1 Mon 10:45 POT 081

Highly efficient photocatalytic water splitting with colloidal CdS nanorods by mediated hole scavenging — •Thomas Simon, Aurora Manzi, Christian Wolff, Jacek Stolarczyk, and Jochen Feldmann — Photonics and Optoelectronics Group, Ludwig-Maximilians-Universität Muenchen, Amalienstr. 54, D-80799

Solar hydrogen production is considered to be as one of the biggest challenges for future energy supply. Colloidal semiconductor nanoparticles, as sunlight absorber with additional noble metal nanoparticles as hydrogen catalyst are well known for photocatalytic hydrogen generation. Many of these systems suffer from low solar to hydrogen efficiencies unless high cost and rare materials like platinum or ruthenium compounds are used as co-catalysts. We demonstrate that it is possible to overcome all these problems with CdS nanorods with a very simple earth-abundant nickel-based co-catalyst. An apparent quantum yield exceeding 50% and long term stability of more than 200h could be achieved. We show that the photocatalytic activity is enhanced ten-fold in highly alkaline environment. Thanks to favourable band alignment the hydroxide anion acts as a redox shuttle relaying the hole from the nanocrystals. Since the hole transfer is considered to be the limiting factor, the quick hole scavenging at high pH is responsible for the enhancement of photocatalytic hydrogen evolution. [1]

[1] T. Simon, M.J. Berr, A. Vaneski, D. Volbers, R. Wyrwich, M. Döblinger, A.S. Susha, A.L. Rogach, F. Jäckel, J.K. Stolarczyk, J. Feldmann, submitted

HL 12.2 Mon 11:00 POT 081

Three-dimensional Ordered Macro-mesoporous Mo:BiVO4 Photoelectrode toward Efficient Photoelectrochemical Water Splitting — •Min Zhou[1,2], Yang Xu[1], Chengliang Wang[1], Liaoyong Wen[1], Yong Lei[1], and Yi Xie[2] — [1]Ilmenau University of Technology, Institute of Physics & IMN MacroNano (ZIK) Prof. Schmidt-Str. 26, 98693 Ilmenau, Germany — [2]University of Science & Technology of China, Hefei, China

In view of the worldwide energy challenge in the 21st century, the technology of semiconductor-based photoelectrochemical (PEC) water splitting has received considerable attention as an alternative approach for solar energy harvesting and storage.BiVO4 has been regarded as a promising material for PEC water splitting, but it suffers from a major challenge on charge migration. In order to meet this challenge, for the first time, we design a three-dimensional(3D) ordered macro-mesoporous architecture of Mo:BiVO4 through a controllable colloidal crystal template method. Within expectation, a superior photocurrent density is achieved in return for this design. This enhancement originates primarily from effective charge migration according to the analysis of electrochemical impedance spectroscopy. All the results highlight the great significance of the 3D ordered macro-mesoporous architecture as a promising photoelectrode model for the application in solar conversion. The cooperating amplification effects of nanoenegineering from composition regulation and morphology innovation provide new opportunities for creating more purpose-designed photoelectrodes with highly efficient performance.

HL 12.3 Mon 11:15 POT 081

Three-dimensional Composite Aerogels and Other Nanostructures for Improved Electrochemical Property — •Liying Liang[1,2], Yimeng Xu[1], Haimei Liu[1], and Yong Lei[2] — [1]Beijing University of Chemical Technology, State Key Laboratory of Chemical Resource Engineering, 100029 Beijing (PR China) — [2]Ilmenau University of Technology, Institute of Physics & IMN MacroNano (ZIK) Prof. Schmidt-Str. 26, 98693 Ilmenau (Germany)

Three-dimensional (3D) graphene aerogels possess a lot of unique properties, such as light weight, high conductivity, large surface area, high mechanical strength, and ample volume with hierarchically porous structure, which make them widely applied in various technological fields. Here, 3D porous composite aerogels have been synthesized via an innovative in situ hydrothermal method assisted by freeze-drying process. In this hybrid structure, one-dimensional (1D) AgVO3 nanowires are uniformly dispersed on two-dimensional (2D) graphene nanosheets surfaces or penetrate through the graphene sheets, forming 3D porous composite aerogels. The composite aerogels as cathode materials for lithium-ion batteries, exhibit high discharge capacity, excellent rate capability, and good cycling stability. We are also preparing more novel nanostructures by using AAO templates, which are expected to provide excellent electrochemical performance.

HL 12.4 Mon 11:30 POT 081

Three-dimensional Metal Oxides Based Nano-arrays Anodes for Sodium Ion Batteries — •Yang Xu, Min Zhou, Huaping Zhao, Chengliang Wang, and Yong Lei — Institute of Physics, Ilmenau University of Technology, 98693 Ilmenau, Germany,

The discovery of new materials/microstructures for electrodes in sodium ion batteries (NIBs) is receiving high levels of scientific attention, as sodium is substantially less expensive and more abundant than lithium. However, there is a limited choice of electrode materials that are suitable hosts to accommodate Na ions and allow for reversible insertion/extraction reactions, since Na ions are 55% larger in radius than Li ions. Of those, most have been identified to be potentially useful as cathodes. On the anode side, hard carbonaceous materials and insertion of Sn, Sb, Pb, and their alloys based anodes have been demonstrated to be highly promising. Another emerging class of materials that remains relatively unexplored in this case is conversion and/or insertion electrodes using transition metal oxides with reasonably low insertion potential. We report the successful utilization combining the nano-structured transition metal oxides and three-dimensional metallic current collector for NIBs anodes, and the results are demonstrated to be promising: the electrodes exhibited a highly stable reversible charge storage capacity over long term cycling, and were able to withstand high rate cycling with fully recovering the initial capacity. This proof-of-principle demonstration opens a way forward for future work on nano-architectures with better NIBs anode performance.

HL 12.5 Mon 11:45 POT 081

First principles study on the electronic properties of NaO_2 — •Markus Heinemann[1], Pascal Hartmann[2], Conrad L. Bender[2], Philipp Adelhelm[2], Jürgen Janek[2], and Christian Heiliger[1] — [1]I. Physikalisches Institut, Justus Liebig University, 35392 Giessen, Germany — [2]Physikalisch-Chemisches Institut, Justus Liebig University, 35392 Giessen, Germany

In the light of the recent discovery of rechargeable room-temperature sodium superoxide (NaO_2) batteries [1], a deeper understanding of the electronic properties of NaO_2 has become of broad interest. We investigate the electronic structure of NaO_2 using the framework of density functional theory and employ a hybrid functional approach for the exchange and correlation interaction. The disordered pyrite structure of the NaO_2 room-temperature phase is modeled by taking into account various superoxide orientations in our computations. Our band structure calculations indicate that NaO_2 is an insulator with an energy band gap in the range of 2 eV and that different superoxide alignments lead to a broadening of the conduction band. We compare our calculations to recent experimental investigations on the conductivity of NaO_2.

[1] P. Hartmann, C. L. Bender, M. Vračar, A. K. Dürr, A. Garsuch, J. Janek, and P. Adelhelm, Nature Mat. 3486, 1 (2012)

HL 12.6 Mon 12:00 POT 081

Photostability of GaN-metal interfaces in aqueous media — •Carina Ehrig[1,2], Ralf Krause[1], Christoph Brabec[2], and Günter Schmid[1] — [1]Siemens AG, CT RTC MAT IEC-DE, Erlangen — [2]Lehrstuhl für Werkstoffe der Elektronik- und Energietechnik, FAU Erlangen-Nürnberg, Erlangen

Gallium nitride (GaN) is a well-established semiconductor in optoelectronic applications. It has a wide band gap of 3.4 eV and is thus excitable in the near UV range. A promising application of GaN is its use as a photo electrode driving electrochemical reactions such as photocatalytic water splitting for generation of hydrogen without consumption of fossil fuel or emission of CO_2. The corrosion resistance of those photo electrodes in aqueous media is one of the main factors determining their lifetimes and thus plays an important role for their applicability for highly efficient solar energy conversion. It has been demonstrated in photocatalytic experiments, that under UV-illumination n-type GaN acts as oxygen evolving photo anode and p-type GaN as hydrogen evolving photo cathode.

In the present work, the corrosion resistance of metal-coated n-GaN

and p-GaN photoelectrodes in aqueous media is investigated by electrochemical measurements. The influence of an externally applied potential under light excitation as well as the effect of long-term photo-induced stress are studied. It is observed that without illumination the GaN surfaces and GaN-metal interfaces are rather stable, whereas they undergo different corrosion processes when exposed to UV light.

HL 12.7 Mon 12:15 POT 081

Growth and characterization of 3D graphene networks for supercapacitors — •Simon Drieschner and Jose Antonio Garrido — Walter Schottky Institut, TU München, Am Coulombwall 4, 85748 Garching

The use of graphene as electrode material in supercapacitors has drawn great interest due to a suitable combination of material properties like high surface to volume ratio, high conductivity, and chemical stability. Since the capacitance of one single graphene sheet is rather limited, a continuous 3D network of graphene is expected to enhance the performance of graphene-based supercapacitors. We demonstrate the growth of 3D graphene by chemical vapor deposition (CVD) using a nickel foam as scaffold and a wet-etching transfer, yielding a free-standing macroporous graphene network of high crystalline quality, as shown by Raman spectroscopy. Cyclic voltammetry, charge-discharge measurements, and electrochemical impedance spectroscopy are used to assess the potential of 3D networks of CVD graphene for energy storage applications. We also compare the electronic double layer capacitance of bare graphene foam to the pseudo-capacitance introduced by conductive polymers.

HL 13: Nitrides: Optical characterization

Time: Monday 11:15–12:45 Location: POT 251

HL 13.1 Mon 11:15 POT 251

Nano-scale characterization of InGaN/GaN core-shell micropillars using helium temperature STEM-CL — •Marcus Müller[1], Sebastian Metzner[1], Anja Dempewolf[1], Gordon Schmidt[1], Peter Veit[1], Frank Bertram[1], Jürgen Christen[1], Steven Albert[2], Ana María Bengoechea-Encabo[2], Miguel Ángel Sánchez-Garcia[2], and Enrique Calleja[2] — [1]Institute of Experimental Physics, OvGU Magdeburg, Germany — [2]ISOM and Departamento de Ingeniería Electrónica, UP Madrid, Spain

In this study we report on the approach of combining top-down and the bottom-up processes to fabricate ordered InGaN/GaN core-shell micropillars by plasma-assisted molecular beam epitaxy. Direct comparison of the cross-section scanning transmission electron microscopy image of a single InGaN/GaN core-shell micropillar with the simultaneously recorded panchromatic cathodoluminescence (CL) mapping at 15 K reveals the highest CL intensity from the thick InGaN cap region and from the InGaN side walls. The CL peak wavelength image exhibits a dominating emission from the GaN near band edge at 359 nm as well as the yellow band at 560 nm from the center of the micropillar. On the side facets we observe an InGaN CL peak at 407 nm. In contrast, the upper part of the micropillar emits a broad luminescence band between 510 nm and 640 nm which can be attributed to different In compositions and strain conditions compared to the side facets. Furthermore, a red shift of the InGaN luminescence in both InGaN regions is observed indicating a gradual increase of the In composition during the growth due to the lattice pulling effect.

HL 13.2 Mon 11:30 POT 251

Time-integrated and time-resolved luminescence studies of hybrid InGaN/GaN MQW microrod structures — •Angelina Vogt[1], Stephanie Bley[1], Jana Hartmann[2], Sebastian Resch[3], Xue Wang[2], Matin Sadat Mohajerani[2], Martin Mandl[4], Martin Strassburg[4], Siegfried Waldvogel[3], Andreas Waag[2], Jürgen Gutowski[1], and Tobias Voss[1] — [1]Institute of Solid State Physics, University of Bremen — [2]Institute of Semiconductor Technology, TU Braunschweig — [3]Institute of Organic Chemistry, Johannes Gutenberg University Mainz — [4]Osram Opto Semiconductors GmbH

Three-dimensional GaN-based microrods with embedded InGaN multi-quantum-well structures (MQW) are promising candidates for sensors and light-emitting diodes in the green-ultraviolet spectral region. In order to extend the available wavelength region or to achieve selectivity in sensing devices, coating of the microrod structures with specific organic compounds can be applied. Here, we study the luminescence properties of GaN-based microrod LED structures coated with a perylene bisimide derivative. The InGaN/GaN LED structures were grown by MOVPE. Prior to the dye-coating process, their luminescence properties were studied in order to investigate their homogeneity. The samples were afterwards wet chemically coated with the perylene dye. The energy transfer from the QWs to the dye layer was studied in time-integrated and time-resolved photoluminescence experiments. We compare and discuss the luminescence dynamics in the bare InGaN/GaN microrod LEDs and the hybrid systems and analyse the energy transfer from the inorganic to the organic part.

HL 13.3 Mon 11:45 POT 251

Optical characterization of quaternary AlInGaN SQW using cathodoluminescene spectroscopy — •Martin Müller[1], Christopher Karbaum[1], Gordon Schmidt[1], Frank Bertram[1], Jürgen Christen[1], Jan Wagner[2], Michael Jetter[2], and Peter Michler[2] — [1]Institute of Experimental Physics, OvGUniversity Magdeburg, Germany — [2]IHFG, Stuttgart University, Germany

The optical properties of quaternary AlInGaN SQW have been investigated using spectrally and time-resolved cathodoluminescence (CL) microscopy at liquid helium temperature. All samples of the set consist of an 1 μm thick optimized GaN buffer on a c-plane sapphire substrat. Subsequently, on top of this a quaternary SQW of varying thickness (2, 3, 6, 10 nm) was grown using pulsed MOVPE and finally capped by a high temperature GaN layer. At low temperatures the CL-spectra are dominated by a blue-shifted near band edge luminescence with respect to relaxed GaN and a broad quaternary SQW emission band at about 370 nm. A slight shift of the SQW emission band to longer wavelengths with increasing thickness possibly caused by the quantum confined Stark effect as a consequence of inherent electric fields could be clearly seen. Addionally, the initial lifetime of the SQW increases from 1.1 ns up to 1.5 ns with the thickness as a result of a decreased electron and hole wave function overlap. The temperature dependent shift of the FX^A and FX^B from the GaN buffer could be observed indicating a high optical quality. The non-Varshni-like shift of the quaternary SQW emission with temperature will be discussed.

HL 13.4 Mon 12:00 POT 251

Valence band order in c-oriented wurtzite AlGaN layers — •Benjamin Neuschl[1], Jeffrey Helbing[1], Manuel Knab[1], Hannah Lauer[1], Tobias Meisch[2], Kamran Forghani[2], Ferdinand Scholz[2], and Klaus Thonke[1] — [1]Institute of Quantum Matter / Semiconductor Physics Group, University of Ulm — [2]Institute of Optoelectronics, University of Ulm

Aluminum gallium nitride (AlGaN) is the key material system for semiconductor-based optical devices emitting in the ultraviolet spectral region of light. Until now, some fundamental properties such as the valence band structure are not safely explored yet for all compositions. Especially the symmetry of the topmost valence band has a major impact on the light extraction behavior of the device.

Different layers of c-oriented wurtzite AlGaN were grown by metalorganic vapor phase epitaxy, and investigated by means of temperature- and polarization-dependent photoluminescence and X-ray spectroscopy. Knowing the samples' strain situation, we derive the valence band order, as a function of the relative amount of Al for a unified strain state. Subsequently, $k \cdot p$ theory allows the simulation of the strain-dependent valence band crossing. These fundamental results allow to design optimal light emitters for different emission wavelengths.

HL 13.5 Mon 12:15 POT 251

Micro-photoluminescence and micro-Raman studies on strained polar GaN layers — •Sebastian Bauer[1], Matthias Hocker[1], Lisa Hiller[1], Frank Lipski[2], Ferdinand Scholz[2], and Klaus Thonke[1] — [1]Institute of Quantum Matter / Semiconductor Physics Group, Ulm University, 89081 Ulm, Germany — [2]Institute of Optoelectronics, Ulm University, 89081 Ulm, Germany

Heteroepitaxial growth of *c*-oriented gallium nitride (GaN) layers by

hydride vapor phase epitaxy (HVPE) on sapphire substrates is always associated with specific strain states in the grown material. The efficiency of optoelectronic devices suffers from strain-induced piezoelectric effects as well as from structural defects caused by strain. Hence, the mechanism of strain relaxation with increasing layer thickness is of great interest.

We investigate a series of samples with different thicknesses grown by HVPE by spatially resolved low temperature microphotoluminescence and room temperature micro-Raman spectroscopy. The correlation between the layer thickness and the strain state of the material is analysed. These results suggest a minimum substrate layer thickness of GaN required for the realization of strain-free device material.

HL 13.6 Mon 12:30 POT 251

Photoluminescence of Zn and Mn doped thick GaN layers — •Friederike Zimmermann[1], Jan Beyer[1], Frank Habel[2], Gunnar Leibiger[2], Berndt Weinert[2], Martin Krupinski[3], Patrick Hofmann[3], and Johannes Heitmann[1] — [1]Institute of Applied Physics, TU Bergakademie Freiberg, Leipziger Str. 23, D-09599 Freiberg, Germany — [2]Freiberger Compound Materials GmbH, Am Junger-Löwe-Schacht 5, D-09599 Freiberg, Germany — [3]Namlab gGmbH, Nöthnitzer Straße 64, 01187 Dresden, Germany

Due to its superior electronic properties, GaN-based devices are suitable for high power, high frequency and high temperature applications. The direct and wide bandgap of GaN makes it an ideal material for bright UV and blue light emitting diodes and lasers. Electronic and optical properties can be tuned by doping with transition metal elements. We report on photoluminescence spectroscopy data of Zn and Mn doped samples grown by HVPE. Zn doped samples exhibit clear exitonic features including the exciton bound to the Zn acceptor. For samples of different Zn content four broad bands in the red, yellow, green and blue spectral region are found to vary in their relative intensities and temperature quenching. Mn doped samples show intense peaks at 1.25 and 1.41 eV which are assigned to intra-d-shell transitions of the incorporated Mn-ions. Sharp features in the exitonic range at room temperature can be ascribed to Raman scattering of the laser. As transition metals are generally expected to suppress the PL Raman contribution cannot be ruled out in Zn doped samples neither.

HL 14: Invited Talk James Lott

Time: Monday 11:45–12:15 Location: POT 151

Invited Talk HL 14.1 Mon 11:45 POT 151

Vertical-cavity surface-emitting lasers (VCSELs) for optical interconnects — •James A. Lott — Zentrum für Nanophotonik, Institut für Festkörperphysik, Technische Universität Berlin, Sekr. EW 5-2, Hardenbergstraße 36, D-10623 Berlin, Germany

Vertical-cavity surface-emitting lasers (VCSELs) are at present the smallest practical breed of laser. Mass-produced 10 Gbit/s VCSELs with an energy efficiency of about 400-800 fJ/bit are the workhorses of modern short-reach (SR $<$ 300 m) optical interconnects (OIs) in data centers and peta-FLOPS-class supercomputers. In this presentation we disclose our methods and wavelength-independent "Principles" of VCSEL design and operation, based on our many years of extensive experimental and numerical materials and device studies, that simultaneously lead to the optimization of three critical VCSEL attributes: 1) energy efficiency; 2) temperature stability; and 3) directly current-modulated bit rate. Our 850 nm VCSELs operate error-free across multi-mode fiber at 25-40 Gbit/s with energy efficiencies in the range 56-108 fJ/bit. We next disclose the results of our work on ultrafast 980 nm VCSELs targeted for very-short-reach (VSR $<$ 1 m) and ultra-short-reach (USR $<$ 1 mm) OIs for on-chip, inter-chip, free-space, and exa-FLOPS-class supercomputers of circa 2020-2030, where billions of OIs are envisioned in each supercomputer. We present record ˜179 fJ/bit operation at 42 and 38 Gbit/s at 25 and 85°C, respectively. We conclude with our perspectives on a practical OI roadmap to guide our work through circa 2050. * in collaboration with: D. Bimberg, W. Hofmann, G. Larisch, H. Li, A. Liu, P. Moser, and P. Wolf.

HL 15: Semicrystalline polymers (organized by CPP)

Lecture on the occasion of the Robert-Wichard-Pohl-Preis 2014 awarded to Gert Strobl

Time: Monday 13:15–13:45 Location: HSZ 02

Invited Talk HL 15.1 Mon 13:15 HSZ 02

Semicrystalline polymers - pathway of crystallization and deformation properties — •Gert Strobl — Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, 79104 Freiburg

On cooling a polymer melt, plate-like crystals with thicknesses in the nano-range are nucleated and grow in the two lateral directions. The final structure is semicrystalline and composed of stacks of such crystallites separated by entangled fluid chain sequences. Structure parameters vary with the crystallization temperature which can be chosen far below the equilibrium melting point, down to the transition into the glassy state. The question about the mechanism of polymer crystallization has always been a central issue in polymer physics. Time- and temperature dependent X-ray scattering experiments carried out during the last two decades now led to the establishment of a set of laws which control the structure formation out of the entangled melt, recrystallization processes, and the final melting. The laws indicate the participation of an intermediate mesomorphic phase in the crystal formation process. The peculiar deformation behaviour of polymeric materials reflects their semicrystalline structure, including in a coupled fashion both the rubber-like properties of the fluid parts and the elasto-plastic properties of the crystallites.

HL 16: Electron spin qubits in semiconductor quantum dots (Focus session with TT)

There have been remarkable new developments in the physics of electron spins confined in semiconductor quantum dots. In articular, silicon quantum dots have come to prominence, following in steps developments in GaAs dots. Spin hot spots — parametric regions with drastically reduced spin relaxation time — have been experimentally observed in both silicon and GaAs, in accord with theoretical investigations. Furthermore, novel ways of controlling and manipulating coherent dynamics of electron and nuclear spins in quantum dots by optics have been developed. This focused session will highlight those recent developments.

Organizer: Jaroslav Fabian, Universität Regensburg, and Jonathan Finley, Walter Schottky Institut, TU München.

Time: Monday 15:00–18:45 Location: POT 051

Topical Talk HL 16.1 Mon 15:00 POT 051

Single Charge Relaxation in a Silicon Double Quantum Dot — •Jason Petta — Department of Physics, Princeton University

Silicon has a weak spin-orbit interaction and can be isotopically purified resulting in an ultra-coherent environment for semiconductor qubits. I will describe recent measurements of single electron double quantum dots formed from undoped Si/SiGe quantum wells. Photon assisted tunneling is used to probe the energy level structure of the charge qubit, revealing the presence of low lying excited states. We measure the interdot charge relaxation time T_1 of a single electron as a function of detuning and interdot tunnel coupling and show that it is tunable over four orders of magnitude, with a maximum of 45 μs.

HL 16.2 Mon 15:30 POT 051

Entanglement Purification with the Exchange Interaction — •Adrian Auer and Guido Burkard — Department of Physics, University of Konstanz, Germany

Entanglement purification techniques provide means to create qubit pairs of arbitrary high fidelity with respect to a maximally entangled state, starting from a larger number of low fidelity pairs. So-called recurrence protocols act iteratively on two or more qubit pairs to produce one pair with higher fidelity, using local unitary operations, measurements, and communication of the measurement results. In this talk, we present a purification protocol that solely uses a single pulsed Heisenberg-type exchange interaction between two qubit pairs, therefore being especially suitable for spin qubits in tunnel-coupled quantum dots. In contrast to previously known protocols, we allow for asymmetric bilateral operations where the two communication parties operate differently on their qubits. In the most efficient version of our protocol, the local two-qubit interactions correspond to the $\sqrt{\text{SWAP}}$ gate and its inverse, which are the natural entangling gates generated from a Heisenberg-type interaction. Furthermore, we show how the same fidelity gain can be reached using XY-type interactions.

HL 16.3 Mon 15:45 POT 051

Reservoir-assisted coherent control of a quantum-dot spin — •Carsten H. H. Schulte[1], Jack Hansom[1], Claire Le Gall[1], Clemens Matthiesen[1], Jacob M. Taylor[2,3], and Mete Atatüre[1] — [1]Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, United Kingdom — [2]Joint Quantum Institute, University of Maryland, College Park, Maryland 20742, USA — [3]National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA

The interaction of a quantum-dot electron spin with the nuclear spins of its environment has attracted a lot of attention recently [1]. In equilibrium, the stochastic polarisation of the unperturbed nuclear spin bath leads to a splitting of the electron spin states. Here, we show that this effective Zeeman splitting is smaller than the linewidth of the charged exciton transition. The transitions in the unperturbed regime represent dynamically evolving Λ-systems. Harnessing these level schemes with sub-linewidth spin splittings, we implement spin-bath enabled coherent population trapping in the absence of an external magnetic field. We verify the coherence of the created spin state by coherent dark- and bright-state basis rotation through phase control of the laser fields, yielding arbitrary spin state initialisation and spin rotation with only hyperfine-induced spin orientation. The shown sub-linewidth level splitting advantageously reduces the influence of Larmor precession in spin manipulation schemes and facilitates photonic cluster state generation by triggered photon emission [2].

[1] Urbaszek et al., Rev. Mod. Phys. 85, 79-133 (2013).

[2] Lindner et al., Phys. Rev. Lett. 103, 113602 (2009).

Topical Talk HL 16.4 Mon 16:00 POT 051

Spin Qubits in Silicon — •Andrew Dzurak — University of New South Wales, Sydney 2052, Australia

Spin qubits in silicon are excellent candidates for scalable quantum information processing [1] due to their long coherence and the enormous investment in Si-MOS technology. Projective readout had proved challenging until single-shot measurement of a single donor electron spin was demonstrated [2] using a Si-SET and spin-to-charge conversion. The high readout fidelities > 90% and spin lifetimes T1 > 6 seconds [2] observed opened a path to electron and nuclear spin qubits in Si.

On-chip ESR of the P donor electron enables Rabi oscillations of the electron spin qubit, while Hahn echo reveals coherence T2 > 0.2 ms [3]. We also achieve single-shot readout of the 31P nuclear spin with fidelity > 99.8% and apply (local) NMR pulses to demonstrate coherent control of the nuclear spin qubit, with T2 > 60 ms [4].

Finally, I discuss recent experiments on both single-atom and Si-MOS quantum dot qubits in isotopically enriched 28Si devices, with even longer spin coherence exceeding 30 seconds.

[1] D.D. Awschalom et al., Quantum Spintronics, Science 339, 1174 (2013).

[2] A. Morello et al., Single-shot readout of an electron spin in silicon, Nature 467, 687 (2010).

[3] J.J. Pla et al., A single-atom electron spin qubit in silicon, Nature 489, 541 (2012).

[4] J.J. Pla et al., High-fidelity readout and control of a nuclear spin qubit in Si, Nature 496, 334 (2013).

HL 16.5 Mon 16:30 POT 051

Combining spin and valley singlet-triplet qubits for universal quantum computing — •Niklas Rohling, Maximilian Russ, and Guido Burkard — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

The valley degree of freedom in silicon or other materials is often considered to be an obstacle for quantum computing based on electron spins in quantum dots. Nevertheless, controlling the valley states opens new possibilities for quantum information processing. Combining qubits encoded in the single-triplet subspace of spin and of valley states allows for universal quantum computing because the exchange interaction directly provides a universal two-qubit gate between those qubits if they are stored in the same two-electron double quantum dot [1]. We show how spin and valley qubits can be separated in order to enable single-qubit rotations. Finally we propose explicit sequences for quantum gates in two kinds of spin-valley quantum registers.

[1] N. Rohling and G. Burkard, New Journal of Physics **14**, 083008 (2012).

HL 16.6 Mon 16:45 POT 051

Optical detection of coherent electron spin states of silicon vacancy defects in silicon carbide — •Matthias Widmann[1], Sang-Yun Lee[1], Nguyen Tien-Son[2], Helmut Fedder[1], Torsten Rendler[1], Adam Gali[3], Erik Janzén[2], and Jörg Wrachtrup[1,4] — [1]3. Physikalisches Institut, Universität Stuttgart — [2]Department of Physics, Chemistry and Biology, Linköping University — [3]Institute for Solid State Physics and Optics, Budapest — [4]Max-Planck Institute for Solid State Research, Stuttgart

Deep defects in wide band gap materials are promising candidates for realizing quantum information processing [QIP]. One candidate is the negatively charged nitrogen-vacancy (NV) center in diamond. NV centers can be used for realization of QIP[1] and nano-scale magnetic field sensing[2]. The diamond serving as a host material, however, is rather

hard to be implemented in existing silicon based semiconducting materials and devices. In order to circumvent this challenge, we focus on 4H silicon carbide (4H-SiC) which houses missing silicon atoms, forming the negatively charged silicon vacancies (T_V centers). Unlike the visible light emissions from NV centers in diamond, T_V centers in SiC also have the advantage of the infrared emissions around 900 nm, in which the optical attenuation is weaker in silica based fibers. We will present that single T_V emissions can be observed and coherent spin manipulation of both ensemble and single T_V centers are possible at room temperature.

[1] Neumann et al, Science, 2010, 329, 542
[2] J. R. Maze et al, Nature 455, 644-647

Coffee break (15 min.)

Topical Talk HL 16.7 Mon 17:15 POT 051

Spin Hot Spots in Quantum Dots — •Peter Stano — RIKEN Center for Emergent Matter Science, 2-1 Hirosawa, Wako, Saitama 351-0198 Japan — Institute of Physics, Slovak Academy of Sciences, 845 11 Bratislava, Slovakia

Spin hot spots are points in parameter space which dominate spin relaxation in quantum dots. The relaxation proceeds through spin-orbit interactions and a phonon emission. In a spin hot spot the otherwise weak spin-orbit effects become non-perturbative and thus unusually strong.

The hot-spot dominance leads to a pronounced anisotropy of the relaxation rate as a function of the quantum dot and/or magnetic field orientation with respect to crystallographic axes. This behavior is very general, occurring for different electron occupations, quantum dot geometry and material composition. Of practical interest is the possibility to individually identify different types of spin-orbit interactions (e.g. Rashba vs Dresselhaus), and obtain their relative strengths in a given sample, from the relaxation rate anisotropy.[1]

The important influence that the spin hot-spots might imply on spin relaxation was first recognized in bulk metals and later in quantum dots. The theoretically predicted spin hot-spots were recently established experimentally in gated Si [2] and GaAs [3] quantum dots.

[1] P. Stano and J. Fabian, Phys. Rev. B 74, 045320 (2006).
[2] C. H. Yang, et al., Nature Comm. 4, 2069 (2013).
[3] V. Srinivasa, et al., Phys. Rev. Lett. 110, 196803 (2013).

HL 16.8 Mon 17:45 POT 051

ESR Spin manipulation in spin light emitting diodes — •Andreas Merz, Jan Siller, Heinz Kalt, and Michael Hetterich — Inst. für angew. Physik KIT, Karlsruhe, Germany

Electron spin resonance is one of the most promising mechanisms to enable coherent quantum information processing. In spin light emitting diodes (spin-LEDs) we are able to initialize single electron spins all electrically by injecting them through a ZnMnSe spin-aligner layer into single self-assembled InGaAs quantum dots (QDs) with up to 100% fidelity. In a 53GHz microwave (MW) cavity we are able to manipulate the 3d Mn spin system of the spin aligner resonantly and detect the spin manipulation after the injection of band electrons into the QDs. We can optically observe the effect by analyzing the circular polarization of the recombination radiation during electrical excitation of the spin-LED for the magnetic field tuned such that the MW is resonant with the spin splitting in the Mn system. Furthermore we are able to differentiate between the resonant spin heating and non-resonant lattice heating of an amplified MW pulse for longer pulse lengths and pure spin heating for sub-microsecond MW pulses. The understanding of these mechanisms plays an important role for MW spin manipulation of single electron spins in semiconductor QDs on a ns timescale.

HL 16.9 Mon 18:00 POT 051

Optical Spin Noise of a Single Hole in a Quantum Dot — •Ramin Dahbashi[1], Jens Hübner[1], Fabian Berski[1], Klaus Pierz[2], and Michael Oestreich[1] — [1]Institute for Solid State Physics, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany — [2]Physikalisch Technische Bundesanstalt, Bundesallee 100, D-38116 Braunschweig, Germany

We present spin noise spectroscopy (SNS) [1] at the extreme limit of single spin detection, i.e., measurements of the spin dynamics of a single heavy hole localized in a self-assembled (InGa)As quantum dot (QD) [2]. Magnetic field dependent measurements reveal a strong dependence of the heavy hole spin relaxation rate T_1^{-1} on the longitudinal external magnetic field ($\propto B_z^{-3/2}$) even for very low magnetic fields up to 31 mT. At very low probe light intensities we detect an extremely long T_1 of > 180 μs at 31 mT and 5 K. The inhomogeneously broadening of a single QD SN spectrum is unveiled by the probe energy dependence of the SN power for finite light intensities. This feature is explained by charge fluctuations in the QD vicinity leading to distinct charge configurations. The corresponding fluctuations of the QD resonance energy are corroborated by a distinct probe intensity dependence of the spin lifetime. We further investigate time correlation effects of single QD SN spectra to gain insight into charging dynamics in the surrounding.

[1] Müller et al., Physica E **43**, 569 (2010).
[2] Dahbashi et al., arXiv:1306.3183 (2013).
[3] Dahbashi et al., Appl. Phys. Lett. **100**, 031906 (2012).

HL 16.10 Mon 18:15 POT 051

Spin-orbit effects on nuclear state preparation at the $S - T_+$ anti-crossing in double quantum dots — •Marko J. Rančić and Guido Burkard — University of Konstanz

We explore the interplay of spin-orbit and hyperfine effects on the nuclear preparation schemes in two-electron double quantum dots, e.g. in GaAs. The quantity of utmost interest is the electron spin decoherence time T_2^* in dependence of the number of sweeps through the electron spin singlet S triplet T_+ anti-crossing. Decoherence of the electron spin is caused by the difference field induced by the nuclear spins. We study the case where a singlet $S(2,0)$ is initialized, in which both electrons are in the left dot. Subsequently, the system is driven repeatedly through the anti-crossing and back using linear electrical bias sweeps. Our model describes the passage through the anti-crossing with a large number of equally spaced, step-like parameter increments. We develop a numerical method describing the nuclear spins fully quantum mechanically, which allows us to track their dynamics. Both Rashba and Dresselhaus spin-orbit terms do depend on the angle θ between the [110] crystallographic and the inter-dot axis. Our results show that the suppression of decoherence (and therefore the enhancement of T_2^*) is inversely proportional to the strength of the spin-orbit interaction, which is tuned by varying the angle θ.

HL 16.11 Mon 18:30 POT 051

Addressing ionized ^{75}As nuclear spin qubits in silicon using nuclear quadrupole interaction — •Florian M. Hrubesch, David P. Franke, Markus Künzl, Andrej Voss, Felix Hoehne, Lukas Dreher, and Martin S. Brandt — Walter Schottky Institut, Technische Universität München, Am Coulombwall 4, 85748 Garching

Electrically detected electron nuclear double resonance (EDENDOR) studies have shown coherence times of $^{31}P^+$ nuclear spins in crystalline ^{nat}Si of 18 ms [1]. In isotopically enriched ^{28}Si these T_2 times can reach up to 3 hours [2], making these nuclear spins promising candidates for quantum information storage. However, these long coherence times are caused by the nearly perfect isolation of the ionized donor nuclear spins from their environment, which hampers selective addressing with e.g. electric fields. We present EDENDOR measurements on $^{75}As^+$ nuclear spins in ^{nat}Si which exhibit similarly long decoherence times as $^{31}P^+$ nuclear spins in ^{nat}Si. By applying elastic strain, the transition frequencies involving the $|m_I| = \frac{3}{2}$ states can be shifted by about 25 kHz, while the transitions between the $|m_I| = \frac{1}{2}$ states remain virtually unaffected. This allows the selective manipulation of the nuclear spin state via magnetic resonance, which could enable the addressing of single $^{75}As^+$ qubits with the help of nanoscale piezoactuators positioned on top of the donors [3]. [1] L. Dreher *et al.*, Phys. Rev. Lett. 108, 027602 (2012) [2] K. Saeedi *et al.*, Science 342, 830 (2013) [3] L. Dreher *et al*, Phys. Rev. Lett. 106, 037601 (2011)

HL 17: Invited Talk Thomas Ihn

Time: Monday 15:00–15:30 Location: POT 081

Invited Talk HL 17.1 Mon 15:00 POT 081

Low-temperature scanning probe investigations of nanostructures at high and low magnetic fields — Nikola Pascher, •Thomas Ihn, Aleksey Kozikov, Richard Steinacher, Clemens Rössler, Klaus Ensslin, Christian Reichl, and Werner Wegscheider — ETH Zurich, Department of Physics, Otto-Stern Weg 1, CH-8093 Zurich

In our investigations we use the conducting tip of a scanning force microscope operated at cryogenic temperatures down to 40 mK for spatially resolved studies of the conductance in semiconductor nanostructures. The spatial resolution of the technique, which is comparable to the Fermi wavelength, gives insights into the *local* peculiarities of integer and fractional edge channel formation on spatial scales of many micrometers. It turns out that particular fractional edge channels are observed in certain regions along the edge but often fade out on a micrometer scale [1]. The macroscopic quantization of the Hall resistance still survives in the presence of these inhomogeneities.

It is an adventure to also apply this scanning gate technique to the *local* investigation the *non-local* transport in fully coherent nanostructures such as ballistic stadii [2]. What sounds like a contradiction at a first glance leads to beautiful images exhibiting the whole zoo of coherent mesoscopic phenomena ranging from irregular conductance fluctuations to regular standing wave patterns and even to the paradigmatic Aharonov-Bohm effect.

[1] N. Pascher *et al*, arXiv:1309.4918, accepted in PRX [2] A. A. Kozikov *et al*, New J. Phys. **15**, 083005 (2013).

HL 18: Carbon: Diamond, nanotubes and Buckyballs

Time: Monday 15:00–16:45 Location: POT 112

HL 18.1 Mon 15:00 POT 112

Calculation of the optical properties of the nitrogen-vacancy center in diamond using a configuration interaction approach — •Denis Antonov[1,2], Gabriel Bester[2], and Jörg Wrachtrup[1] — [1]3. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany

We present calculations of the optical properties of nitrogen-vacancy (NV) centers in diamond. In particular, the negatively charged NV^- center is emerging as a promising candidate in the fields of quantum information, quantum processing and high resolution magnetometry. These applications require a precise prediction, and understanding, of the optical properties of NV^- centers including their many-body multiplet structure. We utilize a new approach, the atomic effective pseudopotential (AEP) method, which is based on the local density approximation (LDA) and an empirical correction to the quasiparticle band structure, to accurately model the NV^- center in diamond. Starting from the AEP wave functions, we calculate the many body effects using a configuration interaction approach that we adapt to the treatment of defects. We will highlight the effect of screening in the calculation of the Coulomb and exchange integrals. Our results of the optical spectrum of the isolated NV^- system, calculated on large supercells, show very good agreement with previous experimental reports, including an accurate reproduction of the experimental zero phonon line.

HL 18.2 Mon 15:15 POT 112

Low dimensional effects in surface conductive diamond — •Patrick Simon, Moritz V. Hauf, Max Seifert, Alexander W. Holleitner, Martin Stutzmann, and Jose A. Garrido — Walter Schottky Institut and Zentrum für Nanotechnologie und Nanomaterialien, Am Coulombwall 4, 85748 Garching

Hydrogen-terminated diamond exhibits a high surface conductivity in air. While theoretical models have suggested that a two-dimensional hole gas is formed shortly beneath the surface, no experimental proof has been reported yet.

In this work, we prove the low dimensional character of the surface conductive channel of hydrogen-terminated diamond. Using e-beam lithography and an oxygen plasma process we selectively oxidize the hydrogen-terminated diamond surface in order to fabricate in-plane gated field effect transistors. We demonstrate the lateral depletion of the conductive channel of devices with widths of up to 250 nm by applying a gate voltage. At liquid helium temperatures we observe a transition from the initial 2D system to a 1D system exhibiting quantized conductance. In a bias regime where the channel is almost fully closed, we observe Coulomb blockade effects characteristic of multiple islands that vary in size with the applied bias. The islands dimension exhibits a gate voltage dependence which is a direct result of the two-dimensional nature of the hole gas formed by the hydrogen-terminated surface.

HL 18.3 Mon 15:30 POT 112

Photocurrent from Hybrid Systems Based on Diamond and Bacterial Reaction Centers — •Réka Csiki, Roberta Caterino, Matthias Sachsenhauser, Philipp Niedermayr, Martin Stutzmann, Anna Cattani-Scholz, and Jose Antonio Garrido — Walter Schottky Institut, TU München, Am Coulombwall 4, 85748 Garching

Photoactive reaction centers (RCs) are protein complexes which can convert sunlight into other forms of energy with high efficiency. These proteins can generate a photocurrent under photostimulation when they are immobilized on and electrically connected to inorganic electrodes. In this contribution we show that heavily boron-doped polycrystalline diamond can be chemically modified by covalently attaching the linker molecule 6-phosphonohexanoic acid to the diamond surface, creating a suitable environment for a subsequent attachment of bacterial reaction centers. Two important mediators are involved in the natural charge transfer process of the bacterial RCs: the coenzyme Q_0 and the redox protein cytochrome c. The role of these two mediators in the photocurrent generation from photoactive RCs immobilized on functionalized diamond electrodes will be reported together with a discussion on the voltage dependence of the induced photocurrent. We demonstrated that OH-terminated diamond surfaces can be functionalized with organophosphonates and, together with the attached reaction centers, represent a suitable biohybrid system for energy harvesting.

HL 18.4 Mon 15:45 POT 112

Diamond-based platforms for long-term growth and investigations of neurons — •Alexandra Voss[1], Hongying Wei[2], Cyril Popov[1], Monika Stengl[2], and Johann Peter Reithmaier[1] — [1]Institute of Nanostructure Technologies and Analytics, University of Kassel, Germany — [2]Department Animal Physiology, University of Kassel, Germany

Due to biocompatibility, large electrochemical potential window and high chemical stability, combined with a number of superior physical properties, all types of diamond films are ideal candidates for platforms for biotechnological applications, such as multielectrode arrays (MEA) for neuronal signal derivation. In our work we investigated the suitability of the integration of diamond into the fabrication process of MEA structures. For this purpose the deposition of our ultrananocrystalline diamond (UNCD) layers was investigated on different glass types and metal layers to achieve closed uniform UNCD layers with good substrate adhesion confirmed by optical microscopy and SEM. For further investigations of transparent layer systems Eagle 2000 was chosen. Better optical quality was achieved by decreasing the UNCD layer thickness. For this purpose several diamond powder dispersions for pretreatment were evaluated to enhance the nucleation leading to shorter deposition times. This increases the transparency as confirmed by ellipsometry and transmission spectroscopy. In earlier experiments the improved adhesion of pacemaker neurons of *R. maderae* was confirmed on UNCD layers with different surface termination. This fact was used to improve the cell culture preparation technique.

HL 18.5 Mon 16:00 POT 112

Unusual Hysteresis Observed in the Magnetoresistance of Multiwall Carbon Nanotubes Bundles — •Jose Barzola-Quiquia[1], Manuel Lindel[1], M. Muallem[2], Gilbert D. Nessim[2], and Pablo Esquinazi[1] — [1]Division of Superconductivity and Magnetism, Institute for Experimental Physics II, University of Leipzig, D-04103 Leipzig, Germany — [2]Department of Chemistry, Bar-Ilan University, Ramat Gan 52900, Israel

The magnetotransport properties of several hundreds of micrometer long multi-walled carbon nanotubes (MWCNT) bundles were studied. The samples were contacted with silver paste and showed ohmic behavior at temperatures above 10 K, i.e. linear current-voltage (I-V) curves. The temperature dependence of the resistance is well described by variable-range hopping mechanism for one-dimensional systems. In this temperature range the magnetoresistance is negative and can be explained using an empirical model based on spin-scattering processes that suggests the existence of magnetic order. No magnetic impurities were found by means of energy dispersive X-ray. At temperatures between 2 K and 12 K, the I-V curves showed a nonlinear behavior, indicating the existence of a potential barrier. In this temperature range and at low magnetic fields and low enough input currents the magnetoresistance changed to positive accompanied by a clear hysteresis. The hysteresis as well as the positive magnetoresistance vanished at large inputs currents. Our results indicate that at $T < 12$ K the unusual butterfly hysteresis in the magnetoresistance is directly related to the nonlinear I-V behavior and suggests superconducting.

HL 18.6 Mon 16:15 POT 112

Ultrasensitive force detection with a nanotube mechanical resonator — Joel Moser[1,2], •Johannes Güttinger[1,2], Alexander Eichler[1,2], Maria Jose Esplandiu[2], Dong E. Liu[3], and Mark I. Dykman[3] — [1]ICFO, Av. Carl Friedrich Gauss, 08860 Castelldefels, Barcelona, Spain — [2]ICN, CIN2-CSIC, Campus UAB, 08193 Barcelona, Spain — [3]Department of Physics and Astronomy, Michigan State University, Michigan 48824, USA

Since the advent of atomic force microscopy, mechanical resonators have been used to study a wide variety of phenomena, such as the dynamics of individual electron spins, persistent currents in normal metal rings, and the Casimir force. Key to these experiments is the ability to measure weak forces. Here, we present force sensing experiments with a sensitivity of 12 zN $Hz^{-1/2}$ at a temperature of 1.2 K using a resonator made of a carbon nanotube [1]. An ultra-sensitive method based on cross-correlated electrical noise measurements, in combination with parametric downconversion, is used to detect the low-amplitude vibrations of the nanotube induced by weak forces. The force sensitivity is quantified by applying a known capacitive force. This detection method also allows us to measure the Brownian vibrations of the nanotube down to cryogenic temperatures. Force sensing with nanotube resonators offers new opportunities for detecting and manipulating individual nuclear spins as well as for magnetometry measurements.

[1] J. Moser et.al. Nature Nanotechnology 8, 493 (2013)

HL 18.7 Mon 16:30 POT 112

Charge carrier scattering with acoustic phonons in chirality enriched carbon nanotubes — •Peter Vogel[1], Olga Dyatlova[1], Ulrike Woggon[1], Christopher Köhler[2], Ermin Malic[2], Andreas Knorr[2], Rishabh Jain[3], Kevin Tvrdy[3], and Michael Strano[3] — [1]Institut für Optik und Atomare Physik, Technical University of Berlin — [2]Institut für theoretische Physik, Technical University of Berlin — [3]Department of Chemical Engineering, Massachusetts Institute of Technology

By using two-color pump-probe measurements we investigate the carrier relaxation dynamics in (7,5) carbon nanotubes at different combinations of pump and probe energies. The sample was characterized by PLE spectroscopy and is highly chirality enriched for (7,5) tubes solved in water with 5% sodium dodecyl sulfate (SDS). For pumping resonant to the E22-transition energy (1.922 eV) and probing resonant to E11-transition energy (1.206 eV), typical multi-exponential decay behaviour occurs[1]. By fixing the pump energy at E22 of the (7,5) species and tuning the probe energy from resonant to E11 up to the band (1.563 eV), we observe an acceleration of the relaxation dynamics of the first ps-component. This result is in agreement with predicted theoretical results[2]. Density matrix formalism is applied obtaining microscopic access to time- and momentum-resolved relaxation dynamics driven by scattering with acoustic phonons.

[1] O.A. Dyatlova et al., Nano Lett. 12, 2249 (2012)
[2] C. Köhler et al., Phys. Status Solidi (b) 249, 2483 (2012)

HL 19: Nitrides: Devices

Time: Monday 15:00–17:15 Location: POT 151

HL 19.1 Mon 15:00 POT 151

Comparison of gallium nitride nanorod growth in MBE and MOVPE on nitridated c-plane sapphire — •Julian Stoever, Marc Sauerbrey, Stephan Figge, Jan Ingo Flege, Timo Aschenbrenner, Gerd Kunert, Jens Falta, and Detlef Hommel — Institute of Solid State Physics, University of Bremen, Bremen

Free-standing, nanocrystalline gallium nitride structures on c-plane sapphire substrates were fabricated by metal-organic vapour phase epitaxy (MOVPE) as well as by molecular beam epitaxy (MBE).
Prior to the growth, a substrate nitridation at high temperature and high ammonia flux in MOVPE was carried out to form AlN islands. These nanoislands act as nucleation centers for the rods. The formation process of the islands was investigated in detail by atomic force microscopy and x-ray photoelectron spectroscopy.
Ga-rich conditions, a sufficient silane supply and MOVPE growth temperatures of 1150 °C result in well separated microcolumns. Structures with diameters up to 3 μm and lengths up to 8 μm were fabricated.
On the other hand, nitrogen-rich growth conditions are necessary to achieve columnar growth in MBE. At temperatures of 835 °C, nanorods with diameters of 50 nm and lengths up to 200 nm occur.
Although the same substrate preparation is used, the growth process differs between MOVPE and MBE resulting in different structures. Scanning electron microscopy and micro photoluminescence investigations performed for both types of columns will be presented.

HL 19.2 Mon 15:15 POT 151

Light Emitters Based on GaN Nano-Stripes with Semipolar Quantum Wells — •Robert Anton Richard Leute[1], Junjun Wang[1], Tobias Meisch[1], Benjamin Neuschl[2], Klaus Thonke[2], and Ferdinand Scholz[1] — [1]Institute of Optoelectronics, Ulm University, 89081 Ulm, Germany — [2]Institute of Quantum Matter / Semiconductor Physics Group, Ulm University, 89081 Ulm, Germany

Patterning of silicon dioxide masks on c-oriented GaN/AlGaN templates by imprint lithography allows to fabricate InGaN/GaN nanostripes with semipolar $\{10\bar{1}1\}$ side facets. These stripes have a triangular cross section and form a 1D grating with a period of 260 nm. Subsequent embedding in GaN creates an asymmetric waveguide. The emission of the quantum wells is investigated under electrical and optical excitation. Photoluminescence measurements are performed at varying temperatures. We discuss the performance and suitability of such nano-structures for optical devices.

HL 19.3 Mon 15:30 POT 151

$(11\bar{2}2)$ **InGaN/GaN LEDs grown on 2" patterned sapphire substrates** — •Tobias Meisch[1], Sabine Schörner[2], Junjun Wang[1], Klaus Thonke[2], and Ferdinand Scholz[1] — [1]Institute of Optoelectronics, University of Ulm, 89081 Ulm, Germany — [2]Institute of Quantum Matter, Workgroup Semiconductor Physics, , University of Ulm, 89081 Ulm, Germany

We have grown high quality $(11\bar{2}2)$ GaN on $(10\bar{1}2)$ patterned sapphire. The patterning of the substrate was done by reactive ion etching to produce periodic trenches with a depth of about 1.5 μm and a width of 1.5 μm, revealing a c-plane-like facet on one side. In the following MOVPE process, GaN nucleates on this unmasked side facet, grows out of the trench and forms a coalesced semipolar surface. By comparing the doping behavior of c-plane and $(11\bar{2}2)$ GaN, a significant reduced magnesium incorporation efficiency on the semipolar surface was detected. To achieve similar electrical properties, an about 10 times higher Mg flux is necessary. However, making use of this conclusion, now we are able to grow LEDs on $(11\bar{2}2)$ GaN. Therefore, five InGaN quantum wells with GaN barriers are deposited on an about 1 μm thick silicon doped GaN layer. On the top, a 200 nm thick p-doped

GaN layer was grown. First EL measurements show very promising results: At 20 mA, an optical output of 0.2 mW at 450 nm was achieved. By increasing the indium flux step by step, the emission wavelength could be shifted to 475 nm. Adjusting the QW properties and inserting an InGaN pre-QW should help to increase the output power further.

HL 19.4 Mon 15:45 POT 151

Al(Ga)N electron blocking heterostructure design for high injection efficient 290 nm light emitting diodes — •Martin Guttmann[1], Christoph Reich[1], Tim Kolbe[1,2], Frank Mehnke[1], Christian Kuhn[1], Jens Rass[1,2], Tim Wernicke[1], Mickael Lapeyrade[2], Sven Einfeldt[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

We report on the optical and electronic properties of AlGaN-based light emitting diodes (LEDs) with a wavelength near 290 nm using different electron blocking heterostructures. Using a conventional $Al_{0.7}Ga_{0.3}N$:Mg electron blocking layer (EBL) carrier injection into 290 nm LEDs proves to be challenging. A broad parasitic luminescence around 350 nm was observed, originating from electron overflow into the Mg-doped $Al_{0.4}Ga_{0.6}N/Al_{0.3}Ga_{0.7}N$ superlattice. Our studies show that by inserting an AlN:Mg interlayer (IL) between active region and EBL, electron overflow can be prevented. This is confirmed by electroluminescence measurements and simulations. With increasing IL thickness the emission output power increases, reaches a maximum at 3 nm and remains constant for thicker IL. We present a detailed analysis of the electron and hole injection into 290 nm LEDs using simulations as well as a study of current-voltage-characteristics and the emission spectra obtained from temperature dependent and pulsed electroluminescence measurements.

HL 19.5 Mon 16:00 POT 151

Characteristics of sub-300 nm AlGaN multiple quantum well lasers grown on epitaxially laterally overgrown AlN/sapphire substrates — •Martin Martens[1], Peter Schneider[1], Frank Mehnke[1], Christian Kuhn[1], Christoph Reich[1], Viola Kueller[2], Arne Knauer[2], Carsten Netzel[2], Jens Rass[1,2], Tim Wernicke[1], 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

We have investigated the characteristics of AlGaN-based multiple quantum well (MQW) lasers emitting in the UV-B to UV-C spectral range. The laser heterostructures were grown by metal organic vapor phase epitaxy in [0001] direction on low defect density epitaxially laterally overgrown AlN/sapphire substrates. The separate confinement heterostructures consist of $Al_xGa_{(1-x)}N/Al_{0.70}Ga_{0.30}N$ MQWs and $Al_{0.70}Ga_{0.30}N/Al_{0.80}Ga_{0.20}N$ waveguiding heterostructures. Opitcally pumped lasing was obtained in a wavelength range between 272 nm and 293 nm with threshold energy densities down to 15 mJ/cm^2 for resonant pumping of the MQW. Laser emission was transverse electric polarized independent of the wavelength. The variable stripe length method was applied to determine the gain spectra of different laser heterostructures. The influence of emission wavelength and sample morphology on the laser threshold and gain characteristics will be discussed.

HL 19.6 Mon 16:15 POT 151

Sub-250 nm LEDs with enhanced charge carrier injection — •C. Kuhn[1], F. Mehnke[1], M. Guttmann[1], C. Reich[1], T. Kolbe[1], V. Kueller[2], A. Knauer[2], T. Wernicke[1], M. Weyers[2], and M. Kneissl[1,2] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Germany — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Berlin, Germany

For AlGaN-based LEDs emitting at 250 nm and below, the aluminum content of the active region and surrounding layers exceeds 60%. For LEDs with such high Al mole fractions, carrier injection is a major challenge due to increasing donor and acceptor activation energies and small band offsets between AlGaN quantum wells (QW), barriers and electron blocking layers (EBL). In this study, we investigate the influence of the $AlN/Al_{0.7}Ga_{0.3}N$:Mg electron blocking heterostructure on the injection efficiency of 245 nm LEDs. Increasing thickness of the AlN EBL leads to a rise of the QW luminescence for Mg-doped and undoped AlN layers. However, there is still strong parasitic luminescence centered at 280 nm which depends on the Mg supply during the AlN EBL growth. AlN EBLs grown without Mg enable a drastic reduction of the parasitic luminescence, if the AlN thickness is larger than 4 nm. We were able to demonstrate 245 nm LEDs with an 8 nm thick undoped AlN EBL with external quantum efficiency of 0.19%. Finally, this improved design was applied to UV-C LEDs with different emission wavelengths. AlGaN-based LEDs in the emission range between 235 nm and 263 nm were demonstrated with maximum EQE of 1.1% at 263 nm.

HL 19.7 Mon 16:30 POT 151

Surface passivation studies of AlInN/GaN based HEMTs grown on Si(111) by MOVPE — •Jonas Hennig, Aqdas Fariza, Hartmut Witte, Juergen Blaesing, Armin Dadgar, and Alois Krost — Institut of Experimental Physics, Otto-von-Guericke-University Magdeburg, Magdeburg, Germany

GaN is a wide bandgap material and therefore a good candidate for building high electron mobility transistors (HEMTs) or switching devices with large breakdown voltages. Furthermore, the high electron mobility predestines this material system for high frequency applications that are needed in the telecommunication industry. The spontaneous polarization difference at the AlInN/GaN heterojunction results in a high carrier density of the two dimensional electron gas (2DEG) and therefore in a higher source drain current compared with well-established AlGaN/GaN HEMTs. Although this makes AlInN/GaN HEMTs promising candidates for the application mentioned above these devices suffer from large gate leakage. To reduce the leakage current different capping layers for surface passivation can be chosen. We will present a comparative study of GaN passivation as well as in-situ and ex-situ SiN capping layer and discuss the impact on the device performance. Structural analyses are carried out by XRD and AFM. The electrical characterization includes Hall-effect, C-V measurements and admittance spectroscopy.

HL 19.8 Mon 16:45 POT 151

Defect characterisation in AlInN/AlN/GaN HEMT structures on Si(111) — •Aqdas Fariza, Hartmut Witte, Jonas Hennig, Oliver Krumm, Jürgen Bläsing, Armin Dadgar und Alois Krost — Institute of Experimental Physics, Otto-von-Guericke-University-Magdeburg, Magdeburg, Germany

AlGaN/GaN based high electron mobility transistors (HEMTs) are well established for many applications and can be improved in carrier density by using AlInN instead of AlGaN. Growing such structures on Si is advantageous due to lower substrate cost and large substrate diameter, as well as simpler processing. But, due to unavoidable traps performance problems occur. They mostly lead to leakage currents but also other limitation in device parameters. Therefore, investigations of these traps are essential to optimize HEMT devices. We have grown capped AlInN/AlN/GaN HEMTs on Si(111) by MOVPE with nearly lattice matched In-content. Samples were prepared with a Ni/Au-Schottky like contact and an annealed Ohmic contact deposited on top of the layers. I-V- and C-V-characteristics were carried out in dependence of frequencies and temperatures. Simultaneously, we measured the frequency and temperature dependent capacitances and conductance. These investigations exhibit several strong interface defect states located between the metal contact and the GaN buffer layer. Based on a complex equivalent circuit we were able to localize two interface defect states. We will also show significant differences in the interface defect densities between the investigated samples.

HL 19.9 Mon 17:00 POT 151

A comparative study of V/Al/Ni/Au and Ti/Al/Ni/Au ohmic contacts on n-AlGaN/GaN — •Christopher Schröter[1], Alexander Schmid[1], Volker Klemm[2], and Johannes Heitmann[1] — [1]Institute of Applied Physics, TU Bergakademie Freiberg, 09599 Freiberg — [2]Institute of Materials Science, TU Bergakademie Freiberg, 09599 Freiberg

A study of ohmic contact formation by V/Al/Ni/Au and Ti/Al/Ni/Au on $n-Al_{0.23}Ga_{0.77}N/GaN$ heterostructures is presented. Vanadium was chosen as a potential alternative for titanium due to lower annealing temperatures required for the ohmic contact formation. For the V/Al/Ni/Au metallization low resistance ohmic contacts were achieved after annealing at 650°C for 30 s. This is a reduction of 150 K compared to the reference Ti/Al/Ni/Au stack. The minimum measured specific contact resistivity was $2.3 * 10^{-6} \Omega cm^2$ at an annealing temperature of 800°C and $2 * 10^{-5} \Omega cm^2$ at an annealing temperature of 650°C. A variation of the vanadium layer thickness from 35 nm to 15

nm showed an improved contact formation for the thinner layer.

After annealing the V/Al/Ni/Au metallization exhibited sharper edges and smoother surfaces compared to the rough Ti/Al/Ni/Au reference stack. For further investigation of the contact microstructure, transmission electron microscopy (TEM), electron energy loss spectroscopy (EELS) and energy dispersive x-ray diffraction (EDX) measurements were performed.

HL 20: Symposium SYCM: Crystallography in materials science

Time: Monday 15:00–17:45 Location: HSZ 02

Invited Talk HL 20.1 Mon 15:00 HSZ 02

Complexity on Compression: The Crystallography of High-Density Matter — •Malcolm McMahon — School of Physics and Astronomy, The University of Edinburgh, Edinburgh, UK.

The crystal structure of iron was determined at *normal* conditions as long ago as 1917. But what is the structure of iron within *Super-Earth* exoplanets where core conditions approach 10 million atmospheres (1 TPa) and 10,000 K, and where carbon exists as either diamond, or as an exotic metallic form.

Until the early 1990s, the consensus was that at high pressures, all materials would become metallic, and assume high-symmetry, close-packed crystal structures. But the advent of modern crystallographic methods on synchrotron sources in the early 1990s revealed completely different behavior: even the simplest materials underwent phase transition to complex, frequently incommensurate, forms, while metals became semiconductors or insulators. This complexity is thought to arise from the constraints placed on the electronic wave functions due to the Pauli exclusion principle, the need to orthogonalise the wave functions of both core and valence electrons, and the reduction in the available interstitial space at high compression

In this talk I will present results from recent diffraction studies of elemental metallic systems showing some of the extreme complexity observed at high pressures. I will also look at the new opportunities in extreme conditions crystallography offered by x-ray lasers such as the LCLS in the Stanford, and XFEL in Hamburg.

Invited Talk HL 20.2 Mon 15:30 HSZ 02

X-Ray Microscopy with Coherent Radiation: Beyond the Spatial Resolution of Conventional X-Ray Microscopy — •Christian G. Schroer — Institut für Strukturphysik, Technische Universität Dresden, 01062 Dresden, Germany

Hard x-ray microscopy has greatly benefited from the high brilliance of modern synchrotron radiation sources and x-ray free-electron lasers (XFELs). Today, the spatial resolution of conventional x-ray microscopes is limited by the x-ray optics to a few tens of nanometers. Scanning coherent diffraction microscopy, also known as ptychography, can overcome this limitation. In ptychography, the sample is scanned through a confined coherent beam, recording at each location of the scan a far-field diffraction pattern. From these data, the complex transmission function (projected complex refractive index) of the sample and the illuminating complex wave field can be reconstructed with a spatial resolution that clearly exceeds the lateral size of the illuminating beam. The spatial resolution in a ptychogram is shown to depend on the shape (structure factor) of a feature and can vary for different features in the object. In addition, the resolution and contrast depend on the coherent fluence on the sample. For an optimal ptychographic x-ray microscope, this implies a source with highest possible brilliance and an x-ray optic with a large numerical aperture to generate the optimal probe beam. Ptychography closes the gap between real space imaging and reciprocal space structure determination and merges these two fields.

[1] A. Schropp, et al., Appl. Phys. Lett. **100**, 253112 (2012).

Invited Talk HL 20.3 Mon 16:00 HSZ 02

Modulated martensite: A scale bridging Lego game for crystallographers and physicists — •Sebastian Fähler — IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — Technische Universität Dresden, Department of Physics, Institute for Solid State Physics, 01062 Dresden, Germany — Technische Universität Chemnitz, Faculty of Natural Sciences, Institute of Physics, D-09107 Chemnitz, Germany

Among various materials exhibiting reversible phase transformations structures with low crystal symmetry, so-called modulated phases, exhibit the best ferroelectric, magnetocaloric or magnetic shape memory properties. Here it is describe how modulated martensite can be built in a kind of Lego game from simple tetragonal building blocks. It's complex crystallographic (micro-) structure is determined by the boundary conditions during the nucleation process. Though this building principle can be describe in terms of continuum mechanics, it is consistent with first principle calculations. Supported by SPP 1239 and SPP 1599.

15 min break

Invited Talk HL 20.4 Mon 16:45 HSZ 02

Switching of magnetic domains reveals evidence for spatially inhomogeneous superconductivity — •Michel Kenzelmann — Paul Scherrer Institut

The interplay of magnetic and charge fluctuations can lead to novel quantum phases with exceptional electronic properties. Magnetic order in such quantum phases can fundamentally affect the underlying symmetry and generate new physical properties. Importantly, it has been predicted that spin-density wave (SDW) order in a singlet d-wave superconductor is coupled to triplet superconductivity. We performed neutron diffraction studies of the Q-phase SDW [1] in $CeCoIn_5$, and we make two important observations [2]. We observe a complete and extremely sharp SDW domain switching that is unexplained by current microscopic theories for $CeCoIn_5$. Using representational theory, we interpret our experimental results as evidence for the presence of p-wave superconductivity that coexists with d-wave superconductivity and SDW order. The triplet component is of p-wave symmetry, similar to that found in the A-phase of superfluid ^{3}He, and is modulated as a Cooper pair density wave. Our findings identify the Q-phase as a unique quantum phase where d-wave and modulated p-wave superconductivity are coupled to SDW order, and which emerges in a magneto-superconducting quantum critical point [2].

[1] M. Kenzelmann et al, Science 321, 1652 (2008). [2] S. Gerber et al, submitted to Nature Physics (2013).

Invited Talk HL 20.5 Mon 17:15 HSZ 02

The key role of magnetic neutron diffraction in materials science — •Laurent C. Chapon — Institut Laue-Langevin, Grenoble, France

Since the 1950s, neutron scattering, and more specifically diffraction, has been a tool of choice for studying magnetism at the atomic scale. From the very first experimental proof of antiferromagnetism, a phenomenon predicted by Louis Néel, to unveiling how complex multiferroic materials work, the technique has always offered information of crucial importance to build the physical models that are required to explain macroscopic properties of materials. I will review briefly the historical development of magnetic neutron scattering and present key neutron diffraction experiments in recent areas of interest for condensed matter physicists, in particular highlighting the use of the technique for multiferroics and frustrated magnetic systems.

HL 21: Organic electronics and photovoltaics II (organized by CPP)

Simulations, Polymers, Solar Cells

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

HL 21.1 Mon 15:00 ZEU 222

Quantumchemical Calculation of Zn-Porphyrine-Indolocarbazole-Conjugates — •Ksenia Korshunova and Wichard J. D. Beenken — Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany

We have investigated the structure of Zn-porphyrin-indolocarbazole conjugates with a different number of indolocarbazol meso-substituents without and with THF and DMF axial ligands by quantumchemical methods in order to interpret experimental data such as Absorption spectra, fluorescence lifetime and quantum yields in different solutions. Contrarily to our expectations, we found very weak deformation the Zn-porphyrin macrocycle under the in uence of axial THF and DMF ligands, which only tend to pull the central Zn-atom out of its equilibrium position in the macrocycle plane. This means that the very different fluorescence yields for Zn-porphyrin-indolocarbazoles in toluole, THF, and DMF cannot be explained by a conformational change.

HL 21.2 Mon 15:15 ZEU 222

Estimating Coulomb model parameters in organic molecules from first principles — •Irina Petreska[1,2], Ljupco Pejov[2], Ljupco Kocarev[3,4], 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 — [3]Macedonian Academy of Sciences and Arts, Skopje, Republic of Macedonia — [4]Faculty of Computer Science and Engineering, Ss. Cyril and Methodius University, 1 000 Skopje, Republic of Macedonia

The Coulomb parameters are estimated from electronic structure calculations based on Density Functional Theory (DFT). Of particular interest are phenylene ethynylene oligomers exhibiting electric-field controlled conductance switching. The charge transport properties are analyzed adopting a simplified two-site model accounting for Coulomb correlation effects. The Coulomb parameters are deduced from a population analysis. The DFT calculations employ a combination of the Becke's three parameter adiabatic connection exchange functional (B3) with the Lee-Yang-Parr correlation one (LYP). The Kohn-Sham SCF equations are iteratively solved using the LANL2DZ basis set, for orbital expansion, on an "ultrafine" grid for numerical integration.

HL 21.3 Mon 15:30 ZEU 222

Theoretical Study of Simultaneous Electron- and Excitation Energy Transfer in a Fullerene-Chromophore Complex — •Thomas Plehn, Jörg Megow, and Volkhard May — Humboldt-Universität zu Berlin, Germany

Mainly during the last decade fullerene based molecular systems have been of increasing interest with regard to future components in dye sensitized solar cells and artificial photosynthetic systems. This theoretical study focuses on the characteristic photoinduced charge separation process in a supramolecular complex containing a single fullerene and six pyropheophorbide-a molecules. For this purpose the excitation energy transfer processes are treated among the six chromophores. Simultaneously electron transfer takes place from the excited chromophores to the fullerene. The whole investigation uses molecular dynamics simulations of the highly flexible complex in explicit solvent environment. The transfer phenomena are described in terms of a special mixed quantum-classical version of the Förster- [1] and the well-known classical Marcus rate. Finally the charge separation process is computed concerning an ensemble of complexes. The resulting dynamics are in very good agreement with appropriate experimental data [2].

[1] J. Megow et al., ChemPhysChem 2011, 12 645-656

[2] M. Regehly et al., J. Phys. Chem. B 2007, 111, 998

Invited Talk HL 21.4 Mon 15:45 ZEU 222

Controlled crystallization of semiconducting polymer thin films — •Sabine Ludwigs — Institute for Polymer Chemistry, University of Stuttgart, Germany

The talk will give an overview over current activities in my team on the morphological control of semiconducting polymers for applications in polymer electronics. Different methods to induce and control crystalline order over large areas in thin films will be presented. These include swelling and deswelling in defined solvent vapour atmospheres of good solvents and crystallization under confinement and with external fields. Regarding polymer materials we are currently extending our studies from conventional p-type semiconductors based on pure thiophenes like P3HT[1] to high performance p-type low bandgap polymers such as PCPDTBT[2] and n-type polymers such as PNDI2OD-2T[3]. The control of molecular orientation over macroscopic distances allows us to study the relationship between the polymer microstructure and the resulting charge transport properties along specific crystallographic directions.

[1] E. Crossland, K. Tremel, F.S.U. Fischer, K. Rahimi, G. Reiter, U. Steiner, S. Ludwigs, Adv. Mater. 2012, 24, 838. [2] F.S.U. Fischer, K. Tremel, A.-K. Saur, S. Link, N. Kayunkid, M. Brinkmann, D. Herrero-Carvajal, J. T. López Navarrete, M. C. Ruiz Delgado, S. Ludwigs, Macromolecules 2013, 46, 4924. [3] K. Tremel, F.S.U. Fischer, N. Kayunkid, R. DiPietro, R. Tkachov, A. Kiriy, D. Neher, S. Ludwigs, M. Brinkmann, Charge Transport Anisotropy in Highly Oriented Thin Films of the Acceptor Polymer P(NDI2OD-T2), submitted.

15 min break

HL 21.5 Mon 16:30 ZEU 222

Conjugated oligomers near surfaces with different physical and chemical nature: MD simulation of adsorption layers — •Olga Guskova[1] and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, D-01069 Dresden — [2]Techische Universität Dresden, Institut für Theoretische Physik, Zellescher Weg 17, D-01062 Dresden

Atomistic molecular dynamics simulations are used to explore some general principles of 2D supramolecular organization of conjugated oligomers on adsorbing substrates. Two systems are studied: (i) terminally substituted dicyanovinyl quaterthiophenes, prototypic absorbers for small molecule organic solar cells on a silica surface [1] and (ii) 2,5-dialkoxy-phenylene-thienylene-based oligomers on epitaxial monolayer graphene [2]. We demonstrate that the driving force of molecular orientation on substrate is embodied by the chemical nature of the surface and the character and position of functional groups the conjugated molecule bearing, i.e. the underlying balance of forces defines the spatial orientation - standing upright or lying-down molecules on substrates. This force balance clearly allows isolated molecules to explore flat, bent or twisted molecular conformations and to exploit force anisotropies to maximize their interactions when crystals are growing.

[1] O.A. Guskova et al. // J. Phys. Chem. C 2013. V. 117. P. 17285. [2] R. Shokri et al. // J. Am. Chem. Soc. 2013. V. 135. P. 5693.

HL 21.6 Mon 16:45 ZEU 222

Frank elastic constants in nematic mesophases of polymeric semiconductors — •Patrick Gemünden, Kurt Kremer, and Kostas Ch. Daoulas — Max Planck Institute for Polymer Research, Mainz

Liquid crystalline (LC) mesophases of polymeric semiconductors[1] can facilitate material processing. We develop a particle-based modeling approach considering poly(alkylthiophenes) as a test system for studying nematic mesophases. The method uses "soft tube" representations of chains where non-bonded potentials are defined by soft, directional interactions.[2,3] Here, we focus on Frank elastic constants (FC). Calculating FCs is important for comparing material properties from the soft model with experiments, studying theoretical questions related to FCs in polymer nematics and linking particle-based and continuum descriptions of LCs. We calculate FCs related to bend, splay and twist deformations from the fluctuations of the local nematic director. Indeed, the magnitudes of the FCs from our simulations agree with experiments on polymer nematics. We study the dependence on system parameters, e.g. chain length, and compare with predictions by analytical field theory.[4] Eventually we study local density fluctuations in the nematic samples, which, as predicted by theory, lead to an anisotropic scattering pattern and can be related to the elastic properties.

[1] Ho et al., Macromolecules 43, 7895 (2010) [2] Gemünden et al.,

Macromolecules 46, 5762 (2013) [3] Daoulas et al., J. Phys.: Condens. Matter 24, 284121 (2012) [4] Le Doussal & Nelson, Europhys. Lett. 15, 161 (1991)

HL 21.7 Mon 17:00 ZEU 222

Modeling LC mesophases in polymeric semiconductors with soft directional interactions — Patrick Gemünden, Carl Poelking, Kurt Kremer, Denis Andrienko, and •Kostas Daoulas — Max Planck Institute for Polymer Research, Mainz

Often in Soft Matter mesoscale behavior couples across a hierarchy of scales to details of molecular architecture and interactions. When modeling such materials, features accounting for the latter must be included even in drastically coarse-grained (CG) representations. Focusing on liquid crystalline (LC) mesophases of polymeric semiconductors, we highlight a top-down strategy for developing such models, projecting classical density functionals on particle-based representations. Poly(3-alkylthiophenes) (P3AT) are considered as an example. Two different CG models are developed, representing: a) the polymer chain with a "soft" flexible tube [1] and b) each alkylthiophene as a plate-like object [2]. The first describes uniaxial nematics and the second captures biaxial nematic ordering, mimicking effects of anisotropy in microscopic interactions and chain architecture. We demonstrate that the model reproduces realistic material properties in nematic mesophases. In biaxial morphologies we discuss how collective orientation and planarization of molecules affects the lengths of conjugated segments, defined via conjugation-breaking torsional defects [3]. First results on the interplay between nematic ordering and phase separation in blends of P3AT with nanoparticles are presented.[1] Daoulas et al, J. Phys.: Condens. Matter (2012) 24, 284121 [2] Gemünden et al, Macromolecules (2013) 46, 5762 [3] Rühle et al, J. Chem. Phys. (2010) 32, 134103.

HL 21.8 Mon 17:15 ZEU 222

Correlating structural order and morphology with transport properties in donor-acceptor block copolymers for organic photovoltaics — •Gaurav Gupta[1], Chetan Raj Singh[2], Ruth Lohwasser[3], Peter Muller Buschbaum[4], Mukundan Thelekkat[3], Harald Hoppe[2], and Thomas-Thurn Albrecht[1] — [1]Martin-Luther-Universität Halle-Wittenberg,Germany — [2]Technische Universität Ilmenau, Germany — [3]University of Bayreuth,Germany — [4]Technische Universität München,Germany

Microphase separated donor-acceptor block copolymers are promising systems for morphology control in OPV's. A nanostructure on exciton diffusion length scale, crystalline order and percolating pathways for charge transport are pre-requisites for obtaining good device properties. We here present a systematic study of the correlation between structure and charge transport in thin films of P3HT-b-PPerAcr after different thermal treatments. Combining AFM, microscopy and GISAXS we show that films annealed in the melt state above the melting temperatures of both components form typical microphase separated structures oriented parallel to the substrate, while films crystallized from the disordered state as obtained from spin coating show no well-defined microphase separated structures. GIWAXS measurements reveal that crystallization from the ordered state leads to strongly textured samples. Charge carrier mobilities as measured by SCLC were improved by 2 orders of magnitude in films crystallized from the disordered state, the unfavorable orientation of the microphase morphology in melt annealed films resulted in poor device performance.

HL 21.9 Mon 17:30 ZEU 222

Origins of Reduced Nongeminate Recombination in P3HT:PCBM Organic Solar Cells — •Michael C. Heiber[1], Julien Gorenflot[1], Vladimir Dyakonov[1,2], and Carsten Deibel[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

Understanding the nongeminate recombination processes that are the dominant loss mechanisms in organic solar cells is critical to improving device performance. In P3HT:PCBM blends, nongeminate recombination has been found to be significantly slower than expected from Langevin theory and also exhibits super-second order kinetics. Several theories for this behavior have been proposed, but a complete model has not yet been reached. To shed light on this problem, we have used a combination of transient absorption spectroscopy experiments and kinetic Monte Carlo simulations. By modeling the temperature dependence of the polaron transients measured in both neat P3HT films and annealed P3HT:PCBM blend films, we demonstrate the effects of phase separation, carrier trapping, and charge transfer states on the magnitude of the recombination rate. Furthermore, we show that while neat P3HT films exhibit second order recombination and mobility behavior indicating a Gaussian density of states (DOS), P3HT:PCBM blends are complicated by super-second order recombination that is indicative of an exponential DOS and mobility measurements that are consistent with a Gaussian DOS. To unify these observations, we show that a separate distribution of charge transfer states must be included.

HL 21.10 Mon 17:45 ZEU 222

Model systems for interchromophoric interactions in conjugated polymer materials — •Thomas Stangl[1], Daniela Schmitz[2], Klaas Remmerssen[2], Dominik Würsch[1], Florian Steiner[1], Sigurd Höger[2], Jan Vogelsang[1], and John Lupton[1] — [1]Universität Regensburg, Regensburg, Deutschland — [2]Universität Bonn, Bonn, Deutschland

A set of pi-conjugated oligomer dimers templated in molecular scaffolds is presented as a model system of the interactions between chromophores in conjugated polymers. Single-molecule spectroscopy was used to reveal electronic aggregation between two oligomers with different well-defined distances and single polymer chains. It is concluded that the model systems can be used to investigate the impact of H-aggregation as a function of interchromophoric distance by simultaneous measurement of lifetime and single-molecule spectra. This reveals a strong heterogeneity in coupling strengths even for identical single molecules. Further, it is shown that the coupling strength varies over time on a single molecule, leading to the conclusion that electronic aggregation has to be understood as a dynamic property. In bulk polymer films, such interchromophoric coupling impacts the functionality, e.g. the emission color and the migration of excitation energy to quenching sites. Realizing the presence and dynamics of such interactions is crucial for understanding limitations in quantum efficiency of larger conjugated polymer materials.

HL 22: Invited Talk Emil List-Kratochvil

Time: Monday 15:30–16:00 Location: POT 006

Invited Talk HL 22.1 Mon 15:30 POT 006

Unveiling the origin of resistive switching in organic electronic devices — •Emil J.W. List-Kratochvil — NanoTecCenter Weiz Forschungsgesellschaft mbH Franz-Pichler-Straße 32 A-8160 Weiz, Austria — Institute of Solid State Physics, TU Graz, Petersgasse 16, Graz, Austria

Electrically tunable resistors realized in two terminal structures seem to be one of the most versatile innovations in the semiconductor industry with many possible applications such as logic circuitry or neuromorphic systems. In particular, inorganic resistive switching devices utilized as memories are close to commercialization. Restive switching was observed from many organic devices as well, however despite vital academic interest a consistent explanation about their working mechanisms is still missing. Different models are proposed in this relation, most commonly a) charging/discharging of metallic particles in the an organic matrix and the related formation of a space charge field capable of influencing current injection and b) the formation of highly conductive filaments. We herein present a set of experiments to explain unipolar resistance switching. For the first we are able to unambiguously rule out all charging based models which were held to be responsible for the switching in organic devices and show that the memory behaviour can be interpreted as the formation and rupture of a conductive filament. We demonstrate that unipolar resistive switching is a universal and largely material independent property in electrode/organic/electrode thin-film structures.

HL 23: Quantum wires: Transport properties (with TT)

Time: Monday 16:00–17:45 Location: POT 006

HL 23.1 Mon 16:00 POT 006

Strongly interacting holes in Ge/Si core/shell nanowires — •Franziska Maier, Tobias Meng, and Daniel Loss — Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland

We consider holes confined to the core of Ge/Si core/shell nanowires subject to strong Rashba spin-orbit coupling and screened Coulomb interactions. We find that both, spin-orbit coupling and Coulomb interactions, are largely dependent on wire radius, shell-induced strain and the magnitude of applied electric fields. This tunability allows to drive the system from a Luttinger liquid phase towards a Wentzel-Bardeen singularity.

HL 23.2 Mon 16:15 POT 006

***In-situ* x-ray diffraction during MBE growth of InAs nanowires on Si** — •Andreas Biermanns[1], Anton Davydok[1], Emmanouil Dimakis[2,3], Masamitu Takahasi[4], Takuo Sasaki[4], Lutz Geelhaar[2], and Ullrich Pietsch[1] — [1]Universität Siegen, Festkörperphysik, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [4]Quantum Beam Science Directorate, Japan Atomic Energy Agency, Hyogo, Japan

Compared to the vapor-liquid-solid growth modes of group III-V semiconductor nanowires (NWs), e.g. Au-assisted growth or the self-assisted growth of GaAs NWs, it is a matter of intense debate whether or not liquid Indium is involved during the self-assisted growth of InAs NWs. Here, we present the results of an *in-situ* study of the nucleation phase of InAs NW growth on Si (111). X-ray scattering and diffraction methods have been employed during NW-growth at the synchrotron beamline 11XU at SPring-8 using a MBE chamber integrated with a surface diffractometer. The characteristic scattering signals from liquid In as well as the diffracted intensity of the crystalline NWs growing in the wurtzite (WZ) phase have been monitored during growth. We find that liquid In is present during the initial stage of growth, associated with the formation of extended WZ segments in the NWs. After the nucleation phase of the NWs, the liquid In vanishes, accompanied by a more defective crystal structure with a large number of stacking faults. The results are in accordance with a growth model, predicting a transition from locally In-rich to locally As rich conditions.

HL 23.3 Mon 16:30 POT 006

Ga droplet templates: Density control of self-assisted GaAs nanowires — •Hanno Küpers, Faebian Bastiman, Claudio Somaschini, and Lutz Geelhaar — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin

The self-assisted growth of GaAs nanowires (NWs) on Si is a popular approach for integrating III-V materials on Si. However, growth on unpatterned Si substrates suffers from a lack of control over nanowire density and a high degree of parasitic growth. We report on a new two-step NW density control technique for self-assisted GaAs nanowires grown on Si(111) by molecular beam epitaxy. The first step involves pre-depositing Ga on the substrate utilising a relatively high Ga flux at elevated temperatures. The Ga droplet density can be controlled by changing the magnitude of the Ga flux and the duration of the Ga pre-deposition time. The resulting Ga droplet template provides selective density control for ensuing NW growth. In this second step a maximum of 50% of the Ga droplets can be successfully converted into vertical NWs. The magnitude of the As flux and the size distribution of the Ga droplets underpins both the observed NW yield and the type of parasitic growth. A 10% improvement in the vertical yield can be gained by including a droplet ripening step before As flux exposure in order to narrow the droplet size distribution, but the Gaussian nature of the distribution prevents access to a 100% vertical yield.

HL 23.4 Mon 16:45 POT 006

Transport measurements of ballistic quantum wires exposed to two magnetic spikes. — •Bernd Schüler[1], Mihai Cerchez[1], Hengyi Xu[1], Thomas Heinzel[1], and Andreas Wieck[2] — [1]Heinrich-Heine-Universität, 40225 Düsseldorf, Germany — [2]Ruhr-Universität, 44780 Bochum, Germany

Quantum point contacts (QPC) are still fascinating elementary structures, which can lead in combination with localized magnetic fields to quite interesting effects [A. Tarasov et al., Phys. Rev. Lett. 104, 186801 (2010)]. We have designed a ferromagnet/semiconductor hybrid structure device which consists of a combination of an AFM-defined QPC and localized magnetic fields in the form of two magnetic spikes (magnetic barriers) at sub-micron distances inside the channel. The transport measurements are performed in the open regime of the QPC as function of a superimposed, homogeneous perpendicular magnetic field and as function of the barrier height. On top of the mode depopulation we found transmission resonances which could be explained with theoretically predicted signatures of zero-dimensional states weakly bound by the magnetic field [H. Xu et al. Phys. Rev. B 84, 035319 (2011)].

HL 23.5 Mon 17:00 POT 006

Resistance profiling of freestanding GaAs nanowires by multitip STM — •Stefan Korte[1], Matthias Steidl[2], Hubertus Junker[1], Weihong Zhao[2], Werner Prost[3], 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

Due to their specific one-dimensional geometry, III-V semiconductor nanowires are promising candidates for future optoelectronic devices. However, for the fabrication of novel high performance nanowire devices a precise control of doping profile is indispensable. We use a multitip STM as nanoprober to reveal the electrical transport properties of freestanding GaAs nanowires. *p*-doped GaAs nanowires are grown by Au-assisted metal-organic vapor-phase epitaxy (MOVPE) on GaAs(111)B and GaP(111)B substrates. Conductance profiles along the nanowires were obtained with four point probe measurements. Nanowires grown on different substrates, using a two temperature step growth mode or constant substrate temperature, all exhibit highly nonlinear axial resistance profiles.

HL 23.6 Mon 17:15 POT 006

Investigation of the electrical properties of freestanding Zn-doped GaAs nanowires by a multitip STM — •Matthias Steidl[1], Hubertus Junker[2], Weihong Zhao[1], Stefan Korte[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

The specific geometry of III-V semiconductor makes III-V semiconductor nanowires (NWs) to promising building blocks for novel semiconductor devices in future electronic and opto-electronic applications. In this context a homogeneous distribution of the dopant over the whole NW is of great importance. We have grown p-type Zn-doped GaAs-NWs 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 apply a multitip STM as a nanoprober and conduct four-point probe measurements on single free-standing NWs. With this technique we are able to measure resistance profiles with a high spatial resolution over almost the whole length of a nanowire. These measurements reveal that the resistivity is both dependent on the growth condition and the part of the NW. Generally, the resistivity at the NW base is orders of magnitude larger compared to the upper part of the NW.

HL 23.7 Mon 17:30 POT 006

Investigation of top-gated InAs nanowires with HfO_2 dielectric — •Marion Rosien[1,2], Torsten Rieger[1,2], Sebastian Heedt[1,2], Torsten Jörres[1,2], Thomas Schäpers[1,2], Detlev Grützmacher[1,2], and Mihail Ion Lepsa[1,2] — [1]Peter Grünberg Institute - 9, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology

Electrical characteristics of top-gated InAs nanowire field effect transistors (FETs) with HfO_2 high-k gate dielectric are presented. The nanowires with diameters of about 60 to 80 nm are grown by molecular beam epitaxy (MBE) and coated with HfO_2. The HfO_2 is deposited ex-situ by atomic layer deposition (ALD), which benefits from a high conformity and a good thickness control. To investigate the impact of the gate, the oxide thickness is varied between 2 and 8 nm. Transfer times between the MBE and ALD are kept as short as possible to avoid any contamination. The nanowires are individually contacted by Ti/Au electrodes. The HfO_2 acts as an omega shaped gate dielectric with Ti/Au gate metal. The quality of the oxide and the interface between the nanowire and the dielectric is analyzed by DC electrical measurements of the FETs. In order to derive transport parameters from the measurements, the capacitance of the top gate is simulated for each individual nanowire. The carrier mobility and concentration, peak transconductance and the on/off ratio are presented and discussed.

HL 24: Topological insulators: mostly interaction with magnetic fields (with MA/TT)

Time: Monday 15:45–17:45 Location: POT 081

HL 24.1 Mon 15:45 POT 081

SQUID devices built form S-TI-S junctions based on mercury telluride (HgTe) — •Luis Maier, Manuel Grimm, Christopher Armes, Christoph Brüne, Hartmut Buhmann, and Laurens W. Molenkamp — Physikalisches Institut (EP3), Universität Würzburg, 97074 Würzburg

In the search for Majorana fermions, one way to show their existence requires an interface of a s wave superconductor and a strong topological insulator (TI) [1]. It has already been shown, that a three-dimensional, strained layer of HgTe shows dominant surface conductance in magnetotransport measurements and thus is considered as a 3D-TI [2]. Here we investigate the interaction of superconducting contacts with Dirac Fermions.

S-TI-S junctions based on HgTe and Nb have already been fabricated and characterized successfully [3]. As a next step in this research we created SQUID structures to further study the current phase relation in these special devices. In this talk we are going to present our recent results searching for deviations from normal behaviour that could point to TI or Majorana interactions.

[1] L. Fu and C. L. Kane, Phys. Rev. Lett. 100, 096407 (2008)
[2] C. Brüne et al., Phys. Rev. Lett. 106, 126803 (2011)
[3] J. Oostinga et al., Phys. Rev. X 3, 021007 (2013)

HL 24.2 Mon 16:00 POT 081

Quantum Interferences of Dirac fermions in Bi2Se3 nanostructures — •Louis Veyrat, Joseph Dufouleur, Romain Giraud, Hannes Funke, Silke Hampel, Christian Nowka, Joachim Schumann, and Bernd Büchner — IFW-Dresden, Dresden, Germany

Recently discovered Z2 topological insulators (TIs) are ideally conducting at their interface only, where a gapless band structure forms. In a strong 3D TI, such as Bi2Se3, surface states are spin-chiral Dirac fermions with an odd number of Dirac cones. However, in real materials, the finite bulk conductivity often prevents the study of surface-state transport. We show that mesoscopic transport measurements can unambiguously reveal the specific properties of spin-chiral Dirac fermions in a Bi2Se3 nanostructure [1]. The quantum conductance of a nanowire exhibits Aharonov-Bohm oscillations which result only from surface-state transport. At very low temperatures, the temperature dependence of their amplitude unveils the quasi-ballistic nature of charge transport, which is the signature of the weak coupling of quasi-particles to their environment. Our results further reveal the weak scattering by structural disorder, giving another evidence of the specific nature of spin-chiral Dirac fermions in a strong 3D TI. Furthermore, new physics evidenced in the study of UCF in a nanowire, could be the signature of a perfectly transmitted mode in a nanowire geometry [2].

[1] J. Dufouleur et al., Phys. Rev. Lett. 110, 186806 (2013)
[2] J. Bardarson et al., Phys. Rev. Lett. 105, 156803 (2010)

HL 24.3 Mon 16:15 POT 081

Thermal and Electrical Transport of Single-Crystalline Bismuth Telluride Nanowires — •Bacel Hamdou[1], Johannes Kimling[1], Johannes Gooth[1], August Dorn[1], Eckhard Pippel[2], Raimar Rostek[3], Peter Woias[3], and Kornelius Nielsch[1] — [1]Institute of Applied Physics, University of Hamburg, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany — [3]Department of Microsystems Engineering, University of Freiburg, Germany

Bi_2Te_3 is a topological insulator (TI), a phase of matter that has a bulk bandgap and gapless electronic surface states protected by time-reversal symmetry. Studying topological surface states via electrical transport measurements is still very difficult due to large bulk contribution to conductivity originating from unintentional doping and the small bulk band gaps, which are typical for TI materials. We report on thermal and electrical transport measurements on individual single-crystalline bismuth telluride nanowires (NWs), synthesized via catalytic growth and post-annealing in a Te-rich atmosphere. The resulting Bi_2Te_3 NWs show reproducible electronic transport properties that are close to those of intrinsic bulk Bi_2Te_3. Further, magnetoresistance measurements were performed at temperatures down to 2 K. The parallel magnetoresistance curves exhibit Aharonov-Bohm oscillations, which indicate the presence of topological surface states. Analyses of Subnikov-de Haas oscillations in perpendicular magnetoresistance yield extremely low two-dimensional carrier concentrations and effective electron masses, and very high carrier mobilities.

HL 24.4 Mon 16:30 POT 081

Ambipolar quantum Hall effect in strained bulk HgTe — •Cornelius Thienel, Jonas Wiedenmann, Steffen Wiedmann, Christoph Brüne, Christopher Ames, Hartmut Buhmann, and Laurens W. Molenkamp — Universität Würzburg, Experimentelle Physik III

Strained bulk HgTe has been identified as three-dimensional topological insulator [Phys. Rev. Lett. **106**, 126803 (2011)]. A Dirac-specific quantum Hall sequence can unambiguously be demonstrated in transport measurements. Furthermore we identify two subsets of Landau levels that originate from the topological surface states.
Improving the quality of the interfaces hosting the surface states by introducing additional buffer and cap layers to the structure increases the carrier mobilities in the topological states and makes it possible to observe the quantum Hall effect of electrons and holes in a wide gate voltage range. The detection of p-type QHE points towards a suppressed interaction between bulk and surface states.

HL 24.5 Mon 16:45 POT 081

Weak antilocalization effects in systems with Dirac-like energy dispersion — •Andreas Budewitz, Mathias Mühlbauer, Bastian Büttner, Grigory Tkachov, Ewelina M. Hankiewicz, Christoph Brüne, Hartmut Buhmann, and Laurens W. Molenkamp — Universität Würzburg, Lehrstuhl für experimentelle Physik III

HgTe quantum wells (QW) have been identified as topological insulator (TI) by appearence of the QSHE [1]. It has been shown that the band structure of HgTe QWs has to be described by a four band model revealing a Dirac like dispersion [2, 3]. Here now we investigate the weak antilocalization (WAL) effect in various n-conducting HgTe QWs. We analyse the magnetoresistance of a set of quasi one-dimensional wires and clearly observe different WAL amplitudes for normal and inverted band ordering which does not depended on the structural inversion asymmetry (SIA). The data demonstrate that a non-universal Berry phase which exceeds π, the characteristic value for gapless Dirac fermions, is needed to explain the different observations in our measurements.

[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] B. A. Bernevig, T. L. Hughes and S. C. Zhang, Science 318, 1757 (2006)
[3] B. Büttner, C.-X. Liu, G. Tkachov, E. G. Novik, C. Brüne, H. Buhmann, E. M. Hankiewicz, P. Recher, B. Trauzettel, S.-C. Zhang, and L. W. Molenkamp, Nature Phys. 7, 418 (2011)

HL 24.6 Mon 17:00 POT 081

Giant Photocurrents in a Dirac Fermion System at Cyclotron Resonance — •C. Zoth[1], P. Olbrich[1], P. Vierling[1], K.-M. Dantscher[1], G.V. Budkin[2], S.A. Tarasenko[2], V.V. Bel'kov[2], D.A. Kozlov[3], Z.D. Kvon[3], N.N. Mikhailov[3], S.A. Dvoretsky[3], and S.D. Ganichev[1] — [1]Terahertz Center, Regensburg, Germany — [2]Ioffe Institute, St. Petersburg, Russia — [3]Institute of Semiconductor Physics, Novosibirsk, Russia

We report on the observation of giant photocurrents in HgTe/HgCdTe quantum wells (QW) of critical thickness at which a Dirac spectrum emerges [1]. Exciting QW of 6.6 nm width by terahertz radiation and varying an external magnetic field we detected a resonant photocurrent. Remarkably, the position of the resonance can be tuned from negative (-0.4 T) to positive (up to 1.2 T) magnetic fields by means of optical doping. The photocurrent data, accompanied by measurements of radiation transmission, as well as, magnetotransport, prove that the photocurrent is caused by cyclotron resonance in a Dirac fermion system. This allows us to obtain the effective electron velocity $v \approx 7.2 \times 10^5$ m/s. We develop a microscopic theory of the effect and show that the inherent spin-dependent asymmetry of light-matter coupling in the system of Dirac fermions causes the electric current to flow.

[1] P. Olbrich, C. Zoth, P. Vierling *et al.*, *PRB* **87**, 235439 (2013)

HL 24.7 Mon 17:15 POT 081

Quantum Oscillations of Photogalvanic Effect and Spin Orbit Interaction Effect in HgTe Quantum Wells — •K.-M. Dantscher[1], C. Zoth[1], P. Olbrich[1], V.V. Belkov[2], M.A. Semina[2], M.M. Glazov[2], L.E. Golub[3], D.A. Kozlov[3], Z.D. Kvon[3], N.N. Mikhailov[3], S.A. Dvoretsky[3], and S.D. Ganichev[1] — [1]University of Regensburg, Regensburg, Germany — [2]Ioffe Institute, St. Petersburg, Russia — [3]Institute of Semiconductor Physics, Novosibirsk, Russia

We report on the observation of quantum oscillations in HgTe/HgCdTe quantum well (QW) structures of different widths, which are characterized by an inverted, normal and even Dirac like bandstructure [1,2]. Exciting the QWs by terahertz radiation and sweeping an external magnetic field we observed a resonant photocurrent [3] which shows pronounced oscillations. The photocurrent data are accompanied by measurement of photoconductivity, radiation transmission, as well as, magneto-transport. A comparison of the results shows that the photosignal is enhanced at cyclotron resonance position and is modulated by Shubnikov-De Haas oscillations. Furthermore we present a microscopic model of a magnetic field dependent oscillating current taking into account the oscillations of spin polarization and of conductivity.

[1] Z.D. Kvon *et al.*, *JETP Letters* **94**, 816-819 (2011)
[2] A. Bernevig *et al.*, *Science* **314**, 1757 (2006)
[3] P. Olbrich *et al. Phys. Lett B* **87**, 235439 (2013)

HL 24.8 Mon 17:30 POT 081

Strong Out-of-Plane Magnetic Anisotropy of Fe Adatoms on Bi_2Te_3 — •Thomas Eelbo[1], Marta Waśniowska[1], Marcin Sikora[2], Michal Dobrzański[2], Andrzej Kozlowski[2], Artem Pulkin[3], Gabriel Autès[3], Ireneusz Miotkowski[4], Oleg Yazyev[3], and Roland Wiesendanger[1] — [1]Institute of Applied Physics, University of Hamburg, Germany — [2]Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Krakow, Poland — [3]Institute of Theoretical Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland — [4]Department of Physics, Purdue University, West Lafayette, USA

Topological insulators (TIs) are currently in the focus of fundamental physics. The interaction of magnetic impurities with TIs is widely unexplored on the local scale and might potentially entail interesting properties of the TIs in view of applications in spintronics. To this end, we studied the structural, electronic, and magnetic properties of individual Fe atoms adsorbed on a $Bi_2Te_3(111)$ surface by means of scanning tunneling microscopy/spectroscopy (STM/STS), X-ray absorption spectroscopy and X-ray magnetic circular dichroism (XMCD) at low temperatures. STM reveals the existence of two different Fe species. Density functional theory-based calculations let us assign these to atoms adsorbed on the fcc/hcp hollow sites. STS proves the existence of characteristic resonances for each type and XMCD evidences a strong magnetic out-of-plane anisotropy of the Fe moments in agreement with our calculations.

HL 25: Transport: Quantum dots, quantum wires, point contacts II (organized by TT)

Time: Monday 16:00–18:30 Location: HSZ 204

HL 25.1 Mon 16:00 HSZ 204

A two-atom electron pump — Benoit Roche[1], Roman-Pascal Riwar[1], Benoit Voisin[1], Eva Dupont-Ferrier[1], Romain Waquez[3], Maud Vinet[3], Marc Sanquer[1], •Janine Splettstoesser[2], and Xavier Jehl[1] — [1]SPSMS, UMR-E, CEA Grenoble, INAC, Grenoble, France — [2]MC2, Chalmers University of Technology, Göteborg, Sweden — [3]CEA, LETI, MINATEC, Grenoble, France

In recent years there has been a lot of interest in time-dependently driven quantum systems, such as quantum-dot pumps, both in the adiabatic regime of slow driving as well as in the high-frequency regime. However, all experiments so far were carried out in either one of these regimes, but were not subsequently tuned to both. I will present an experimental realization [1] of electron pumping through two phosphorus donors in series implanted in a silicon nanowire. While quantized pumping is achieved in the low-frequency adiabatic regime, remarkable features are observed at higher frequency, when the charge transfer is limited either by the tunnelling rates to the electrodes or between the two donors. We model the transitions between quantum states involving a Landau-Zener transition, allowing to reproduce in detail the characteristic signatures observed in the non-adiabatic regime. Interestingly, the breakdown of the adiabatic limit can thus accurately be associated to the relation of the respective time-scales of tunneling to the electrodes or between the donors, compared to the time-scales of the driving. Consequently, information on the time-scales can be extracted from a detailed inspection of the pumping signal.

[1] B. Roche, *et al.*, Nat. Commun. 4, 1581 (2013)

HL 25.2 Mon 16:15 HSZ 204

Functional renormalization group in Floquet space and its application to periodically driven quantum dots — •Katharina Eissing[1,2], Stefan Göttel[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 (RG) was recently extended to study interacting, low-dimensional systems out of equilibrium. This includes correlated quantum dot setups with explicitly time-dependent Hamiltonians as e.g. realized in quantum quenches or in the presence of time-dependent bias voltages [Phys. Rev. B 85, 085113 (2012), Phys. Rev. B 85, 245101 (2012)]. However, following this route periodic pumping processes, which are of particular interest in e.g. nanoelectronics and quantum information science, can only be described in an inefficient way. Taking advantage of the periodicity, we combine the Floquet theorem with the functional RG. This allows us to transform the double-time self-energy and Green functions in the Floquet basis [J. Phys.: Condens. Matter 20 085224] and the functional RG treatment resembles the stationary formalism. This makes it feasible to study transport in periodically driven systems. In my talk, I will shortly introduce this Floquet theorem based functional RG and present first results on transport through a quantum dot described by the interacting resonant level model.

HL 25.3 Mon 16:30 HSZ 204

Interplay of edge state polarization and a Zeeman split quantum dot — •Benedikt Probst[1], Pauli Virtanen[2], and Patrik Recher[1] — [1]Institute for Mathematical Physics, TU Braunschweig, Braunschweig, Germany — [2]O.V. Lounasmaa Laboratory, Aalto University, Finland

Topological insulators are a novel state of matter showing interesting physics. One of the effects realized in these materials is the quantum spin Hall effect in which electrons with different spin propagate in different directions on the edge of the system. Applying a bias to the system therefore leads to a spin bias for the edge state. We consider

a system in which a quantum dot in the Coulomb blockade regime is attached to a helical Luttinger liquid. This quantum dot is treated as a localized spin, which can be manipulated by a magnetic field. The dynamics of the dots are described by setting up a general master equation. From the steady state of the system the polarization of the dot and the differential edge conductance is calculated. We discuss a regime in which the dot polarization exhibits a strong bias dependence and a regime in which the transport shows a characteristic bias asymmetry which allows to identify the relative orientation of the spin polarization in the edge state with respect to the magnetic field.

15 min. break.

HL 25.4 Mon 17:00 HSZ 204

Entanglement detection in an interacting beam-splitter device — •Alexander Schroer[1], Bernd Braunecker[2], Alfredo Levy Yeyati[3], and Patrik Recher[1] — [1]Institute for Mathematical Physics, TU Braunschweig, Germany — [2]Department of Theoretical Condensed Matter Physics, Universidad Autónoma de Madrid, Spain — [3]School of Physics & Astronomy, University of St Andrews, UK

We investigate a tunnel contact between two Luttinger liquids, e.g. realized as two crossed one-dimensional nanowires. When injecting one of two electrons with opposite spin in each wire, the current measured behind the crossing differs for singlet, triplet or product states. This is an apparent non-Fermi liquid feature because the current has been shown to be independent of spin-entanglement for Fermi liquid beam-splitters before. It can be understood in terms of collective excitations and by taking spin-charge separation into account. This behavior may offer an easier alternative to traditional entanglement detection schemes based on current noise, which turns out to be suppressed by the electron-electron interaction.

HL 25.5 Mon 17:15 HSZ 204

Hierarchical Equation of Motion Investigation of Decoherence and Relaxation Dynamics in Nonequilibrium Transport through Interacting Quantum Dots — •Rainer Härtle[1,2], Guy Cohen[3], David R. Reichman[3], and Andrew J. Millis[2] — [1]Institut für theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany — [2]Department of Physics, Columbia Universtiy, New York, USA — [3]Department of Chemistry, Columbia Universtiy, New York, USA

A recently developed hierarchical quantum master equation approach [1,2] is used to investigate nonequilibrium electron transport through an interacting double quantum dot system in the regime where the inter-dot coupling is weaker than the coupling to the electrodes. The corresponding eigenstates provide tunneling paths that may interfere constructively or destructively, depending on the energy of the tunneling electrons [3]. Electron-electron interactions are shown to quench these interference effects in bias-voltage dependent ways, leading, in particular, to negative differential resistance, population inversion and an enhanced broadening of resonances in the respective transport characteristics [2]. Relaxation times are found to be very long, and to be correlated with very slow dynamics of the inter-dot coherences. The ability of the hierarchical quantum master equation approach to access very long time scales is crucial for the study of this physics.

[1] J. Jin *et al.*, J. Chem. Phys. 128, 234703 (2008).
[2] R. Härtle *et al.*, arXiv:1309.1170 (2013)
[3] R. Härtle *et al.*, Phys. Rev. B 87, 085422 (2013)

HL 25.6 Mon 17:30 HSZ 204

Detection of the decay rates in interacting quantum dots — •Jens Schulenborg[1,2], L. Debora Contreras- Pulido[3], Michele Governale[4], and Janine Splettstoesser[1,2] — [1]Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, Göteborg, Sweden — [2]Institut für Theorie der Statistischen Physik, RWTH Aachen University, Germany — [3]Institut für Theoretische Physik, Universität Ulm, Germany — [4]School of Physical and Chemical Sciences, Victoria University of Wellington, New Zealand

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, the relaxation rates in the dynamical response of an interacting single-level quantum dot, weakly tunnel coupled to an electronic reservoir and brought out of equilibrium by a step pulse, have been investigated [1].

This theoretical work focuses on the readout of these relaxation rates with a capacitively coupled sensor quantum dot (SQD). Using a generalized master equation approach for the combined system of dot and SQD, we investigate the measurability of the dot relaxation behavior via the SQD current, especially accounting for back-action effects.

Our results reveal parameter regimes in which back-action leads to a decrease of the dot decay rates and to a mixing of relaxation modes that decay independently in the absence of a measurement. However, avoiding these regimes, we show that the original dot rates can still be extracted from the SQD current.

[1] L. D. Contreras-Pulido et al., Phys. Rev. B **85**, 075301 (2012).

HL 25.7 Mon 17:45 HSZ 204

Hybrid Microwave Cavity Heat Engine — Christian Bergenfeldt[1], Peter Samuelsson[1], •Björn Sothmann[2], Christian Flindt[2], and Markus Büttiker[2] — [1]Physics Department, Lund University, Box 118, SE-22100 Lund, Sweden — [2]Département de Physique Théorique, Université de Genève, CH-1211 Genève 4, Switzerland

We propose and analyze the use of hybrid microwave cavities as quantum heat engines. A possible realization consists of two macroscopically separated quantum dot conductors coupled capacitively to the fundamental mode of a microwave cavity. We demonstrate that an electrical current can be induced in one conductor through cavity-mediated processes by heating up the other conductor. The heat engine can reach Carnot efficiency with optimal conversion of heat to work. When the system delivers the maximum power, the efficiency can be a large fraction of the Carnot efficiency. The heat engine functions even with moderate electronic relaxation and dephasing in the quantum dots. We provide detailed estimates for the electrical current and output power using realistic parameters.

[1] C. Bergenfeldt, P. Samuelsson, B. Sothmann, C. Flindt and M. Büttiker, arXiv:1307.4833v1 (2013).

HL 25.8 Mon 18:00 HSZ 204

Vibration-induced thermoelectric effects in quantum dots — •Matti Laakso and Volker Meden — Institut für Theorie der Statistischen Physik, RWTH Aachen, Aachen, Germany

We study the thermoelectric transport through a quantum dot coupled to a single vibrational mode described by the Anderson-Holstein model. We use analytical methods in the linear response regime as well as the functional renormalization group (FRG) in the non-linear regime. We predict relatively large thermoelectric effects in the parameter regime where the phonon-mediated electron-electron interaction dominates over the bare Coulomb repulsion.

HL 25.9 Mon 18:15 HSZ 204

Superexchange transport and blockade in triple quantum dots — •Rafael Sánchez[1], Ghislain Granger[2], Fernando Gallego-Marcos[1], Sergei A. Studenikin[2], Andrew S. Sachrajda[2], and Gloria Platero[1] — [1]Instituto de Ciencia de Materiales de Madrid, CSIC, E-28049 Madrid, Spain — [2]National Research Council Canada, Ottawa, ON K1A 0R6 Canada

We present recent experimental evidence of long range transport in triple quantum dots. Superexchange is responsible for the spin-dependent indirect coupling of the two outer quantum dots, mediated by virtual transitions through the middle one. They are manifested in the form of sharp current resonances at the degeneracy points of states with left-right symmetric charge distributions [1,2]. The transition can take two paths: two electrons in different dots tunnel simultaneously [1] or a single electron tunnels twice [2].

We analyze a configuration where the two paths with different virtual intermediate states are possible and lead to quantum interference. Remarkably, we find conditions where the destructive interference of these transitions completely cancels the transport, what we call superexchange blockade [3]. Spin correlations play an essential role by avoiding certain transitions. This effect, known as spin blockade, leads to the suppression of certain resonances whose observation gives a measure of spin decoherence times.

[1] M. Busl et al., Nature Nanotech. 8, 261 (2013).
[2] R. Sánchez et al., submitted.
[3] R. Sánchez, F. Gallego-Marcos and G. Platero, submitted.

HL 26: Graphene: Structural properties (organized by O)

Time: Monday 16:00–19:00 Location: WIL C107

HL 26.1 Mon 16:00 WIL C107

Vertical height of quasi-free standing monolayer graphene on SiC(0001): an XSW study — •J. Sforzini[1], T. Denig[2], T. L. Lee[3], C. Kumpf[1], S. Subach[1], U. Starke[2], F. C. Bocquet[1], and F.S. Tautz[1] — [1]Peter Grünberg institute (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany — [3]Diamond light source ltd, Harwell oxford, Didcot, Oxfordshire, United Kingdom

We investigated a quasi-free standing monolayer graphene sample[1] on SiC(0001) obtained by decoupling the buffer-layer from Si-terminated surface by hydrogen intercalation. We used X-ray Standing Wave technique (XSW), combining dynamical diffraction and X-ray photoelectron spectroscopy, to detect the coherent distribution of the chemically different species (Si and C) at the interface. Our analysis shows two different carbon species (C in the graphene layer and C in the SiC bulk); we find that the adsorption height of the graphene layer is slightly higher than theoretically predicted. The discrepancy, attributed to the very weak graphene-substrate intercation, is still challenging for theory[2].

[1]Riedl, et. al., PRL, 103, 246804 (2009)
[2]Deretzis , et. al., Nanoscale, 5, 671-680 (2012)

HL 26.2 Mon 16:15 WIL C107

Epitaxial graphene nanostructures on SiC — •Alexander Stöhr[1], Stiven Forti[1], Ulrike Waizmann[1], Thomas Reindl[1], Jens Baringhaus[2], Alexei Zakharov[3], Christoph Tegenkamp[2], and Ulrich Starke[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]Institut für Festkörperphysik, Leibniz-Universität Hannover, Hannover, Germany — [3]MAX IV Laboratory, Lund University, Lund, Sweden

In recent years a lot of effort was put into the realization of graphene devices, in view of their unique electronic properties and the potential application in logical circuits. However, for the use in logical electronics a band gap would be required. This can be achieved by confining the electrons into quasi-onedimensional graphene stripes, called graphene nanoribbons. When patterning graphene, the altering of the electronic properties by the mechanical attack on the ribbon edges as well as residual resist is always an issue. For that matter we chose to structure the SiC-samples before growing graphene, using electron beam lithography and reactive ion etching. Subsequently, the graphene was grown at elevated temperatures, which also removed the residual resist. As a result onedimensional stripes could be obtained and were decoupled from the substrate by intercalation of hydrogen. Characterization by low-energy electron microscopy and angle-resolved photoemission spectroscopy proves the development of quasi-free standing monolayer graphene ribbons.

HL 26.3 Mon 16:30 WIL C107

Moiré-induced Brillouin zone backfolding of graphene phonons on Ir(111) — •Michael Endlich[1], Alejandro Molina-Sánchez[2], Henrique Miranda[2], Ludger Wirtz[2], and Jörg Kröger[1] — [1]Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau — [2]Physics and Material Sciences Research Unit, University of Luxembourg, L-1511 Luxembourg

The moiré superstructure of graphene on Ir(111) leaves its characteristic footsteps in the phonon dispersion. Replica of the phonon dispersion branches of singly oriented graphene on Ir(111) have been determined throughout the entire surface Brillouin zone with angle-resolved inelastic electron scattering. These replica are rationalized in terms of phonon backfolding induced by the graphene moiré superlattice.

HL 26.4 Mon 16:45 WIL C107

Back Focal Plane Imaging of Raman Scattering from Graphene — •Harald Budde, Xian Shi, Nicolai Hartmann, and Achim Hartschuh — Department Chemie und CeNS, LMU München, Germany

Raman Scattering Spectroscopy is a powerful technique for studying graphene and other sp2 carbon materials [1]. We combined Raman Spectroscopy with back focal plane (BFP) imaging , a method used to visualize the angular distribution of emitted or scattered light. As an example BFP imaging allows to determine the orientation of single dipolar emitters [2, 3]. For graphene on glass Raman BFP images mainly reflect the polarization characteristics of the different phonon modes. On thin gold films emission from graphene leads to the excitation of propagating surface plasmon polaritons.

[1] A. Ferrari, D. Basko, Nat. Nanotech 8, 235-246, 2013.
[2] M. Lieb, J. Zavislan, L. Novotny, J. Opt. Soc. Am. B 21, 1210-1215, 2004.
[3] N. Hartmann, G. Piredda, J. Berthelot, G. Colas des Francs, A. Bouhelier, A. Hartschuh, Nano Lett. 12, 177-181, 2012.

HL 26.5 Mon 17:00 WIL C107

Ion Irradiation of Metal-Supported Graphene: Exploring the Role of the Substrate — •Charlotte Herbig[1], Harriet Åhlgren[2], Sabina Simon[1], Carsten Busse[1], Jani Kotakoski[2,3], Arkady V. Krasheninnikov[2,4], and Thomas Michely[1] — [1]II. Phys. Inst., Universität zu Köln, Germany — [2]Dept. of Phys., University of Helsinki, Finland — [3]Faculty of Phys., University of Vienna, Austria — [4]Dept. of Appl. Phys., Aalto University, Finland

Ion irradiation effects on 2D materials are an emerging subject, triggered by graphene's (Gr) potentials in applications. For supported Gr the effect of the substrate on ion beam damage and annealing is important. We investigate the behavior of high quality Gr, weakly coupled to Ir(111), to low energy noble gas ion irradiation by scanning tunneling microscopy (STM), molecular dynamics simulations, and density functional theory (DFT). For a freestanding layer, sputtered atoms leave the layer either in forward or backward direction. For metal-supported Gr, only C atoms carrying backward momentum are sputtered while atoms carrying forward momentum are trapped. As evident from STM and DFT, trapped C atoms form nm-sized Gr platelets at the interface upon annealing at 1000K, assisted by substrate defects. The incorporation into the Gr layer is suppressed due to high migration barriers, while diffusion into the Ir is energetically unfavorable. By measuring the area fraction of the platelets, we obtain the trapping yield, i.e., the number of trapped C atoms per incident ion. Interestingly, compared to the sputtering yield, the trapping yield for Gr on Ir(111) displays a distinctly different dependence on the ion beam angle of incidence.

HL 26.6 Mon 17:15 WIL C107

***Ab initio* study of graphene on O-intercalated Ir(111) surface and its functionalization via molecular adsorption** — •Vasile Caciuc, Nicolae Atodiresei, and Stefan Blügel — Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

To integrate graphene in molecular electronics and spintronics devices it is crucial to understand how the strength of the graphene–metal electrode interaction can be specifically tuned. One possibility to loose or strengthen this interaction is to intercalate adatoms with different chemical reactivity between graphene and the metal surface in question. We will analyse this approach from first principles by considering the case of the O-intercalated graphene on Ir(111) [1]. Another path is to analyse how the adsorption of $\pi-$conjugated organic molecules can affect the electronic structure of a quasi-freestanding graphene layer. We investigated this issue by performing spin-polarized density functional theory (DFT) for a trioxotriangulene-derivate molecule [2] on graphene. Importantly, as already demonstrated in [3], for such systems it is mandatory to include the dispersion interaction and in our *ab initio* study these long-range van der Waals interactions were considered at a semi-empirical [4] or first-principle [5] level.

[1] E. Gråsäs *et al.*, ACS Nano. **6**, 9951 (2012).
[2] Y. Morita *et al.*, Nat. Mater. **10**, 946 (2011).
[3] C. Busse *et al.*, Phys. Rev. Lett. **107**, 036101 (2011).
[4] S. Grimme, J. Comput. Chem. **27**, 1787 (2006).
[5] M. Dion *et al.*, Phys. Rev. Lett. **92**, 246401 (2004).

HL 26.7 Mon 17:30 WIL C107

From two to three dimensions: The effect on the Coulomb interaction by increasing the dimensionality in layered materials — •M. Rösner[1], E. Sasioglu[2], C. Friedrich[2], S. Blügel[2], A.I. Lichtenstein[3], M.I. Katsnelson[4], and T.O. Wehling[1] — [1]Institut für Theoretische Physik and Bremen Center for Computational Materials Science, Universität Bremen, Bremen, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Jülich, Germany — [3]I. Institut

für Theoretische Physik, Universität Hamburg, Hamburg, Germany — [4]Radboud University Nijmegen, Institute for Molecules and Materials, AJ Nijmegen, The Netherlands

We study the Coulomb repulsion and the dielectric screening in mono-, bi- and tetralayer graphene as well as in graphite. We discuss the transition from 2D systems to the bulk structure in layered materials with regard to the (non) local Coulomb interactions. Therefore, we use *ab initio* constrained random phase (cRPA) calculations to get reliable data in a first step. By tailoring the resulting Coulomb interaction in classical electrostatic models afterwards, we find the following: In addition to the effective height of each layer especially the direction dependence and the non-locality of the dielectric function are the keys to understand the screening effects in these structures. Thereby, we discuss models to estimate the Coulomb interaction of the 2D systems by using exclusively the bulk data as input. We apply these rules to calculate the Coulomb interaction in graphene on iridium and find a very good agreement with *ab initio* data.

HL 26.8 Mon 17:45 WIL C107

Graphene nanolithography with 2.5 nm precision: combining bottom-up and top-down techniques — •Antonio J. Martínez-Galera[1,2], Iván Brihuega[1,3], Ángel Gutiérrez-Rubio[1], Tobias Stauber[1,3], and José M. Gómez-Rodríguez[1,3] — [1]Departamento Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [2]Present address: II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany. — [3]Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain.

The selective modification of pristine graphene represents an essential step to fully exploit its potential. The work presented here overcomes one of the remaining challenges key for the comprehensive integration of graphene in real devices: the realization of lithography below 10 nm sizes. Specifically, we have developed a perfectly reproducible nanolithographic technique for graphene that allows, by means of an STM tip, to modify with 2.5 nm accuracy the electronic properties of graphene monolayers epitaxially grown on Ir(111) surfaces. This method can be carried out also on micrometer sized regions and the structures so created are stable even at room temperature. As a result, we can strategically combine graphene regions presenting large differences in their electronic structure to design graphene nanostructures with tailored properties. Therefore, this novel nanolithography method could open the way to the design of nanometric graphene-based devices with specific functionalities. In particular, we explore here the possibility of developing a new platform for plasmonics.

HL 26.9 Mon 18:00 WIL C107

Relaxation of compressive stresses in graphene through mobile nanoripples — •Peter Klaver, Shouen Zhu, Marcel Sluiter, and Guido Janssen — Delft University of Technology, Delft, Netherlands

Graphene monolayers have a far smaller thermal expansion coefficient than the Cu substrates on which they are often grown through CVD at high temperature. Once the Cu substrate and graphene monolayer are cooled down to room temperature, the Cu contracts 1.5-2.0% more than the graphene. Yet various experiments do not show graphene layers on Cu to be under significant compressive stress. We present molecular dynamics simulations that show that under compressive stress, small ripples of just a few nm wide appear that absorb the excess graphene area. These ripples are quite mobile, even at room temperature. Their movement offers a mechanism to remove the compressive stress in graphene while keeping it flat, by absorbing the ripples into larger ripples (like those that have formed around bunches of step edges) or by eliminating the ripples at the edges of graphene islands. The relaxation of stresses through the movement of nanoripples is somewhat analogous to flattening out a red carpet by gradually moving a wrinkle away to the carpet edge instead of pulling the entire carpet all at once. The ease with which stresses in graphene relax, is not directly determined by the corrugation energy.

HL 26.10 Mon 18:15 WIL C107

Epitaxial graphene nanoflakes on Au(111) and Ag(111) — •Julia Tesch[1], Philipp Leicht[1], Lukas Zielke[1], Riko Moroni[1], Bernd Illing[1], Luca Gragnaniello[1], Felix Blumenschein[1], Elena Voloshina[2], Lukas Hammerschmidt[3], Lukas Marsoner Steinkasserer[3], Beate Paulus[3], Yuriy Dedkov[4], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz — [2]Institut für Chemie, HU Berlin — [3]Institut für Chemie und Biochemie, FU Berlin — [4]Fritz-Haber-Institut der MPG, Berlin

In zig-zag edge terminated graphene nanoribbons or nanoflakes (GNFs), confinement of electrons is predicted to give rise to edge states with magnetic moments. However, the experimental observation of edge effects is impeded by the inevitable presence of substrates that interact with the flake edges, hence masking the GNFs' intrinsic properties. In the attempt of reducing the graphene substrate interaction, we use an entirely UHV based approach for the preparation of GNFs on Au(111) and Ag(111) surfaces allowing for flake sizes down to 10 nm. GNFs on Ir(111) are prepared by temperature programmed growth [1] and subsequently covered by deposition of several nm of Au or Ag. After post-annealing, the flakes diffuse through the Au or Ag film and form embedded or floating graphene flakes. In scanning tunnelling microscopy (STM), the edges of floating GNFs are found to be singly hydrogen terminated and entire flakes can be laterally displaced with the STM tip on both Au and Ag surfaces, suggesting a considerable reduction of graphene-substrate interactions compared to other metals. [1] Coraux et al., New J. Phys. 11, 023006 (2009)

HL 26.11 Mon 18:30 WIL C107

Scatttering and electronic structure in graphene nanoflakes on Au(111) — •Philipp Leicht[1], Lukas Zielke[1], Samuel Bouvron[1], Julia Tesch[1], Felix Blumenschein[1], Luca Gragnaniello[1], Lukas Marsoner Steinkasserer[2], Beate Paulus[2], Elena Voloshina[3], Yuriy Dedkov[4], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz — [2]Institut für Chemie und Biochemie, FU Berlin — [3]Institut für Chemie, HU Berlin — [4]Fritz-Haber-Institut der MPG, Berlin

Confinement of electrons in graphene quantum dots and nano ribbons with atomically well defined edges represents an exciting field of research, owing to predicted peculiar electronic and magnetic properties.

Here, we present scanning tunneling microscopy (STM) investigations of graphene nano flakes (GNFs) prepared by temperature programmed growth on Ir(111) [1] and subsequent intercalation of Au for electronic decoupling. The electronic properties of the graphene flakes are addressed by scanning tunneling spectroscopy. Within our atomically resolved constant-energy maps we can probe the electronic states of the graphene electrons exploiting the intervalley scattering. The hereby obtained dispersion relation shows a linear behavior and can be unambiguously discriminated from the parabolic dispersion relation of the Au(111) surface state electrons. The intervalley scattering of graphene electrons forms discs in the Fourier transforms of constant-energy maps, which include additional scattering features compared to monolayer graphene.

[1] Coraux, J. et al., New J. Phys. 11, 023006 (2009)

HL 26.12 Mon 18:45 WIL C107

Improved effective theories for edge magnetism — •Cornelie Koop and Manuel Schmidt — Institut für Theoretische Festkörperphysik, RWTH Aachen University, Deutschland

We consider the effective interaction between edge states in graphene nanoribbons. Low-energy edge states come along with a strongly enhanced density of states near the graphene edges, which makes electron-electron correlation important and gives rise to the so-called edge magnetism. In a pristine nanoribbon in first order, there is a direct ferromagnetic intra-edge coupling and an antiferromagnetic interaction between opposite edges. We study the coupling by means of an effective model yielding a separation between edge and bulk states. In particular we investigate the influence of the bulk states on the effective edge state theory via a second order Schrieffer-Wolff transformation. Using both numeric and analytic methods, we calculate various correlation functions. We discuss the results for the effective correlations between smooth edges as well as between the strongly localized states at rough edge structures.

HL 27: Frontiers of electronic structure theory - Non-equilibrium phenomena at the nano-scale II (organized by O)

Time: Monday 16:00–18:45 Location: TRE Ma

Topical Talk HL 27.1 Mon 16:00 TRE Ma

Simulating heat transport: from large scale molecular dynamics to first-principles calculations — •Davide Donadio — Max Planck Institute for Polymer Research, Mainz, Germany

The necessity to design materials and devices able to harness thermal energy, and possibly convert it into more amenable energy forms, has stimulated a major effort in the scientific community to understand heat transport at the mesoscale and the nanoscale. In this talk I will discuss different atomistic approaches to simulate nanoscale heat transport, ranging from large scale molecular dynamics simulations with classical empirical potentials at equilibrium and non-equilibrium conditions, to lattice dynamics calculations with force-constants computed by first principles. Applications will include silicon and carbon nanostructures, phase-change materials and molecular junctions.

HL 27.2 Mon 16:30 TRE Ma

First principles study of thermal conductivity cross-over in nano-structured Zinc-Chalcogenides — •Ankita Katre[1], Atsushi Togo[2], Ralf Drautz[1], and Georg K. H. Madsen[1] — [1]ICAMS, Ruhr-Universität Bochum, 44801 Bochum, Germany — [2]ESISM, Kyoto University, Sakyo, Kyoto 606-8501, Japan

Nano-structured Zinc-Chalcogenides are interesting for thermoelectric applications due to their low thermal conductivity.[1] A simple model study has reported how the thermal conductivity of ZnS, ZnSe and ZnTe can potentially show a cross-over as a function of the maximal mean free path of the phonons.[2] We have applied the Boltzmann transport equation in the relaxation time approximation to verify this. We find that thermal conductivity of ZnS crosses ZnSe and ZnTe and explain this in terms of the different contributions of phonon modes in these materials. Furthermore, the cross-over is found to be strongly influenced by isotope scattering. The calculated thermal conductivity is found to be strongly dependent on the volume and we explain the observed differences between LDA and GGA calculations. We compare further calculated thermal properties, such as the thermal expansion coefficient, to experiment to validate our approach.

[1] L.Zhen, S.Qiao, D.Y.Xiang, H.Z.Zhong, and Q.L.Gao, J. Mater. Chem. 22, 22821 (2012). [2] N.Mingo and D.Broido, Phys. Rev. Lett. 93, 246106 (2004).

HL 27.3 Mon 16:45 TRE Ma

Density-functional perturbation theory for lattice dynamics with numeric atom-centered orbitals — •Honghui Shang, Christian Carbogno, Patrick Rinke, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin

The response of the electronic structure to atomic displacements gives rise to a variety of interesting physical phenomena, which can be probed by experimental techniques such as infrared or Raman spectroscopy or neutron diffraction. The response can be conveniently computed from first principles by means of density-functional perturbation theory (DFPT). Here we present our implementation in the all-electron atom-centered numeric orbital code FHI-aims [1]. Our approach combines the accuracy of an all-electron full-potential treatment with the computationally efficiency of localised atom-centered basis sets that is necessary to study large and complex systems. We verified the accuracy of our DFPT implementation by comparing the vibrational frequencies to finite-difference reference calculations and literature values. Due to the atom-centered nature of the integration grids in FHI-aims, the portion of the grid that belongs to a certain atom also moves when this atom is displaced. Here we demonstrate that, unlike for first derivatives (i.e. forces) [2], this moving-grid-effect plays an important role for second derivatives (i.e. vibrational frequencies). Further analysis reveals that predominantly diagonal force constant terms are affected, which can be bypassed efficiently by invoking translational symmetry.

[1] V. Blum et al. Comp. Phys. Comm. 180, 2175 (2009)
[2] B. Delley, J. Chem. Phys. 94, 7245 (1991).

HL 27.4 Mon 17:00 TRE Ma

Breakdown of Fourier law in layered materials — •Andrea Cepellotti[1], Giorgia Fugallo[2], Francesco Mauri[3], and Nicola Marzari[1] — [1]THEOS, École Polytechnique Fédérale, Lausanne — [2]IMPMC, Universite Pierre et Marie Curie, Paris — [3]LSI, École Polytechnique, Paris

We compute the thermal conductivity in crystalline layered materials by solving the Boltzmann Transport Equation (BTE) for phonons [1], with the phonon-phonon collision rates obtained from density-functional perturbation theory. We find that in 2D materials, such as graphene and related compounds, and even in 3D layered materials, like bulk graphite, the single-mode relaxation time approximation (SMRTA) cannot describe heat transport correctly, underestimating by one order of magnitude or more thermal conductivities and phonons' mean free paths. Instead, we show that the exact self-consistent solution of the BTE provides results in excellent agreement with experimental measurements [2]. The shortcomings of the SMRTA lie in the assumption that heat flow is transferred only by individual phonon excitations, whereas in layered materials the transport can only be explained in terms of collective phonon excitations. The characteristic length of these collective excitations is often comparable with that of the experimental sample - as a result, Fourier's law become questionable, since its statistical nature makes it applicable only to systems larger than a few mean free paths.

[1] G. Fugallo et al., Phys. Rev. B, **88**, 045430 (2013).
[2] A. A. Balandin, Nat. Mater. **10**, 569 (2011).

HL 27.5 Mon 17:15 TRE Ma

High Temperature Thermal Conductivity from First Principles — •Christian Carbogno[1], Rampi Ramprasad[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Chemical, Materials & Biomolecular Engineering, University of Connecticut, Storrs, USA

In spite of significant research efforts, a first principles determination of the thermal conductivity at high temperatures has remained elusive. Under such conditions, Boltzmann transport techniques [1] that include anharmonic effects only perturbatively become inaccurate or even inapplicable. In this work, we overcome this limitation by performing first-principles Green-Kubo simulations [2], in which all orders of anharmonicity are incorporated by the means of *ab initio* molecular dynamics. The thermal conductivity is then assessed from the autocorrelation function of the heat flux in thermodynamic equilibrium. We discuss the details of our implementation and the definition of our heat flux that is based on the virial theorem. We validate our approach by presenting calculations for ZrO_2 that also showcase the importance of higher order anharmonic effects in materials with low thermal conductivities. Eventually, we discuss how our technique can be coupled to multi-scale models to achieve a computationally efficient and accurate description of the thermal conductivity at the nanoscale.

[1] D. A. Broido *et al.*, *Appl. Phys. Lett.* **91**, 231922 (2007).
[2] R. Kubo, M. Yokota, S. Nakajima, *J. Phys. Soc. Jpn.* **12**, 1203 (1957).

HL 27.6 Mon 17:30 TRE Ma

Accurate Modelling of the Polymorphism and Elastic Response of Molecular Materials from First Principles — •Anthony Reilly and Alexandre Tkatchenko — Fritz-Haber-Institut der MPG, Berlin, Germany

Molecular materials are of great fundamental and applied importance in science and industry, with numerous applications in pharmaceuticals, electronics, sensing, and catalysis. A key challenge for theory has been the prediction of their stability, polymorphism and response to perturbations. While pairwise models of van der Waals (vdW) interactions have improved the ability of density functional theory (DFT) to model these systems, quantitative and even qualitative failures often remain. Here, we show how a many-body description of vdW interactions can dramatically improve the accuracy of DFT for molecular materials, yielding quantitative description of stabilities and polymorphism for these challenging systems. Moreover, the role of many-body vdW interactions goes beyond stabilities to response properties. In particular, we have studied the elastic properties of a series of molecular crystals, finding that many-body vdW interactions can account for up to 30% of the elastic response, leading to quantitative and qualitative changes in elastic behavior. We will illustrate these crucial effects with the challenging case of the polymorphs of aspirin, leading to a

better understanding of the conflicting experimental and theoretical studies of this system.

HL 27.7 Mon 17:45 TRE Ma

Surface chemistry on nanostructured oxides: do we have to go beyond hybrid DFT? — •Daniel Berger, Harald Oberhofer, and Karsten Reuter — Technische Universität München, Germany

Nanostructured oxide surfaces are promising candidates for a wide range of energy and catalysis applications. For first-principles modeling of corresponding surface chemical reactions the current state-of-the-art is generally defined by hybrid-level density-functional theory (DFT). Systematic work assessing the achieved accuracy at this level is nevertheless scarce, also owing to the fact that higher-level reference methods are often not available for standard periodic boundary condition supercell calculations. To this end, we present a study benchmarking semi-local and hybrid DFT against (renormalized) second-order perturbation theory (MP2,rPT2) as recently implemented in the FHI-aims package [1]. We make the efficient usage of the latter theories for oxide surfaces possible through a solid-state embedding framework, in which a central cluster region is described quantum mechanically, the long-range electrostatic interactions in the oxide are accounted for through a polarizable monopole field, and a shell of norm-conserving pseudopotentials correctly connects the two regions. We illustrate the performance of the various levels of theories using the water-splitting reaction at ideal and defected TiO_2(110) surfaces as showcase. [1] X. Ren *et al.*, Phys. Rev. B **88**, 035120 (2013)

HL 27.8 Mon 18:00 TRE Ma

Atoms-in-solids perspective on polarizabilities and van der Waals coefficients in semiconductors — •Guo-Xu Zhang, Anthony M. Reilly, Alexandre Tkatchenko, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, Germany

The calculation of response properties of solids including their polarizabilities and van der Waals (vdW) coefficients usually requires the knowledge of the full electronic bandstructure. For non-covalently bound solids, such as noble-gas and ionic crystals, atoms-in-solids model can be successfully utilized to define their polarizabilities. Here we critically assess the atoms-in-solids model for covalently-bound solids, ranging from wide-gap (10 eV) to narrow-gap (below 1 eV) semiconductors. We model their response by assigning a single quantum harmonic oscillator to every atom, where the parameters of the oscillators are defined as functionals of the electron density, following the Tkatchenko-Scheffler method [1]. The response function is then calculated by solving self-consistent screening equations of classical electrodynamics, without any explicit information about the electronic bandstructure [2]. The calculated polarizabilities and vdW coefficients for 23 semiconductors are compared with TDDFT and experimental benchmark data, revealing an overall agreement within 10%. The efficiency of our method and the accuracy of the calculated vdW parameters allows us to demonstrate the crucial role of vdW interactions in the cohesive properties of the 23 semiconductors. [1] Tkatchenko and Scheffler, PRL (2009); [2] Tkatchenko, DiStasio, Car, Scheffler, PRL (2012).

HL 27.9 Mon 18:15 TRE Ma

Adsorption at semiconductor surfaces - an energy analysis method — •Ralf Tonner and Marc Raupach — Fachbereich Chemie & Materials Sciences Centre, Philipps-Universität Marburg, Germany

The chemical bond is one of the most fundamental concepts in chemistry. Classifications such as covalent, ionic or metallic bonding are central in discussing trends in different compounds and predicting new reactivity. Several very helpful concepts and methods were developed to understand the chemical bond at surfaces.[1] The question about energetic contributions to surface chemical bonds on the other hand did not receive great attention although energy changes are the ultimate driving force in bond formation.

Starting from preliminary work by Philippsen and Baerends,[2] we implemented all terms of an Energy Decomposition Analysis (EDA) to obtain quantitative data about energetic contributions to chemical bonding in periodic systems. This periodic EDA method was applied to questions of chemisorption of organic molecules at semiconductor surfaces where it can shed light on the nature of the surface-adsorbate bonds.

[1] a) A. Nilsson, L. G. M. Pettersson, J. Nørskov, Chemical Bonding at Surfaces and Interfaces, Elsevier, Amsterdam, 2007; b) A. Groß, Theoretical Surface Science, Springer, Berlin, Heidelberg, 2009. [2] P. H. T. Philipsen, E. J. Baerends J. Phys. Chem. B 2006, 110, 12470.

HL 27.10 Mon 18:30 TRE Ma

Non-local density functionals meet many-body dispersion: A hybrid approach for van der Waals interactions — •Jan Hermann, Matthias Scheffler, and Alexandre Tkatchenko — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Different approaches to treating van der Waals (vdW) interactions in density-functional theory can be loosely divided into the atom-based and the ones based on non-local functionals. The first type comprises a range of methods from atom-pairwise additive schemes by Grimme to many-body dispersion (MBD) approach of Tkatchenko et al. Usually, these methods require precalculated atomic parameters and thus rely on information not explicitly contained in the electron density. The other category consists of nonlocal functionals either of the Langreth and Lundquist or the Vydrov and van Voorhis (VV) type. In these approaches, the vdW interaction is obtained as a functional of the electron density and at most a few tuning parameters are needed.

Here, we show that these two contrasting approaches can be synergistically combined. We use the polarizability from the nonlocal functional of VV within the MBD method of Tkatchenko et al. Such a combination is worthy for several reasons. First, it is an atom-centered approach with no atomic parameters. Second, it puts aside the problem of partitioning electron density between atoms, which can be problematic in some cases. Third, it enables more direct comparison of so far unrelated methods. Fourth, it highlights the idea of combining working elements from different approaches.

HL 28: Organic electronics and photovoltaics I (organized by DS)

Time: Monday 18:00–19:45 Location: CHE 91

HL 28.1 Mon 18:00 CHE 91

Studying the electric potential of organic solar cells — •Michael Scherer[1,2,3], Tobias Jenne[1,2,3], Rebecca Saive[1,2,3], Felix Schell[1,2,3], Robert Lovrincic[1,2,3], and Wolfgang Kowalsky[1,2,3] — [1]InnovationLab GmbH, Heidelberg — [2]TU Braunschweig — [3]Universität Heidelberg

Despite steadily increasing efforts in the research on organic semiconductors, many of the models applied in the field are restricted to small clusters of molecules or model systems only, thus lacking prediction when it comes to full devices. With scanning Kelvin probe microscopy (SKPM) accompanied by device simulations we try to access the physics of entire OSC devices and bridge the gap between the molecular and the macroscopic understanding.

Our scanning probe station is placed within the vacuum of a scanning electron microscopy (SEM)/focused ion beam (FIB) cross beam system. We prepare OSC cross sections with the FIB and place the cantilever under SEM observation right at the cross section. Thus we are able to investigate the potential distribution of OSCs in situ with SKPM.

The SKPM measurements are backed by IV characterization and device simulations. Varying the parameter of the active layer/contact interface, we investigate their impact on the potential distribution and the device characteristics of the OSC. In IV measurements and cross sectional SKPM measurements we check the validity of the applied models and identify loss mechanisms and their localization in the solar cell device.

HL 28.2 Mon 18:15 CHE 91

Correlation of electric properties and interface band alignment in organic light-emitting diodes — •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, Surface Science Division — [2]InnovationLab

GmbH, Heidelberg — [3]Merck KGaA, Darmstadt

Organic light-emitting diodes consist of several functional organic layers sandwiched between two electrodes with different work functions. At the current onset voltage the applied electric field is high enough that charge carrier injection and transport begins. In some device structures the onset voltage increases with increasing thickness of the emission layer. We present a detailed study on this up to now unpredictable phenomenon by combining IV-measurements and interface investigations using photoelectron spectroscopy (XPS/UPS). We focus on two isomers synthesized by Merck that serve as matrix material in the emission layer-one showing the changes in onset voltage the other not. The complex device architecture was reduced to a model device system using NPB as hole-transport layer and the undoped isomers as emission layer. The shift in onset voltage can still be observed in the model devices as well in hole-only devices derived from the model system. By stepwise evaporation of the respective isomer onto NPB we performed PES-interface experiments and analyzed the band alignment between NPB and the isomers in an integrated UHV system. It was found that the hole injection barrier is larger by about 200 meV in case of the isomer showing the observed shift in onset voltage.

HL 28.3 Mon 18:30 CHE 91

Temperature dependent exciton diffusion length in ZnPc — •Bernhard Siegmund[1], Johannes Widmer[1], Simone Hofmann[1], Moritz Riede[2], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, Dresden, Germany — [2]Current address: Clarendon Laboratory, Oxford, England

The photo-current of organic solar cells is the result of a multi-step process. It includes the generation and diffusion of excitons as well as their separation into free charge carriers, the transport to the electrodes, and their final extraction. One bottleneck for highly efficient devices is the short exciton diffusion length in organic materials.

In this work, the singlet exciton diffusion length ℓ_{diff} in the absorber material ZnPc is studied. For this purpose, the photo-current of organic solar cells, incorporating ZnPc and C_{60} in a flat heterojunction architecture, is measured and modelled as a multi-step process. ℓ_{diff} is extracted from a thickness variation of the absorber layer, as not yet encountered in the context of modelling the photo-current to determine ℓ_{diff} before. Measurements at varying temperature between 200 K and 370 K reveal a thermal activation of the diffusion length above 310 K. This is interpreted as promotion of the excitons to higher energies with a density of states allowing for enhanced hopping transport. The activation energy is considered as a measure for the energetic disorder of the excitonic states. These investigations aim for a better understanding of exciton migration in order to design materials with longer exciton diffusion lengths for highly efficient organic solar cells.

HL 28.4 Mon 18:45 CHE 91

The effect of gradual fluorination on the opto-electronic properties of F_nZnPc/C_{60} bilayer cells — •M. Brendel[1], A. Steindamm[1], A. Topczak[1], and J. Pflaum[1,2] — [1]Exp. Phys. VI, JMU Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

The respective position of energy levels at the donor/acceptor heterojunction is crucial for the resulting parameters of an organic solar cell. For instance the open circuit voltage (V_{oc}) is correlated to the energy difference between the highest occupied molecular orbital (HOMO) of the donor and the lowest unoccupied molecular orbital (LUMO) of the acceptor, the so-called effective band gap ($E_{g,eff}$). To gain insights into this correlation, tailoring of energy levels by chemical modification is a powerful approach. In this contribution, we investigate the impact of gradual fluorination of zinc phthalocyanine on the opto-electronic properties of F_nZnPc/C_{60} (n=0,4,8,16) bilayer cells. Upon fluorination, HOMO and LUMO levels are shifted towards lower energies. The gain in V_{oc} for F_4ZnPc/C_{60} and F_8ZnPc/C_{60} by 11% and 23% respectively, compared to ZnPc/C_{60}, confirms qualitatively the expected energy level scheme. Besides, the differences between $e \cdot \Delta V_{oc}$ and $\Delta E_{g,eff}$ hint at the occurrence of dipoles and their gain in strength with increasing degree of fluorination. As will be shown, this dipol can be correctly accounted for in a plate capacitor geometry, considering image charges at the interface induced by electronegative fluorine in the immediate vicinity of C_{60} molecules. We thank S. Sundarray and P. Erk from BASF for providing F_4ZnPc. Financial support by the DFG (program SPP1355) and the BMBF (GREKOS program).

HL 28.5 Mon 19:00 CHE 91

Effect of Counter-Anions During Electrodeposition on the Charge Transport Dynamics in Sensitized ZnO Solar Cells — •Christoph Richter, Max Beu, and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany

Thin porous $ZnO/EosinY$ films have been electrochemically deposited from oxygen-saturated aqueous solution. During the electrochemical deposition chloride or perchlorate as different counter-anions have been used. After the removal of $EosinY$ with KOH the films have been sensitized with the indoline dye D149. These electrodes were used in dye-sensitized solar cells (DSCs) and the charge transport dynamics were studied with electrochemical impedance spectroscopy (EIS), intensity modulated current/voltage spectroscopy (IMPS/IMVS) and IV-curves. Doping of the ZnO films by Cl alters the charge transfer dynamics by filling of otherwise unoccupied states in ZnO and changing the concentration of available trap states. By changing the counter-anion to perchlorate well-reproducible results could be obtained which open the way to further improvements in DSCs.

HL 28.6 Mon 19:15 CHE 91

Efficiency roll-off in organic light-emitting diodes: influence of emitter position and orientation — •Caroline Murawski[1], Philipp Liehm[1,2], Simone Hofmann[1], Karl Leo[1], and Malte C. Gather[1,2] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]present address: SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews KY16 9SS (UK)

In this contribution, we study the efficiency decrease of organic light-emitting diodes (OLEDs) at high brightness (so-called roll-off).[1] We find a strong influence of the emitter-cathode distance and the transition dipole orientation of the emitter molecules on the roll-off by comparing two phosphorescent emitters (Ir(MDQ)2(acac) and Ir(ppy)3).[2] The measurements are modeled using triplet-triplet-annihilation (TTA) theory. A comparison of experiment and theory reveals the critical current density and the TTA rate constant and shows that the differences in roll-off behavior are predominantly caused by a change of the decay rates inside the OLED cavity. In order to provide guidelines for designing OLEDs with optimal high-brightness efficiency, we model the roll-off as a function of the emitter-cathode distance, emitter dipole orientation, and radiative efficiency.

[1] C. Murawski, K. Leo, and M.C. Gather, Adv. Mater. 10.1002/adma.201301603 (2013).

[2] C. Murawski, P. Liehm, K. Leo, and M.C. Gather, Adv. Funct. Mater. 10.1002/adfm.201302173 (2013).

HL 28.7 Mon 19:30 CHE 91

Solution-based planarization layers for organic solar cells on flexible silver nanowire transparent electrodes — •Jan Ludwig Bormann[1], Franz Selzer[1], Nelli Weiss[2], Lars Müller-Meskamp[1], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, TU Dresden — [2]Physikalische Chemie, TU Dresden

Flexible transparent electrodes made of silver nanowires (AgNWs) are an emerging research field for different optoelectronic devices such as organic transistors, organic light emitting diodes (OLED) and organic photovoltaics (OPV). They exhibit excellent electrical and optical properties (sheet resistance of 11 Ohm/sq at 85% transmittance) and are suitable for the application on flexible substrates. These transparent electrodes show high roughness and therefore require a planarization layer for fabricating efficient small molecule devices.

In this work, solution-based organic materials are processed with spin coating to planarize the AgNW electrode. A solution processed small molecule layer acts as planarizing layer and as hole transport layer in organic solar cells with a bulkheterojunction comprising the fullerene C60 as acceptor and different small molecule donor layers (oligothiophenes and phtalocyanines) . The efficiency of these devices is comparable or even better to reference devices with indium tin oxide (ITO) as transparent electrode.

HL 29: Poster: Organic semiconductors and hybrid organic-inorganic heterostructures / Organic photovoltaics

Time: Monday 17:00–20:00 Location: P2

HL 29.1 Mon 17:00 P2

Photoemission and photoluminescence spectroscopies of hybrid inorganic-organic heterostructures — •Mariel Grace Dimamay[1,2], Abebe Tarekegne[3], Aina Quintilla[3], David Talaga[4], Jules Oriou[2], George Hadziioannou[2], Thomas Mayer[1], and Wolfram Jaegermann[1] — [1]Materials Science Institute, Technische Universität Darmstadt, Darmstadt, Germany — [2]Laboratoire de Chimie des Polymères Organiques, CNRS, Université Bordeaux 1, Pessac, France — [3]Light Technology Institute, Karlsruher Institut für Technologie, Karlsruhe, Germany — [4]Institut des Sciences Moléculaires, CNRS, Université Bordeaux 1, Talence, France

Organic emitters are in general brighter than their inorganic counterparts, but their low carrier mobility still poses limitations to device efficiency. Several schemes are being developed to circumvent such problem by utilizing inorganic phases for carrier injection and transport. Through subsequent direct charge carrier transfer or Förster energy transfer from the inorganic semiconductor to the organic emitter, followed by a radiative recombination, photons could be emitted efficiently. In this study, two hybrid inorganic-organic material systems, namely, ZnSe - Ir(4-tBupiq)2(acac) and nanocrystalline TiO2 - squaraine-derived dye are investigated. Interface properties and energy level lineups are obtained by measurements involving XPS and UPS on evaporated Ir complex emitter molecules on ZnSe and on drop-casted squaraine-derived dye on TiO2. Photoluminescence of composite films are obtained to show a possible Förster transfer of exciton energy from matrix to emitter dopants.

HL 29.2 Mon 17:00 P2

Electronic and structural properties of a novel Picene - F4TCNQ based charge transfer material — •Torsten Hahn[1] and Benjamin Mahns[2] — [1]Institute for Theoretical Physics, TU Freiberg, D-09596 Freiberg — [2]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Based on the resolved crystal structure the electronic structure, optical excitations and transport properties of novel Picene-F4TCNQ mixed crystals have been investigated using experimental as well as theoretical techniques. The results are compared to those of the pure compounds as well as to other charge transfer salts. The density functional theory (DFT) based theoretical calculations together with electron energy loss spectroscopy (EELS) and transport measurement results reveal the details of the charge transfer process and resolve the electronic structure close to the Fermi level.

HL 29.3 Mon 17:00 P2

Charge transfer and electrical conductance at the F_{16}CoPc-Rubrene interface — •Yulia Krupskaya[1], Susi Lindner[2], Benjamin Mahns[2], Martin Knupfer[2], and Alberto Morpurgo[1] — [1]University of Geneva, CH-1211 Geneva, Switzerland — [2]IFW Dresden, D-01171 Dresden, Germany

Here we present an electronic transport study of the F_{16}CoPc-Rubrene interface. Originally both materials Rubrene (5,6,11,12-tetraphenyltetracene) and F_{16}CoPc (cobalt(II) 1,2,3,4,8,9,10,11,15,16,17,18,22,23,24,25-hexadecafluoro-29H,31H-phthalocyanine) are large-gap undoped semiconductors and eventually insulators. The interfaces were prepared by evaporating the F_{16}CoPc film on top of the Rubrene single crystal. Four-probe electronic transport measurements were performed at applied voltages up to 40 V and temperatures between 30 K and 300 K. The measurements reveal the resistivity per square of the interface of approximately 300 kΩ at room temperature, which is in general rather low in comparison to previously studied organic interfaces [1] and lowest after outstanding TTF-TCNQ interface [2]. The obtained temperature dependence indicates slight metallic behavior of the resistivity which decreases by 20 % while cooling from 300 K to 100 K. Below 100 K the resistivity increases reaching 370 kΩ at 30 K. The observed electrical conductance originates from a rather big charge transfer between the two materials that takes place at their interface.

[1] I. Gutiérrez Lezama et al. *Nature Mat.* **11**, 588-794 (2012)
[2] H. Alves et al. *Nature Mat.* **7**, 574-580 (2008)

HL 29.4 Mon 17:00 P2

Correlation between structural and electrical properties of co-evaporated doped organic thin films — •Daniela Donhauser[1,2], Anne K. Kast[1,2,3], Martin Pfannmöller[3], Rasmus R. Schröder[3], Markus Gölz[2,4], Alexander Müller-Brand[2,4], Michael Kröger[1,2], Robert Lovrincic[1,2], and Wolfgang Kowalsky[1,2] — [1]Institut für Hochfrequenztechnik, Technische Universität Braunschweig — [2]InnovationLab GmbH, Heidelberg — [3]CellNetworks, Universität Heidelberg — [4]Kirchhoff-Institut für Physik, Universität Heidelberg

Nowadays, organic devices like OLEDs or OPV are often realized by employing electrochemically doped transport layers to enhance device performance and stability. However, a comprehensive and detailed understanding of the doping process in organic semiconductors is still missing. In this work the organic semiconductor CBP (4'-Bis(N-carbazolyl) -1,1'-biphenyl) doped with the transition metal oxide MoO3 was used as a model system and structural as well as electrical measurements were conducted to gain a better understanding of the fundamentals of electrochemical doping. Electron tomography revealed that the dopant forms a filamentous structure with nanofilaments preferentially orientated perpendicular to the substrate. To investigate whether the structural anisotropy influences the electrical properties, IV- and cryo-IV characteristics of device structures with current flowing along and perpendicular to the substrate were measured. Based on these results a model for charge transport in CBP:MoO3 composites will be presented.

HL 29.5 Mon 17:00 P2

External Quantum Efficiency of novel PTCDA derivatives — •Robin Döring, Nils Rosemann, Eduard Baal, Jörg Sundermeyer, and Sangam Chatterjee — Philipps-Universität Marburg, Marburg, Germany

3,4,9,10 perylene tetracarboxylic dianhydride (PTCDA) is a well-studied and widely commercially available dye and n-channel organic semiconductor. A major disadvantage of PTCDA is its low solubility in organic solvents. We studied the optical properties of novel PTCDA derivatives featuring high solubility in organic solvents such as CH_2Cl_2 and C_7H_8. A "flourophore-spacer-receptor" configuration based photoinduced electron transfer (PET) is assumed. If the PET between the receptor (amine group) and fluorophore (perylene core) within the molecule is suppressed, the PL intensity is expected to increase significantly. Hence, protonation of the amine functional group should disallow PET. This, in turn, makes applications like non-contact sensing of pH possible. The experimental setup features an integrating sphere which allows measurements of the absolute photoluminescence. These measurements then yield the external quantum efficiency η of the samples. In combination with time resolved photoluminescence measurements this enables us to determine the true radiative (τ_r) and non-radiative (τ_{nr}) decay times of the excited states. Our results confirm a strong dependency of the quantum efficiency on the fact whether or not PET is enabled.

HL 29.6 Mon 17:00 P2

Vapour-phase absorption of aromatic molecules — •Niklas Kraus, Sangam Chatterjee, and Andre Rinn — Philipps Universität, Marburg, Deutschland

Organic semiconductors are promising materials for future electronic applications. To understand the complex optical properties of organic molecular crystals, one needs to obtain the single molecular response first. Hence, we investigated the optical properties of different molecules in solution and in the vapour phase. Therefore, we construct an evaporation cell where the optical transmission through a 5cm long gas volume is measured in the 1-6eV energy range. Using this apparatus, we analyzed the vapour-phase absorption and photoluminescence of the aromatic molecules perylene. pentacene, and perfluoropentacene at temperatures up to 590K.

HL 29.7 Mon 17:00 P2

Time-resolved spectroscopy of interfacial states in P3HT-PCBM blends — •Marina Gerhard[1], Andreas Arndt[2], Aina Quintilla[2], Ulrich Lemmer[2], and Martin Koch[1] — [1]Faculty of Physics and Material Sciences Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]Light Technology Insti-

tute, Universität Karlsruhe, Kaiserstrasse 12, D-76131 Karlsruhe, Germany

We have studied the time-resolved photoluminescence (PL) of organic donor-acceptor bulk heterojunctions based on the polymer poly(3-hexylthiophene) (P3HT) blended with varying concentrations of the fullerene derivative [6,6]-phenyl-C61 butyric acid methyl ester (PCBM). Those blends represent a well-known material for potential solar cell applications. By comparing the emission of the blends to that obtained for neat polymer and fullerene films, most of the contributions could be allocated to radiative recombination inside the polymer domains. In addition, we identified a weak but slower decaying signature in the IR-regime that was only present in the blends. We thus attributed this feature to carriers recombining at the interfaces between donor and acceptor. Currently, the role of such interfacial "charge transfer" states in the process of free carrier generation is intensely being discussed. We discovered that the dynamics of the interfacial state was almost independent of temperature and excitation density. These findings indicate that the electrons and holes which cause the interfacial PL-emission are trapped inside isolated states where further diffusion is unlikely.

HL 29.8 Mon 17:00 P2

Effect of the donor-acceptor morphology on the recombination behavior in polymer-fullerene bulk heterojunction solar cells — •Sebastian Wilken, Michael Koopmeiners, Jürgen Parisi, and Holger Borchert — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, Carl-von-Ossietzky-Str. 9-11, 26129 Oldenburg, Germany

In this study, we discuss the impact of the donor-acceptor morphology on the recombination behavior in polymer-fullerene bulk heterojunction solar cells based on poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl-C_{61}-butyric acid methyl ester (PCBM). Different amounts of nanoscale phase separation have been obtained by using 1,2-dichlorobenzene and chlorobenzene as spin-casting solvents, respectively, as is visualized by atomic force microscopy (AFM) and transmission electron microscopy (TEM). Both the current-voltage characteristics and the white-light bias external quantum efficiency with respect to varying illumination intensities suggest that the dominant recombination mechanism, i.e., monomolecular and bimolecular recombination, is strongly correlated with the respective nanomorphology of the P3HT:PCBM blend. To further evaluate the influence of charge carrier trapping, transient photocurrent measurements have been performed and analyzed in terms of emssion time constants $\tau_{e,i}$, assuming that each $\tau_{e,i}$ is characteristic for one distinct trap level i. In addition, the temperature dependence of $\tau_{e,i}$ was investigated to gain information about the thermal activation energy ΔE_i of the corresponding emission process.

HL 29.9 Mon 17:00 P2

Measurement of the harvesting factor under realistic conditions for organic solar cells — •Trinath Reddy Pinnapa, Benjamin Oesen, Johannes Widmer, Rico Meerheim, Christian Koerner, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany

The efficiency of organic solar cells is usually measured under standard reporting conditions (SRC). The efficiency measurements carried out under SRC disregard the influence of varying parameters such as temperature, illumination intensity of sun, angle of incidence, and spectrum of the sunlight, although these varying parameters are very important for the overall energy harvesting. Thus, measurement conditions which are on par with real time data should be used to obtain precise efficiency values. To measure the harvesting factor, the realistic efficiency of cells for a period of one year, the accumulated solar irradiation energy and the efficiency at SRC are to be compared. This study is aimed at measuring the harvesting factor by investigating the performance of a pin structured organic solar cell under realistic conditions, then, the harvesting factor of organics are compared with an equivalent silicon cell. To understand the performance of organic solar cells, efficiency measurements of DCV5T-Me and F4-ZnPc donor cells with respect to changing illumination intensity and temperature are performed and then their respective harvesting factors are estimated.

HL 29.10 Mon 17:00 P2

Charge Carrier Mobility of a Quinquethiophene Derivative Deposited on Heated Substrates — •Julia Oelker, Johannes Widmer, Christian Koerner, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden

The absorber material DCV5T-Me has been successfully used in small molecule organic solar cells. Fundamental properties of this material are of special interest to learn more about the mechanisms that lead to highly efficient solar cells. For organic solar cells with DCV5T-Me and C_{60} as donor-acceptor blend layer, the power conversion efficiency is strongly dependent on the substrate temperature during the deposition of the absorber layer. This parameter is known to change the morphology and the degree of disorder in the blend layer which affects the transport properties.

In this contribution, the carrier mobility as one of the key parameters to achieve highly efficient solar cells is investigated. Electric potential mapping by thickness variation (POEM) is applied to pip-hole-only-devices with DCV5T-Me:C_{60} as intrinsic layer to measure the hole mobility in the blend. The substrate temperature during the deposition of the intrinsic layer is varied to get particular insight into the influence of substrate heating.

HL 29.11 Mon 17:00 P2

White top-emitting OLEDs with nanoparticle scattering layers — •Tim Schaefer[1], Tobias Schwab[1], Simone Hofmann[1], Karl Leo[1], and Malte C. Gather[1,2] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Straße 1, 01069 Dresden, Germany — [2]School of Physics & Astronomy, University of St Andrews, North Haugh, St Andrews, KY16 9SS, Scotland, UK

We present white top-emitting organic light-emitting diodes (OLEDs) with a random nanoparticle scattering layer as outcoupling structure on top of the OLED stack. The nanocomposite scattering layer consists of titanium dioxide particles embedded into a transparent photoresist matrix. The scattering layer can be deposited directly on top of the small molecule OLED stack by solution-based dip- or spin-coating, without affecting the electrical performance of the device. The optical properties of the scattering layer are widely tunable by adjusting particle size and concentration. In first proof-of-principle experiments, the spectral radiant intensity for the blue spectral range of a white top-emitting OLED is nearly doubled and the overall external quantum efficiency at 1000 cd/m^2 is increased by 18% in comparison to a reference device with standard organic capping layer for outcoupling. Furthermore, light scattering by the randomly distributed nanoparticles strongly improves the color stability with viewing angle. The proposed process is cost-efficient, scalable and compatible with different types of substrates and OLED architecture. It is expected that it can be readily adopted for large area OLEDs and is thus promising for lighting applications.

HL 30: Poster: Quantum dots and wires: Preparation, characterization, optical properties and transport

Time: Monday 17:00–20:00 Location: P2

HL 30.1 Mon 17:00 P2

Raman and AFM Characterization of Ultrasmall CdS Nanoparticles Incorporated in Polymeric Matrix — •Dmytro Solonenko[1], Volodymyr Dzhagan[2], Oleksandra Raevska[3], Oleksandr Stroyuk[3], Ovidiu D. Gordan[1], and Dietrich R. T. Zahn[1] — [1]Semiconductor Physics, Technische Universität Chemnitz, Chemnitz, Germany — [2]E. Lashkaryov Institute of Semiconductor Physics, Kyiv, Ukraine — [3]L.V. Pysarzhevskiy Institute of Physical Chemistry, Kyiv, Ukraine

Semiconductor nanoparticles (NPs), or quantum dots, gain wide interest due to anumber of striking features: tunable and narrow features in photoluminescence (PL) and absorption spectra, high chemical and photophysical stability, and high PL quantum yields. Theunique properties of ultrasmall NPs include broadband PL. They can also be strongly influenced by environment and stabilizing ligands. However, both ordinary and ultrasmall NPs should be processed before their applicationin various optoelectronic devices. In this work we investigated the interactions between ultrasmall CdS NPs stabilized by mercaptoacetic acids and ammonia (N2H4) with polymers such as polyethyleneimine (PEI), polyethylene glycol (PEG), and surfactant sodium dodecyl sulfate (SDS) by Raman spectroscopy and AFM. Thin polymer films containing NPs were prepared by spin- and spray-coating. We concluded that neutral polymers such as PEG as well as SDS refrain from chemical interaction with the negatively charged NPs surface, while polycationic PEI chemically reacts with the NPs resulting in the formation of agglomerates in a colloidal phase.

HL 30.2 Mon 17:00 P2

Synthesis and characterization of quantum sized InP nanowires prepared by UTAM surface nano patterning and reactive-ion etching technique — •Lin Cheng, Kin Mun Wong, and Yong Lei — Ilmenau University of Technology, Institute of Physics & IMN MacroNano (ZIK) Prof. Schmidt-Str. 26, 98693 Ilmenau (Germany)

The electronic properties of ultra-small indium phosphide (InP) nanowires had been rarely investigated. When the size of the nanowires is smaller than its Bohr radius, due to the quantum confinement effects, there are many interesting properties in the nanowires. In this study, single crystalline InP nanowires with diameter smaller than its Bohr radius are synthesized by first preparing ultra-thin alumina mask (UTAM) in 0.3M Oxalic acid for 1 min. Then the UTAM was transferred onto a single crystalline InP substrate and the pore size of the UTAM was reduced by atomic layer deposition. Gold or titanium was deposited by physical vapor deposition at the bottom of the pore openings in the UTAM to be used as the mask on the top surface of the InP substrate. Finally, the UTAM was removed and reactive-ion etching was used to prepare the arrays of quantum sized InP single crystalline nanowires in a vacuum chamber. We predict that our quantum sized InP nanowires will have very interesting electronic and transport properties that will be verified with the first-principles simulations on the nanowires.

HL 30.3 Mon 17:00 P2

Characterization of InP-quantum dots in AlGaInP for integration in vertical-cavity surface-emitting lasers as active medium — •Sergey Gelhorn, Susanne Weidenfeld, Thomas Schwarzbäck, Roman Bek, Christian Kessler, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen and Research Center SCoPE, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

With reduction of the dimensionality of the laser active media, differential gain increases which brings advantages like simultaneous low threshold current and high modulation bandwidth. Quantum dots (QDs) are zero-dimensional structures and their usage as laser active media can provide a temperature independent laser threshold current [1]. However, if the difference between QD-energy and bandgap of the surrounding barrier is small, carriers can be thermally excited from QD in the barrier. Therefore thermal stability of QD-layers needs to be controlled to allow their integration as active medium in a laser device. We report about spectral and thermal characterization of InP-QD layers, which were integrated in AlGaInP-barrier during metal-organic vapor-phase epitaxy. The integration of stacked InP-QD layers in vertical-cavity surface-emitting lasers is shown, where we took care that the averaged emission energy properly match the energy of the optical resonator. Finally, experiments to increase the energetic confinement of the InP-QDs are presented.

[1] Y. Arakawa and H. Sakaki, Appl. Phys. Lett. **40**, 939 (1982)

HL 30.4 Mon 17:00 P2

Analysis of the nucleation behavior of quantum dots on planar and prepatterned GaAs substrates for the integration in single-photon devices — •Marc Sartison, Matthias Paul, Ulrich Rengstl, Elisabeth Koroknay, Susanne Weidenfeld, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen and Research Center SCoPE, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

In the last decade, the potential of semiconductor quantum dots for the application in single-photon devices has been widely demonstrated. Most approaches deal with the self-assembly of the quantum dots, but for the functionalization into complex arrangements a precise positioning is essential. In this contribution, we show our routes for the fabrication of single addressable quantum dots (QDs). The growth of the QDs takes place in a metal-organic vapor-phase-epitaxy (MOVPE) system. We have concentrated on two approaches for prepatterning the GaAs substrates for different QD material systems. The first one is to produce a hexagonal hole pattern by microsphere photolithography and wet chemical etching, followed by an overgrowth with GaAs, InGaAs and InAs. The higher expected accumulation of In inside the holes, after InGaAs overgrowth, leads to strain effects changing the nucleation probability above. The second approach of site controlled nucleation of InP is done by wet chemical etched ridges and aperture oxidation. The resulting strain field is expected to support the nucleation probability of InP QDs above the aperture. Structural and optical characterization will show our first efforts.

HL 30.5 Mon 17:00 P2

InAs Quantum Dots at Telecom Wavelengths — •Fabian Olbrich[1], Jan Kettler[1], Matthias Paul[1], Katharina Zeuner[1], Sven Markus Ulrich[1], Michael Jetter[1], Matusala Yacob[2], Mohamed Benjoucef[2], Johann Peter Reithmaier[2], and Peter Michler[1] — [1]University of Stuttgart, Institut für Halbleiteroptik und Funktionelle Grenzflächen (IHFG), Allmandring 3, 70569 Stuttgart, Germany — [2]University of Kassel, Institute of Nanostructure Technologies and Analytics (INA), Heinrich-Plett-Str. 40, 34132 Kassel, Germany

Semiconductor quantum dots have proven to be bright, well-defined and controllable single photon sources with the possibility of creating entangled photon pairs by utilizing the biexciton-exciton-cascade.

Hence they are good candidates to serve as emitters of non-classical light in fiber-based quantum networks with possible applications for quantum cryptography and quantum computers.

Under these circumstances it is desirable for QDs to emit at 1.31 μm (telecom O-band) or 1.55 μm (telecom C-band), which show low absorption. In order to manipulate the emission range of our QDs, mainly three approaches have been made to tune the original GaAs/InAs QDs (920 nm) towards these telecom wavelengths: The deposit of a strain reducing layer, the incorporation of Ga or the usage of an InP substrate.

We are able to show that these QDs are excellent single photon sources and find strong indications for the biexciton-exciton-cascade.

HL 30.6 Mon 17:00 P2

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

To investigate the morphology, structure and behavior of individual one-dimensional nanostructures, so called nanowires (NWs), we have grown single localized Au seeded InAs NWs on GaAs(111)B substrate by molecular beam epitaxy. 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 to increase the aspect-ratio up to 300:1. 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 30.7 Mon 17:00 P2

Indirect exchange interaction between quantum dots in a magnetic field — •Alexander W. Heine[1], Katharina Janzen[2], 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

Quantum dots with an odd number of electrons have a non-zero spin which is a possible realization of a qubit in quantum information processes. An indirect exchange interaction between magnetic moments, the so-called Ruderman-Kittel-Kasuya-Yosida interaction, is a possible mechanism to control this spin qubit.

We investigate the exchange constant J of two localized moments mediated by the electrons in a large circular quantum dot in a perpendicular magnetic field. Our results for the effective interaction show signatures known for both, the exchange couplings in metals and in molecules. This is consistent with the fact, that the quantum dot is intermediate between a large molecule and a metal.

A second effect observed for the localized spin of a quantum dot is the Kondo effect. In our system of two quantum dots separated by an open conducting region the Kondo effect can be used as a spectroscopic tool to demonstrate the presence of the indirect exchange interaction. Measurements are performed in a temperature range of 25 mK to 900 mK. A high perpendicular magnetic field up to 5.5 T is applied. The temperature dependence of the differential conductance is analyzed for varying magnetic field.

HL 30.8 Mon 17:00 P2

Numerical determination of the non-equilibrium many-body statistical operator for a nanowire-based field-effect transistor — •Jose Maria Castelo and Klaus Michael Indlekofer — RheinMain University of Applied Sciences, IMtech / Faculty of Engineering, D-65428 Rüsselsheim, Germany

We present a numerical approach to construct a non-equilibrium many-body statistical operator ρ_{MB} for a semiconductor nanowire-based field-effect transistor (NWFET). As a constraint for ρ_{MB}, we assume that the single-particle density matrix ρ_1 is a given quantity, resulting from a non-equilibrium Green's function calculation for the NWFET for a given set of applied voltages. Two different ON eigenbases for ρ_{MB} are considered in this presentation: (i) a Slater determinant basis of natural orbitals (eigenstates of ρ_1) and (ii) the eigenbasis of the projected many-body Hamiltonian H_{MB} within a relevant Fock subspace of the system. As for the eigenvalues w_K of ρ_{MB}, we furthermore assume that w_K have a generalized Boltzmann form, parameterized by effective chemical potentials of natural orbitals and a given temperature. From the determined ρ_{MB}, in turn, one can calculate expectation values for any observable of the system. As an example, we analyze the electron density and the density-density correlation function for a set of representative equilibrium and non-equilibrium conditions of the NWFET.

HL 30.9 Mon 17:00 P2

Thermal noise in AlGaAs/GaAs-nanostructures — •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, D-33098 Paderborn — [3]Angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum

Transport properties of low-dimensional mesoscopic systems strongly differ from those of bulk materials. When the width of a conducting channel has the scale of the Fermi wavelength, these properties are dominated by the electron's wave characteristics and the channel is referred to as electronic waveguide. We investigate the heat transport through a one-dimensional quantum-wire ring structure fabricated from a AlGaAs/GaAs heterostructure in the presence of an electron temperature gradient at 4.2 K. The temperature gradient is established by the current heating technique. The experimental setup [1] enables the measurement of the Johnson noise and thus the detection of a change in the electron temperature. A global top-gate allows the change of the waveguide's conductance. We present and discuss the results of the heat transport in dependence of the participating one-dimensional transport modes.

[1] S. S. Buchholz, et al, Phys. Rev. B 85, 225301 (2012)

HL 30.10 Mon 17:00 P2

A New Structure for Time-Resolved Transport Spectroscopy of InAs-Quantum Dots — •Sergej Markmann, Patrick A. Labud, Arne Ludwig, Dirk Reuter, and Andreas D. Wieck — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum

Time-Resolved Transport Spectroscopy (TRTS) is a powerful method for the electrical investigation of Quantum Dots (QDs) and provides an access to the equilibrium and the non-equilibrium electron configurations in QDs. Typically the investigation of QDs with TRTS method is done on High Electron Mobility Transistor Structure in which QDs are embedded[1]. In this case, a time resolved conductivity change of the two-dimensional electron gas is an indicator for the charge configuration in the QDs. In this work, we demonstrate a new structure, which could be even more sensitive to charging and discharging events of the QDs. The new structure consists of p+-doped GaAs layer followed by an intrinsic GaAs layer in which InAs-QDs are embedded. On top of the intrinsic layer, a n+-doped GaAs layer is grown, which acts as a sensor for the QDs. Charging and discharging of QDs is controlled by the back-gate (p+-doped GaAs). With a top-gate, it is possible to deplete the channel (n+-doped GaAs layer) and hence control the conductivity of the channel such that the charged QDs may deplete the channel completely.

[1]B. Marquardt, M. Geller, B. Baxevanis, D. Pfannkuche, A. D. Wieck, D. Reuter and A. Lorke, Nature Commun. 2, 209 (2011).

HL 30.11 Mon 17:00 P2

Electron counting in a quantum dot system — •Timo Wagner, Eddy P. Rugeramigabo, and Rolf. J. Haug — Institut für Festlörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany

We study the properties of a topgate defined quantum dot in a GaAs/AlGaAs heterostructure. Besides electronic transport measurements through the dot, we perform charge measurements with an adjacent quantum point contact (QPC) that serves as sensitive detector. These methods allow the characterisation of the dot over a wide range of tunnel couplings and electron numbers.

The analysis of the charge stability diagram reveals a region of a second capacitively coupled quantum dot. In this region electron counting experiments were performed. We are able to detect signals for tunneling rates beween Hz and kHz and for temperatures up to 1.5 K. Further we analyse the stability of the signals.

HL 30.12 Mon 17:00 P2

Top-down fabrication and characterization of silicon nanowire RFETs — •Dipjyoti Deb, Artur Erbe, Manfred Helm, and Jochen Grebing — Helmholtz-Zentrum Dresden-Rossendorf, Center for Advancing Electronics Dresden

The following work illustrates top-down fabrication and characterization of reconfigurable, undoped silicon nanowire field effect transistor with Schottky junctions. The nanowires are fabricated on SOI wafer by electron beam lithography and oxidized for passivation. Two Nickel-Silicide Schottky junctions are formed by Nickel deposition and annealing from source and drain region creating silicide-silicon-silicide contacts. Diffusion of Ni-Si is precisely controlled by radial crystal orientation of the nanowire and annealing temperature. The Schottky junctions are electrostatically controlled by surround gates. Transport properties of these nanowires can be modulated by changing local electrostatic gradient at the gates. One gate can modulate the current density while the other gate can be electrostatically programmed to shift the polarity of the device from N-type to P-type and vice-verse. Nanowire performance is optimized by reducing the edge roughness of the nanowires (lowering the scattering) and accurate alignment of the metal gates.

HL 30.13 Mon 17:00 P2

Electronic Structure and Photoluminescence of Bare Core and Core/shell CdSe QDs — •Ghazal Tofighi[1], Martin Möbius[2], Jörg Martin[3], Christian Spudat[3], Thomas Otto[2], Thomas Gessner[2,3], Ovidiu D. Gordan[1], and Dietrich R.T. Zahn[1] — [1]Technische Universität Chemnitz, Semiconductor Physics, Chem-

nitz, Germany — [2]Technische Universität Chemnitz, ZfM, Chemnitz, Germany — [3]Fraunhofer Institute for Electronic Nano Systems, Chemnitz, Germany

CdSe quantum dots (QDs) exhibit interesting properties including narrow emission bands, good photostability, and bright photoluminescence (PL) which can be tuned by the size of QDs and surface ligands. Therefore, we can integrate them with piezoelectric materials in order to make extremely small film-based sensors. Electrical charges generated by mechanical stress within the piezoelectric film can be injected into QDs, resulting in quenching their photoluminescence. Subsequently, e.g. material failure could thus be detected at an early stage through a color change of the photoluminescence.

For this purpose, we prepared thin layers of CdSe (core) and CdSe/ZnS (core/shell) QDs on gold substrates using the Langmuir-Blodgett method and investigated the electronic structure of QDs by photoemission spectroscopy (PES) and inverse photoemission spectroscopy (IPS). Furthermore, PL measurement and Raman spectroscopy were also performed on the QD layers, and the optical band gap was compared to the electronic band gap achieved from the IPS/UPS measurements.

HL 30.14 Mon 17:00 P2

Capacitance-Voltage Spectroscopy of InAs Quantum Dots Under External Applied Strain — •Sascha René Valentin[1], Arne Ludwig[1], Dirk Reuter[2], and Andreas D. Wieck[1] — [1]Lehrstuhl für Angewandte Festkörperphysik, Ruhr Universität Bochum — [2]Department Physik, 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 30.15 Mon 17:00 P2

All optical approach to determine the spatial extension of bound wave functions in semiconductor quantum dots using intraband spectroscopy — •Sandra Kuhn, Judith Specht, Andreas Knorr, and Marten Richter — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany

Self-assembled semiconductor quantum dots are one of the most extensively studied nanostructures and a variety of applications are based on them. High quality devices require precise information about the structural quantum dot properties, especially about the quantum dot shape and size. However, sophisticated experimental methods such as electron microscopy to identify the quantum dot size have several significant drawbacks.

We propose an all optical spectroscopic pump-probe method to determine the spatial extension of nanoscale electron wave functions in semiconductor quantum dots. In particular, we use intraband transitions between unbound continuum states in the host medium and the bound states to adress the extension of the quantum dot wave function. The developed theoretical scheme is readily applicable to quantum dots embedded in bulk material and can be applied to quantum dots embedded in two dimensional host materials as well with slight modifications. We present an analytical and easy to use formula to extract information about the spatial extension of bound quantum dot states from pump-probe experiments.

HL 30.16 Mon 17:00 P2

Theory of simultaneous time- and frequency-gated fluorescence and Raman spectroscopy in quantum dots — •Anke Zimmermann, Marten Richter, and Andreas Knorr — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstrasse 36, 10632 Berlin, Germany

Time-dependent light scattering and fluorescence of quantum dots are in the focus of current experimental and theoretical research. In particular the combination of time- and frequency-resolved fluorescence allows to inspect dephasing and relaxation mechanisms specifically for single quantum dot spectroscopy. Here, we study the interaction of a laser pulse with the dominant excitonic transition in a quantum dot coupled to phonons.

To determine simultaneously frequency and time-resolved emission properties, a spectral filter is combined with temporal gated detection.

In this way, it is possible to investigate the time and frequency gated fluorescence and the Raman signal including the interaction of electrons and phonons. The resulting equations and numerical evaluations are applied to different kinds of excitation conditions and filters.

HL 30.17 Mon 17:00 P2

Simulation of Correlation Measurements of Exciton and Trion Recombination in Single Quantum Dots, Coupled to a Two-Dimensional Electron Gas — •Benjamin Merkel[1], Annika Kurzmann[1], Arne Ludwig[2], Andreas D. Wieck[2], Axel Lorke[1], and Martin Geller[1] — [1]Faculty of Physics and CeNIDE, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany — [2]Chair of Applied Solid State Physics, Ruhr-Universität Bochum, Universitätsstr. 150, 44780 Bochum, Germany

For optical spectroscopy and coherent exciton state control, self-assembled quantum dots (QDs) are often embedded in a diode structure with a n-doped back contact that allows fast electron tunnelling from the reservoir into the dot states. We use here a different sample structure to investigate the slower electron tunnelling between a single QD and a two-dimensional electron gas and simulate the correlation measurements between the exciton and trion lines.

The occupation of the QD can be controlled with single charge resolution by an applied gate voltage and monitored by measuring the exciton and trion transition line, respectively. However, under non-resonant excitation, different excitonic recombination lines from different charge states can be observed simultaneously in a wide range of gate voltages. We use a model, which describes the capture and escape of QD charges as well as the recombination of exciton states by rate equations. Based on the model, we can simulate correlation measurements of the emitted radiation and are able to reproduce the experimental results.

HL 30.18 Mon 17:00 P2

Simulation and characterisation of an integrated optical beamsplitter based on multimode GaAs/AlAs waveguides with embedded InGaAs/GaAs quantum dots — •Markus Oster[1], Ulrich Rengstl[1], Klaus D. Jöns[1,2], Samir Bounouar[1], Sven M. Ulrich[1], Michael Jetter[1], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]Kavli Institute of Nanoscience Delft, Quantum Transport, Delft University of Technology, PO Box 5046, 2600 GA Delft, The Netherlands

The miniaturization and high-density integration of electronic logic elements into single chip architecture has been a revolutionary development for electronic data processing in the past decades. Nevertheless, in the future perspective to create novel all-optical types of quantum logic structures, the integration of tailored quantum emitters as non-classical light sources into dedicated optical waveguide structures is one of the major aims of research in this field.

Here we report on investigations on multimode GaAs/AlAs waveguides using integrated single InGaAs/GaAs quantum dots as light sources to study the light propagation and beamsplitter operation of the waveguide structures. Our studies reveal waveguide losses of $\alpha = 15.7\,\mathrm{cm}^{-1}$, wavelength-dependent beamsplitter ratios around 0.5/0.5, and a photon polarisation of over 90 %. These results represent an important step towards the realization of semiconductor based integrated photonic quantum circuits.

HL 30.19 Mon 17:00 P2

Spectroscopy and photon-statistics of InP/AlGaInP quantum dots with reduced spatial density — •Mario Schwartz, Christian A. Kessler, Elisabeth Koroknay, Thomas Schwarzbäck, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Allmandring 3, 70569 Stuttgart, Germany

We investigate the optical properties of self-assembled InP/AlGaInP quantum dots (QDs) with a reduced spatial QD density grown by metal-organic vapor-phase epitaxy. We examine how effective an interruption in the phosphine flow (PH_3-stop) during the growth decreases

the spatial QD density, with the aim of finding background free single emission lines without any pre- or postprocessing of the samples. The influence of the PH_3-stop on the decay dynamics of the QD emission is also investigated. They exhibit a second large decay time which arises from a second excitation of the QD due to carriers trapped in the vicinity of the QDs. We found that the magnitude of the second decay channel reduces using lower excitation energies in the range of the band gap of the AlGaInP barrier. In second order correlation measurements performed at low excitation energies $g^{(2)}(0) = 0.015$ is achieved when background emission is neglected.

HL 30.20 Mon 17:00 P2

Simulating SiGe/Si Self-Assembled Quantum Dots — •Torsten Wendav[1], Inga Fischer[2], and Kurt Busch[1,3] — [1]Humboldt Universität zu Berlin, Institut für Physik, AG Theoretische Optik & Photonik, Berlin, Germany — [2]Institute for Semiconductor Engineering, University of Stuttgart, Stuttgart, Germany — [3]Max-Born-Institut, Berlin, Germany

The integration of optoelectronic functionality into Silicon-based devices has been of interest for quite some time. However, this has proven to be difficult, mainly due to material properties of Silicon [1]. A promising approach to circumvent these difficulties is the integration of Germanium quantum dots into Silicon.

While it is easy to grow Germanium quantum dots on Silicon it is hard to experimentally tune their optoelectronic properties, largely due to the sheer amount of growth parameters [3].

In order to obtain a deeper understanding of the relationship between growth parameters and optoelectronic properties of Germanium quantum dots, numerical simulations were performed. Combing both experimental and numerical results leads to a consistent physical picture of SiGe/Si self-assembled quantum dots [4].

[1] R. A. Soref, Proceedings of the IEEE **81**, 1687 (1993).
[2] Y.-H. Kuo, *et al.*, Nature **437**, 1334, 2005.
[3] M. Brehm, *et al.*, J. Appl. Phys. **109**, 123505-1, 2011.
[4] I. Fischer, *et al.*, (In preparation).

HL 30.21 Mon 17:00 P2

Quantum coherence in semiconductor quantum dot molecules — •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 coherence effects such as electromagnetically induced transparency and amplification without inversion are well known in atomic few-level systems. Quantum dots, which are arguably the closest realization of an atomic-like system in semiconductors, are natural candidates for the realization of quantum coherence phenomena in solids. However, typical room temperature dephasing times limit the achievable quantum coherence effects. We present theoretical results of electromagnetically induced transparency and group-velocity slowdown for optical pulses in InGaAs-based double quantum dot molecules. These are designed to exhibit a long lived coherence between two electronic levels whereby a V-type pump-probe scheme for the investigation of quantum coherence effects is achievable. We apply a many-particle approach including microscopic scattering and dephasing based on realistic semiconductor parameters that allows us to calculate the spatio-temporal material dynamics coupled to the propagating optical field. The dependences of slowdown and shape of the propagating probe pulses on lattice temperature and pump intensities are investigated. The probe pulse slowdown in the double quantum dot molecule is shown to be substantially higher than what is achievable from similar transitions in typical InGaAs-based single quantum dots.

HL 30.22 Mon 17:00 P2

Computational study of CdSe and PbSe quantum dot structures — •Farzana Aslam and Christian von Ferber — AMRC, Coventry University, Coventry, UK

Applying computational time dependent density functional techniques we analyse small structures of potential quantum dot material. In particular, we focus on the optical properties of these dots observing the effects of cluster size, the cluster composition, capping ligands and complexation.

HL 30.23 Mon 17:00 P2

Optical Spectroscopy of Site-Controlled InAs Quantum Dots — •Julia Susan Wiegand[1], Ramin Dahbashi[1], Christian Mayer[2], Jens Hübner[1], Daniel Schaadt[2], and Michael Oestreich[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, Abteilung Nanostrukturen, Appelstraße 2, D-30167 Hannover, Germany — [2]Technische Universität Clausthal, Institut für Energieforschung und Physikalische Technologien, Leibnizstraße 4, D-38678 Clausthal-Zellerfeld, Germany

Site-controlled quantum dots (SCQDs) are well suited candidates for a number of future applications in quantum-optronics. For device applications with novel functionalities - such as deterministic single photon sources - controlled positioning of QDs with high structural and electronic quality is desirable for scalable fabrication. We investigate SCQDs grown by molecular beam epitaxy on pre-patterned GaAs substrates [1] by optical high precision low-temperature microphotoluminescence spectroscopy. The optical spatial resolution shows the successful controlled nucleation at the predefined sites. The photoluminescence spectra yield a measure of the SCQDs' optical quality which is influenced by defects created in the prepatterning process.

[1] Helfrich *et al.*, Growth and characterization of site-selective quantum dots, Phys. Stat. Sol. A **209**, 2387 (2012).

HL 30.24 Mon 17:00 P2

Investigation of CdS nanowire lasing emission — Robert Röder[1], •Max Riediger[1], Daniel Ploss[2], Adrian Kriesch[2], Ulf Peschel[2], and Carsten Ronning[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena — [2]Institut für Optik, Information und Photonik, Friedrich-Alexander Universität Erlangen-Nürnberg, Staudstraße 7, 91058 Erlangen

Nanophotonic on-chip integrated components are a promising approach to overcome forthcoming limitations of electronic integrated circuits. Optical data transmission and processing by exploiting semiconductor nanowires, which offer efficient waveguide properties and mark the lower size limit of photonic laser systems, builds a possible route to overcome these challenges. High quality cadmium sulfide nanowires (CdS NW) open up the green spectral range around 2.4 eV acting as Fabry-Pérot laser resonators with a remarkable low threshold of 10 kW/cm^2 at room temperature [Geburt et al, Nanotechnology 23, 365204 (2012)] and operating even in cw emission mode [Röder et al, Nano Letters 13, 3602 (2013)]. Since optical processing is specified by the direct emission of the device, a head-on setup was developed to investigate the light output originating from the end facet of a single nanowire laser. This setup is suited to determine super luminescence (ASE) as well as lasing emission dependent on the polarization of the optical pump beam. Furthermore the angular distribution of nanowire lasing emission can be measured.

HL 30.25 Mon 17:00 P2

Intense intra-3d luminescence and waveguide properties of single Co doped ZnO nanowires — Sebastian Geburt[1], •Markus Schwiderke[1], Robert Röder[1], Uwe Kaiser[2], Wolfram Heimbrodt[2], and Carsten Ronning[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, D-07743 Jena — [2]Fachbereich Physik, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg

The transition metal Co is well-known as optically active luminescence center in semiconductors. Cobalt doped nanowires would therefore take advantage of their morphology in providing photonic waveguiding for new optoelectronic nano-devices such as nanowire LEDs or nanolasers. Homogeneous doping of ZnO nanowires (NW) with transition metal Co is achieved by ion implantation and subsequent annealing procedures provide excellent optical activation of the luminescence centers. Excitation of the Co ions was observed by either resonant absorption or by energy transfer from the ZnO host with lifetimes of ˜ 8 ns. The waveguide properties of single doped NWs were characterized using spatially resolved microPL-measurements [Geburt et al, Phys. status solidi (RRL), 10/2013, 886].

HL 30.26 Mon 17:00 P2

InGaN/GaN nanowire heterostructures as optical probes for oxygen-related surface processes — •Pascal Hille[1], Marius Günther[1], Paula Neuderth[1], Pascal Becker[1], Jörg Teubert[1], Jörg Schörmann[1], Matthias Kleine-Boymann[2], Mariona Coll[3], Jordi Arbiol[3,4], Jürgen Janek[2], Bernd Smarsly[2], and Martin Eickhoff[1] — [1]I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Germany — [2]Physikalisch-Chemisches Institut, Justus-Liebig-Universität Gießen, Germany — [3]Ciencia de Materials de Barcelona,CSIC, Campus de la UAB, 08193 Bellaterra, CAT, Spain

— [4]ICREA, Campus de la UAB, 08193 Bellaterra, CAT, Spain

InGaN/GaN nanowire heterostructures (NWHs) show a high sensitivity of their photoluminescence (PL) intensity to the ambient atmosphere rendering them as promising candidates for gas-sensor applications with all-optical readout in the visible spectral range. InGaN/GaN NWHs were grown by plasma-assisted molecular beam epitaxy. Exposure to ppm-concentrations of oxygen leads to a quenching of the PL intensity. This PL response behaviour is investigated for undoped and Ge-doped InGaN/GaN NWHs. A comparison with GaN NWs yields much longer (≈10x) response times of undoped InGaN/GaN NWHs. These time constants, however, can be significantly reduced by Ge-doping. Possible mechanisms will be discussed. Additionally, InGaN/GaN NWHs covered with CeO_2 were investigated in order to assess the potential of NWHs for an optical detection of ad-/desorption processes at catalytic materials.

HL 30.27 Mon 17:00 P2

Optical Properties of Rare-Earth doped InAs Quantum Dots — •Markus K. Greff, Arne Ludwig, and Andreas D. Wieck — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Opto-electronical devices like LEDs or lasers are included in nearly every technical product nowadays. One point that has led to their importance, is the broad tunability of optical properties of these devices. For example, by doping Gallium-Nitride (GaN) with rare-earth materials (RE) it is now possible to build full-colour LEDs and lasers. Here, we concentrate on systems with a lower bandgap: Combining RE with spintronics, exploiting both charge and spin of carriers, will allow to tune the optical and electrical properties of these devices further. In this work we show the successful doping of Indium-Arsenide (InAs) Quantum Dots (QDs) in a Gallium-Arsenide (GaAs) matrix with the rare-earth element Europium (Eu). We assume that the doping significantly shifts the photoluminescence (PL) spectrum of the QDs towards higher energies (blue shift) due to a diffusion-driven process in which a new sub-ensemble of Eu-doped QDs is formed during an additional annealing step. This is a first step towards further optical and electrical experiments and future spintronic applications of these QDs.

HL 31: Poster: Nitrides

Time: Monday 17:00–20:00 Location: P2

HL 31.1 Mon 17:00 P2

Time-resolved photoluminescence studies of Ge-doped gallium nitride nanowires — •Evelyn Röder[1], Nils Rosemann[1], Pascal Becker[2], Jörg Teubert[2], Martin Eickhoff[2], and Sangam Chatterjee[1] — [1]Philipps-Universität Marburg, Marburg, Germany — [2]I. Physikalisches Institut Justus-Liebig-Universität Gießen, Gießen, Germany

GaN nanowires (NWs) exhibit their large surface-to-volume ratio makes them ideal systems to investigate surface-related effects such as the influence of, e.g., band bending. Additionally, these NWs exhibit a low defect density due to the self-assembly during growth. This makes them an ideal system to investigate the influence of doping on the crystal structure and the related optical properties. Previous studies investigated the influence of Si- and Mg-doping on such NWs[1]. These structures show a quenching of the luminescence due to surface band bending. This quenching also shows a non-linear dependence on the doping. As a next step the doping was changed to the germanium, which has a much larger covalent radius than Si or Mg. We studied several Ge-doped ensembles of GaN nanowires using a standard streak-camera setup. By this the spectral shift and changes in the dynamics of carriers, due to the doping are obtained.[1] J. Appl. Phys. 104(7), 074309, (2008)

HL 31.2 Mon 17:00 P2

The role of Si during the growth of GaN micro- and nanorods — •Christian Tessarek[1], Martin Heilmann[1], Christel Dieker[2], Erdmann spiecker[2], and Silke Christiansen[1,3] — [1]Max Planck Institute for the Science of Light, Erlangen — [2]University Erlangen-Nuremberg, Center for Nanoanalysis and Electron Microscopy, Erlangen — [3]Helmholtz Centre Berlin for Materials and Energy, Berlin

Self-assembled GaN micro- and nanorods on sapphire substrates have been grown by metal-organic vapor phase epitaxy via a self-catalyzed vapor-liquid-solid (VLS) growth mode [1]. The aspect ratio/vertical growth of the rods is strongly dependent on the Si/Ga ratio. Furthermore, Si improves the rod morphology and rods with a regular hexagonal shape, smooth sidewall facets and sharp edges are obtained. Whispering gallery modes are observed in optical investigations representing the high quality of the rods [2].

Structural investigations have been carried out utilizing transmission electron microscopy and energy dispersive X-ray spectroscopy. A SiN layer is existing on the sidewall facets of the GaN rods. The SiN layer acts as an antisurfactant for GaN and is thus stabilizing the sidewall facets. The influence of the SiN layer on the thermal resistivity and on the subsequent InGaN quantum well growth will be discussed. Finally, a model will be presented explaining the role of Si during the VLS GaN rod growth [3].

[1] C. Tessarek et al., J. Appl. Phys. **114**, 144304 (2013). [2] C. Tessarek et al., Opt. Express **21**, 2733 (2013), and Jpn. J. Appl. Phys. **52**, 08JE09 (2013). [3] C. Tessarek et al., Cryst. Growth Des., submitted.

HL 31.3 Mon 17:00 P2

Terahertz spectroscopy of electron transport in GaN — •Thomas Rene Arend[1], Stefan Gerhard Engelbrecht[1], Menno Johannes Kappers[2], and Roland Kersting[1] — [1]Photonics and Optoelectronics Group, Ludwig-Maximilians-Universität München, Germany — [2]Department of Materials Science and Metallurgy, University of Cambridge, UK

Structural imperfections in epitaxial GaN, such as threading dislocations and surface inhomogeneities limit the electronic conductivity. Terahertz (THz) spectroscopy is applied for characterizing charge transport in n-doped GaN fabricated by MOVPE. We use Schottky devices that allow for switching the electron density. The resulting differential THz signal is proportional to the high frequency conductivity of the electrons. Devices with low threading dislocation density (4e8cm-2) and low doping density (5e16cm-3) show the classical Drude response. Increasing the dislocation density to 4e9cm-2 leads to unexpected deviations from Drude behavior, such as a negative imaginary conductivity at low frequencies. Even more drastic is the impact of a high doping concentration (4e18cm-3), which leads to a negative imaginary conductivity over the entire THz spectrum accessible. The experimental data are well reproduced by the Bruggeman model, where we assume a conducting and an insulating phase. The calculations deliver the ratios of the components as well as scattering times and mobilities. In all samples, the scattering times are about 50fs. But increasing the doping concentration or the density of threading dislocations decreases the volume fraction of the conducting phase from 95% to about 50%.

HL 31.4 Mon 17:00 P2

Oxidative chemical vapor deposition of p-conductive polymers on ZnO and GaN — •Max Rückmann[1], Stephanie Bley[1], Florian Meierhofer[2], Jens Reinhold[2], Lutz Mädler[2], Jürgen Gutowski[1], and Tobias Voss[1] — [1]Institute of Solid State Physics, Semiconductor Optics, University of Bremen, 28359 Bremen, Germany — [2]Foundation Institute of Materials Science (IWT), Department of Production Engineering, University of Bremen, Germany

Semiconducting ZnO and GaN nanowires can be used as optoelectronic components if a pn-junction can be realized. One possibility to create such a junction is the deposition of organic p-conductive polymers (here: polypyrrole (PP) and poly(3,4)-ethylenedioxythiophene (PEDOT)) on to the surface. For the deposition of polymer layers, we use oxidative chemical vapor deposition (oCVD), with a monomer and an oxidizing agent (here: $FeCl_3$) in the gaseous phase, respectively. A constant flow of the monomer, supported by nitrogen carrier gas, passes the reaction chamber while the oxidizing agent evaporates and initiates the polymerization and thus p-doping directly on the sample surface. We demonstrate that a homogenous, thickness controlled coating of different ZnO and GaN samples can be achieved by carefully adjusting the process parameters like reaction time, substrate temperature, and the oxidizing agent's amount and evaporation temperature. We

discuss the results of structural, optical and electrical characterization of the hybrid structures for different deposition parameters.

HL 31.5 Mon 17:00 P2

Optical investigations of exciton-phonon coupling in GaInN quantum wells — •Manuela Klisch, Fedor Alexej Ketzer, Torsten Langer, Heiko Bremers, Uwe Rossow, and Andreas Hangleiter — Institut für Angewandte Physik, TU Braunschweig

The photoluminescence of GaInN quantum wells shows asymmetric luminescence spectra, which can be consistently explained via sidebands due to coupling of excitons with longitudinal optical phonons (LO-phonons) and due to Fabry-Perot interferences. Therefore we investigate different GaInN quantum well structures grown via low pressure MOVPE by continuous wave photoluminescence. The Huang-Rhys factor, which describes the coupling strength between electron-hole pairs and LO-phonons, is determined by a fit considering Fabry-Perot interferences and up to three LO-phonon sidebands. To determine the origin of the strong coupling between LO-phonons and the recombining electron-hole pairs we change several parameters. The Huang-Rhys factor is analysed as a function of temperature, well width and indium content. We observe that the Huang-Rhys factor increases with the well width and indium content. For this effect we provide an explanation that compares excitons to donor-acceptor pairs considering the Huang-Rhys factor. We observe a thermally activated behavior of the Huang-Rhys factor. At temperatures below 120 K, this behavior is consistent with a thermalization of excitons and the S-shaped temperature dependence of the emission energy. Towards higher temperature, monotonously increasing Huang-Rhys factors are observed likely due to contributions of excitonic 2s states.

HL 31.6 Mon 17:00 P2

GaInN/GaN multiple quantum well structures grown via plasma-assisted MBE — •Patricia Herbst, Christopher Hein, Andreas Kraus, Fedor Alexej Ketzer, Ronald Buss, Heiko Bremers, Uwe Rossow, and Andreas Hangleiter — Institute of Applied Physics, TU Braunschweig, Germany

The material system containing the group-III-nitrides takes an important role for optoelectronic devices, e.g. light-emitting diodes (LED). In particular, the promising features of GaInN/GaN multiple quantum wells (MQW) need further studies because the physical processes taking place are not fully understood. The growth of GaInN/GaN single layers as well as MQW was investigated using a RF-MBE (RIBER 32). Indium concentrations, surface morphologies, relaxation and layer thicknesses were analyzed in the growth temperature range from 470°C up to 750°C at different fluxes. Varying layer thicknesses (1-45nm) were analyzed revealing a correlation between indium concentration, relaxation and layer thickness. With increasing layer thickness InGaN relaxes and a higher indium concentration is detected. A five fold $Ga_{0.89}In_{0.11}N$/GaN MQW was realized emitting at 2.84 eV (15K). Superlattice fringes with pendellösungen appear in XRD measurements around the (0002)-Bragg reflection. The predicted In-concentration via XRD corresponds to the photoluminescence spectroscopy data. Even at 300K a quantum well emission could be observed corresponding to an internal quantum efficiency of 0.2%.

HL 31.7 Mon 17:00 P2

RF-MBE growth of AlN on sapphire utilizing AlN nucleation layers — •Christopher Hein, Andreas Kraus, Heiko Bremers, Uwe Rossow, and Andreas Hangleiter — Institute of Applied Physics, TU-Braunschweig, Germany

AlN is a promising material for laser as well as quantum well structures due to its high thermal conductivity and stability as well as large bandgap. Further AlN can be used to grow self assembled GaN quantum dots. We report on our AlN growth on sapphire with a Riber 32P RF-MBE. Experiments cover the investigation of the influence of nucleation layers. Before growth a nitridation step at a temperature of 200°C was performed. AlN nucleation layers were grown at 400°C. 500 nm thick epilayers were grown at 700°C using either continuous or metal modulated epitaxy. Growth rates were 3.4 nm/min with a III/V ratio of ~ 1. AFM micrographs of samples with increasing nucleation layer thickness show a decreasing RMS roughness down to 0.7 nm. Strikingly a narrow peak in symmetric XRD omega scans was observed, whose FWHM was resolution limited. The appearance of the narrow peak is also seen in MOVPE grown AlN on sapphire for layer thicknesses below 1-2 μm. It is assumed to originate from an interference effect of small crystallites highly ordered in c-direction. This assumption can be confirmed by our experiments with increasing AlN nucleation layer thicknesses giving rise to smaller grains as seen by AFM. Relating this to the results from omega scans, the intensity of the narrow peak decreases with increasing nucleation layer thickness, hinting at a correlation between grain size and the interference.

HL 31.8 Mon 17:00 P2

Photoreflectance studies on InGaN/GaN multi-quantum well structures — •Stefan Freytag[1], Christoph Berger[1], Pavel Y. Bokov[2], Armin Dadgar[1], Rüdiger Goldhahn[1], Alois Krost[1], and Martin Feneberg[1] — [1]Institut für Experimentelle Physik , Otto-von-Guericke-Universität, Magdeburg, Germany — [2]Moscow State University, Moscow, Russia

Wurtzite(0001) oriented InGaN/GaN multi-quantum well structures were investigated by photoreflectance spectroscopy at variable temperatures. To achieve a systematic understanding, structures were varied from sample to sample, i.e. quantum well thickness, barrier thickness, number of quantum wells and the width of the cap layer. We clearly observe free excitons in the GaN matrix and find a very prominent photoreflectance feature from the InGaN quantum wells. The energy position of this contribution as a function of temperature is compared to photoluminescence yielding data on localization effects. Finally, additional features in photoreflectance which are located energetically between the quantum wells and the GaN excitons are found and possible origins are discussed.

HL 31.9 Mon 17:00 P2

Structural and luminescence properties of an AlInN/AlGaN based microcavity structure — •Max Trippel, Gordon Schmidt, Peter Veit, Frank Bertram, Christoph Berger, Armin Dadgar, Alois Krost, 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. In addition, the temperature dependence of the spectral characteristics of the active medium were investigated by photoluminescence.

The MC structure was grown by metal-organic vapor phase epitaxy (MOVPE) on a c-plane sapphire substrate with an optimized AlGaN buffer structure. A lattice matched 45 pairs $Al_{0.85}In_{0.15}N/Al_{0.2}Ga_{0.8}N$ distributed Bragg reflector (DBR) operates as the bottom mirror. The active medium consists of an InGaN/AlGaN multiple quantum well (MQW) embedded in a λ-cavity.

At 4.2 K the photoluminescence spectrum is dominated by the MQW emission at about 360 nm followed by sideband peaks at 370 nm and 383 nm which are assigned to longitudinal optical phonon replica. The STEM-CL images clearly resolve the complete stacking sequence of the MC structure. Highly spatially resolved STEM-CL linescans reveal a constant MQW peak position along growth direction indicating spectrally identical QWs. Within the DBR stack, we observe an emission at about 335 nm originating from the AlGaN layers.

HL 31.10 Mon 17:00 P2

MOVPE growth of group III-Nitrides on ruthenium coated silicon and sapphire substrates — •Silvio Neugebauer, Armin Dadgar, Jürgen Bläsing, Peter Veit, and Alois Krost — Institute of Experimental Physics, Otto-von- Guericke-University Magdeburg, Germany

We present results on MOVPE growth of group III-Nitrides on ruthenium coated sapphire and high index silicon substrates. The growth on high index silicon substrates is a promising way for achieving semipolar GaN and hence a possibility to overcome the spontaneous and piezoelectric polarization field in conventionally grown c-axis devices. Unfortunately, the received GaN c-axis tilt angle with respect to the surface normal is a function of AlN seed layer thickness for a given high index silicon substrate. Higher tilt angles were achieved for thinner AlN seed layers with the drawback of an increased chance of melt-back etching. Therefore we investigated the application of a ruthenium layer deposited on the silicon substrate serving the purposes of a higher GaN c-axis tilt angle and reduced melt-back etching. On the other hand the deposition of ruthenium on sapphire substrates seems to be quite promising for the growth of III-Nitrides. The lattice mismatch of ruthenium compared to sapphire is as small as -1.5% and -1.1% along the a- and c-direction respectively. This is an excellent requirement for the epitaxial growth of film bulk acoustic wave resonators, which essentially consists of a piezoelectric thin film in a matrix of two electrodes. Unfortunately the growth of III-Nitrides on ruthenium is quite challenging. The possibilities and limitations are discussed.

HL 31.11 Mon 17:00 P2

Morphology and atomic structure of GaN surfaces and InGaN/GaN quantum wells — •Sabine Alamé[1], Andrea Navarro-Quezada[1], Daria Skuridina[2], Tim Wernicke[2], Michael Kneissl[2], Patrick Vogt[2], and Norbert Esser[1,2] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V. — [2]Technische Universität Berlin, Institut für Festkörperphysik, Germany

We present a study on the morphology and optoelectronic properties of buried group-III polar $In_{0.11}Ga_{0.89}N$ and $In_{0.07}Ga_{0.93}N$ single quantum wells (SQWs) upon (0001) surface preparation. The SQWs were grown in a GaN matrix by MOVPE on sapphire substrate, with thicknesses of 3 to 5 nm, the thicknesses of the GaN cap layers were varied from 1 to 10 nm. For the surface preparation the samples underwent thermal annealing between 400°C and 800°C under ultra high vacuum conditions and in nitrogen plasma. X-ray photoelectron spectroscopy revealed, that annealing up to 650°C in nitrogen plasma ambient removes about 90 % of surface oxides and carbons from the oxidized surface without affecting the emission of the underlying SQW, as determined by photoluminescence spectroscopy. It was found, that the indium content of the QWs decreases, whereas the emission wavelength seems not to be changed within the error margin. Low energy electron diffraction showed a (2x2) surface symmetry for the annealed GaN (0001) cap layers, with an increasing surface order for higher annealing temperatures. Clean surfaces in combination with conserved optical properties of the SQWs serve as a starting point for further studies on the interaction of adsorbates with the SQW layers.

HL 31.12 Mon 17:00 P2

Analysis of semipolar gallium nitride layers by μ-Raman spectroscopy — •Lisa Hiller[1], Philipp Schustek[1], Matthias Hocker[1], Sebastian Bauer[1], Marian Caliebe[2], Tobias Meisch[2], Ferdinand Scholz[2], and Klaus Thonke[1] — [1]Institute of Quantum Matter / Semiconductor Physics Group, Ulm University, 89081 Ulm, Germany — [2]Institute of Optoelectronics, Ulm University, 89081 Ulm, Germany

In recent years, great efforts have been undertaken to explore semipolar gallium nitride (GaN) layers, which are predicted to reduce significantly the built-in electric fields. We investigate thick semipolar $(11\bar{2}2)$-oriented GaN layers grown on pre-structured sapphire by a sequence of metalorganic vapour phase epitaxy and hydride vapour phase epitaxy.

Confocal Raman spectroscopy with micron-scale resolution gives access to bulk information by non-destructive depth resolved scanning of the sample. The strain analysis on the basis of Raman tensor elements provides a tool of determining local strain fields, which we compare to finite element based simulations. It allows us to characterize different structural domains resulting from the two different growth processes. Furthermore, uncontrolled high dopant concentrations could be identified by the observation of coupled phonon-plasmon modes. Spatially and spectrally resolved cathodoluminescence and secondary ion mass spectrometry confirm these findings.

HL 31.13 Mon 17:00 P2

Development of a dedicated low noise EBIC measurement system — •Manuel Knab[1], Matthias Hocker[1], Ingo Tischer[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 Optoelectronics, University of Ulm

The homogeneity of the active region has a major impact on the efficiency of semiconductor-based light emitting devices. Electron beam induced current (EBIC) is a measurement technique for the characterization of semiconductors inside a scanning electron microscope (SEM). It is mainly used to visualize and locate the active region of light emitting diodes (LED) and for other regions with built-in fields. It also allows to determine the minority carrier diffusion length in semiconductors.

The concept of our system is the amplification of the signal directly inside the SEM in close vicinity of the sample to avoid stray capacitances, and to obtain a low noise EBIC signal with maximum bandwidth. An optimized current amplifier is integrated directly into the sample holder in order to amplify the electron beam induced current in the nA range. Furthermore, it is possible to obtain sample images by recording directly the current absorbed by the specimen. The advantage of this method is to have no detector shading contrast by the sample surface shape.

HL 32: Poster: ZnO and its relatives

Time: Monday 17:00–20:00 Location: P2

HL 32.1 Mon 17:00 P2

Method of choice for the fabrication of high-quality ZnO thin film based Schottky diodes — •Stefan Müller[1], Holger von Wenckstern[1], Florian Schmidt[1], Robert Heinhold[2], Martin Allen[2], and Marius Grundmann[1] — [1]Universität Leipzig, Semiconductor Physics Group, Institut für Experimentelle Physik II, Leipzig, Germany — [2]The MacDiarmid Institute for Advanced Materials and Nanotechnology, University of Canterbury, Christchurch 8043, New Zealand

In this contribution we present a comprehensive comparison of electrical properties of differently fabricated high quality Schottky contacts on ZnO thin films grown by pulsed laser deposition. Thermally evaporated Pd/ZnO Schottky contacts exhibit ideality factors as low as 1.06 due to their high lateral homogeneity. The effective Richardson constant of such Schottky contacts is with $7.7 \pm 4.8\,\mathrm{A\,cm^{-2}\,K^{-2}}$ close to the theoretical value of $32\,\mathrm{A\,cm^{-2}\,K^{-2}}$. At the same time the on/off ratio of such Schottky contacts is at most five orders of magnitude due to their comparably small effective barrier height ($\approx 0.7\,\mathrm{eV}$). The largest effective barrier heights up to 1.11 eV and on/off ratios up to 7×10^{10} were obtained for reactively sputtered PdO_x/ZnO Schottky contacts. However, the ideality factors are increased to 1.3. Eclipse pulsed laser deposited IrO_x/ZnO Schottky contacts combine the very good homogeneity ($n \approx 1.1$), the large barrier height (0.96 eV) and large on/off ratio (≈ 9 orders of magnitude) of evaporated and sputtered contacts.

HL 32.2 Mon 17:00 P2

Low frequency noise in ZnO-based MESFETs — •Fabian J. Klüpfel, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Fakultät für Physik und Geowissenschaften, Linnéstr. 5, 04103 Leipzig

We examined the sources of noise in metal-semiconductor field-effect transistors (MESFETs) based on n-type ZnO channels on a-plane sapphire substrates for frequencies up to 100 kHz. Measurements have been performed in dependence on the channel geometry prior and after gate deposition. The noise has also been characterized depending on the applied source-drain voltage. In addition to thermal noise a contribution with a 1/f power density spectrum can be observed at ZnO channels without gate, which is best described by a generation-recombination process in the semiconductor with a broad range of attributed time constants. To realize MESFETs we used reactively sputtered platinum Schottky contacts. The noise measured at ungated channels and at Schottky contacts was compared with the drain current noise of the transistors, in order to identify the dominating source of noise and its dependence on geometrical parameters. The results can be used to improve the signal-to-noise ratio in ZnO-based sensor applications.

HL 32.3 Mon 17:00 P2

Electrical and optical properties of (Mg,Zn)O:Al thin films for solar cell application — •A. Mavlonov, H. von Wenckstern, S. Richter, R. Schmidt-Grund, and M. Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig, Germany

We investigated electrical, and optical properties of $Mg_xZn_{1-x}O$:Al thin films in dependence on the aluminum concentration. For that we used a thin film with two perpendicular, lateral composition gradients (of Al and Mg, respectively). The sample was grown by pulsed-laser deposition (PLD) using a single but threefold segmented PLD target [1]. The spatial variation of chemical composition was investigated by energy dispersive X-ray (EDX) spectroscopy. The free carrier density and the mobility were determined by Hall-effect measurement. For a fixed Al concentration the bandgap increases systematically with increasing

Mg content, and the plasma frequency, determined from IR spectroscopic ellipsometry decreases due to an increase of the effective electron mass. As expected, increasing the Al dopant concentration led to an increase of the free carrier density (varying between $2-9\times10^{20}\mathrm{cm}^{-3}$) and conductivity, and a minor decrease of the mobility. The absorption edge increases also with increasing Al concentration due to the Burstein-Moss effect. The reduced electron mass was calculated for different Mg content x, being $0.62\mathrm{m}_e$, $0.71\mathrm{m}_e$ and $0.78\mathrm{m}_e$ for x=0.01, 0.03 and 0.05, respectively.

[1] H. von Wenckstern *et al.*: CrystEngComm 15, 10020-10027 (2013).

HL 32.4 Mon 17:00 P2

Terahertz spectroscopy on electron transport in disordered zinc oxide — •Stefan Gerhard Engelbrecht, Ludovica De Angelis, Marc Tönnies, and Roland Kersting — Photonics and Optoelectronic Group, Physics Department and Center for NanoScience (CeNS), Ludwig-Maximilians-Universität München, Germany

The characterization of disordered semiconductors by conventional electronic techniques is challenging since slow processes such as hopping transport or scattering at grain boundaries mask the fast transport within the crystallites. Terahertz (THz) time-domain spectroscopy offers an alternative approach for characterizing charge transport in disordered semiconductors. We report on THz spectroscopy of electron transport in nanocrystalline zinc oxide deposited by spray pyrolysis. In our experiments, the electromodulation of charge carriers in the ZnO films leads to a differential THz signal, which provides the AC conductivity. The experiments reveal an unexpected deviation from Drude transport that exhibits a negative imaginary conductivity over the accessible frequency range. Both, the Drude-Smith model as well as the Bruggeman model reproduce the experimental data well. The analysis delivers the fundamental scattering times and reveals the percolated nature of high frequency conductivity in disordered films.

HL 32.5 Mon 17:00 P2

IR absorption study of cobalt doped ZnO — •Preeti Pandey[1,2], Edward V. Lavrov[1], and Jörg Weber[1] — [1]Technische Universität, 01062 Dresden, Germany — [2]Indian Institute of Technology Roorkee, Roorkee, India

Ferromagnetic Diluted Magnetic Semiconductors (DMSs) are expected to be a potential candidate for spin dependent electronics known as spintronics. Prediction of room temperature ferromagnetism in transition metal doped ZnO has initiated extensive research in this area [1]. Although much of research has been done regarding the electrical and magnetic properties of the material, it is equally important to analyze the optical properties. Vapor phase grown ZnO crystals doped with cobalt have been investigated by means of FTIR spectroscopy. Along with the temperature dependent spectra, polarized spectra of $Co^{2+}(d^7)$ ions occupying substitutional Zn sites have been studied. Absorption lines due to $^4A_2(F) \rightarrow {}^4T_2(F)$ transitions positioned at 3609.4, 3614.9, 3628.5 and 3634.1 cm^{-1} are observed. Effect of hydrogen treatment on the cobalt-related complexes has also been probed.
[1]. T. Dietl et al., Science, Vol. 287, 1019, 2000

HL 32.6 Mon 17:00 P2

Low-temperature ZnO buffer for high-quality ZnO epitaxy on Si(111) substrate grown by molecular beam epitaxy — •Manuel H. W. Bader and Cedrik Meier — University of Paderborn, Experimental Physics & CeOPP, Warburger Str. 100, 33098 Paderborn.

Due to its unique properties such as the large direct bandgap of 3.37eV and its high exciton binding energy of 60meV, zinc oxide (ZnO) is a very promising semiconductor for optoelectronic and photonic applications even at room temperature. Especially quantum wells and multi-quantum wells can function as light emitting sources inside photonic devices. Therefore, thin ZnO films have been grown in a plasma-assisted molecular beam epitaxy system using Silicon (111) substrates. Growth conditions were systematically studied using ex-situ atomic force microscopy (AFM), x-ray diffraction (XRD) and photoluminescence (PL). Due to the large mismatch between the in-plane lattice constants of ZnO(0001) and Si(111), usually granular films are obtained. A solution capable of overcoming the effects of the undesired mismatch is achieved by inducing a low-temperature ZnO buffer layer between the substrate and the ZnO film. The effects of the additional buffer layer are studied and optimized in order to obtain a high-temperature ZnO film on top of the buffer layer with high-quality.

HL 32.7 Mon 17:00 P2

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

A very striking characteristic of ZnO is the persistent photoconductivity (PPC). During illumination with light in the UV region, the conductivity increases, and after switching off the light, the photocurrent persists with decay times of hours. This effect is related to oxygen vacancies acting as shallow donors, which can undergo a large lattice relaxation. Also the ambient plays a important role in the PPC behaviour, especially the adsorption and desorption of oxygen from the surface. Overall this effect is still not completly understood.

In this contribution we investigate the role of temperature and different gases on the decay of the PPC. By this method, the oxygen concentration can be detected down to the lower ppm range.

HL 32.8 Mon 17:00 P2

Patterned growth of ZnO nanowires on the 10 μm to 200 nm scale — •Florian Huber[1], Manfred Madel[1], Julian Jakob[1], Dominik Heinz[2], Manuel Hartmann[3], Alfred Plettl[3], Ferdinand Scholz[2], and Klaus Thonke[1] — [1]Institute of Quantum Matter / Semiconductor Physics Group, Ulm University — [2]Institute of Optoelectronics, Ulm University — [3]Institute of Solid State Physics, Ulm University

Two different approaches for the structured growth of ZnO nanowires via chemical vapour deposition (CVD) were realized. On the one hand GaN pyramids grown via metalorganic vapour phase epitaxy (MOVPE) were used to control the alignment of the nanowires. On the other hand several types of substrates were patterned using PS-lithography. Both methods show a very good alignment over wide ranges. The diameter of the nanowires could be controlled from 400 nm down to less than 100 nm. Furthermore different filling factors could be realized. An additional method for a controlled positioning of single nanowires via dielectrophoresis was established. This enables the investigation of the gas sensing behaviour of single nanowires with varying diameters via an optical readout in micro-photoluminescence measurements under different gas atmospheres.

HL 32.9 Mon 17:00 P2

Linear and nonlinear optical deformation potentials in bent ZnO microwires — •Sherzod Khujanov, Christof P. Dietrich, Jörg Lenzner, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnestr. 5, 04103 Leipzig, Germany

The wide-band gap semiconductor ZnO has outstanding optical and piezoelectrical properties that can be modified under tensile and compressive strain [1]. The piezoelectric coefficient of ZnO is at least twice as high as for other II-IV compounds with wurtzite crystal structure. Hexagonal zink oxide microwires were fabricated by using a vapor-phase transport process [2] at temperature of 1150 °C . The grown wires have diameters in the range of $0.5-50\ \mu m$ and lengths between 0.1 and 20 mm. For low temperature cathodoluminescence measurements, the microwires were transferred onto silicon substrates, mechanically bent and fixed with silver paste. Linescans (in steps of 100 nm) from the tensile to the compressivly strained part of the wires revealed different strain regimes. We observe a linear energy shift for uniaxial strain up to $\pm1.5\%$ and deduce a deformation potential which is in very good agreement to previous studies [1]. For higher strain values (up to $\pm3\%$), we are observed the onset of nonlinear effects.

[1] C. P. Dietrich, *et al*: Appl. Phys. Lett. 98, 031105 (2011).
[2] M. Lorenz *et al*: Phys. Stat. Sol.(b) 247, 1265 (2010).

HL 32.10 Mon 17:00 P2

Effect of external magnetic field on the photoresistance of ZnO based wires — •Israel Lorite[1], Carlos Ivan Zalandazini[2], Silvia Perez[2], and Pablo Esquinazi[1] — [1]Division of Superconductivity and Magnetism, Institute for experimental Physics II, Fakultät für Physik und Geowissenschaften, Linnéstrasse 5, 04103 Leipzig, Germany — [2]Laboratorio de Física del Sólido, Dpto. de Física, FCEyT, Universidad Nacional de Tucumán, 4000 Tucumán, Argentina

An exhaustive study of the effect of the external magnetic field on the transient photoresitance of Hydrogen implanted Li doped ZnO was carried out. The wire was illuminated with light at different wavelength; 549 nm, 500 nm and 370 nm, respectively. A variation of the relaxation time is observed when external magnetic field is applied. This variation changes as a function of the used light to illuminate the wire

and the intensity of the magnetic field. This variation is interpreted by means of the electronic state variation of the point defects of ZnO, such as oxygen vacancies, Vo, after illumination. The Vo can be single ionized, Vo+. Since the Vo+ presents net magnetic moment, the external magnetic field could change its spin state. This change would increase the probability of the photo generated electron-hole recombination to reduce the transient photo resistance time.

HL 32.11 Mon 17:00 P2

Comparative study of deep defects in ZnO microwires, thin films and bulk single crystals — •Florian Schmidt[1], Thorsten Schultz[1], Stefan Müller[1], Holger von Wenckstern[1], Christof Peter Dietrich[1], Robert Heinhold[2], Hyung-Suk Kim[2], Martin Ward Allen[2], and Marius Grundmann[1] — [1]Universität Leipzig, Institut für Experimentelle Physik II, Abteilung Halbleiterphysik, Linnéstraße 5, 04103 Leipzig — [2]The MacDiarmid Institute for Advanced Materials and Nanotechnology, University of Canterbury, Christchurch 8043, New Zealand

In this study we report on the electrical properties and deep-level defects of a ZnO microwire grown by carbo-thermal evaporation, a pulsed laser deposited ZnO thin film and a hydrothermally grown ZnO bulk crystal. Deep defects were investigated by means of deep-level transient spectroscopy. The origin of a defect labelled T2 is assumed to be a donor-acceptor complex, with its concentration being limited by the acceptor involved [1]. Our investigations suggest the zinc vacancy V_{Zn} as a possible candidate for the acceptor. From first-principles studies it is known that V_{Zn} has a smaller formation energy for a higher Fermi level which is proportional to the net-doping density in our samples. That would suggest that the formation of such an acceptor is most likely in the PLD thin film, followed by the bulk sample and the microwire which is supported by the experiment [2].

[1] M. Schmidt *et al.*, phys. stat. sol. **249**, 588 (2012).
[2] F. Schmidt *et al.*, Appl. Phys. Lett. **103**, 062102 (2013).

HL 33: Optical properties I

Time: Tuesday 9:30–11:00 Location: POT 006

HL 33.1 Tue 9:30 POT 006

Investigation of the Purcell effect in rolled-up active metamaterials by means of time-resolved photoluminescence measurements — •Hoan Vu[1,3], Marvin Schulz[1], Stephan Schwaiger[1], Tobias Korn[2], Christian Schüller[2], David Sonnenberg[1], Christian Heyn[1], Tobias Kipp[3], and Stefan Mendach[1] — [1]Institut für Angewandte Physik, Universität Hamburg, Jungiusstraße 11, D-20355 Hamburg, Germany — [2]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D-93040 Regensburg, Germany — [3]Institut für Physikalische Chemie, Universität Hamburg, Grindelallee 117, D-20146 Hamburg, Germany

In materials with hyperbolic light dispersion a broadband Purcell effect was predicted and recently experimentally investigated [1]. Here, we probe the Purcell effect of a GaAs quantum well embedded in rolled-up radial metamaterials, which we prepare exploiting the self-rolling mechanism of strained semiconductor layers [2]. We varied the thickness ratio η of rolled-up Ag/GaAs layer systems to tune the effective permittivity at the quantum well emission energy (1.63 eV) and thereby change the effective dispersions' iso-frequency surface from a closed ellipsoidal iso-frequency surface ($\eta < 0.53$) to an open hyperboloidal iso-frequency surface ($\eta > 0.53$). We show by means of time-resolved photoluminescence measurements that the lifetime of GaAs quantum wells is enhanced by a factor of 2.5. We acknowledge financial support by the Deutsche Forschungsgemeinschaft (DFG) via ME 3600/1. [1] H. N. S. Krishnamoorthy et al., Science 336, 6078 (2012) [2] S. Schwaiger et al., Phys. Rev. B 84, 155325 (2011)

HL 33.2 Tue 9:45 POT 006

Optical semiconductor microtube resonators coupled to chemically synthesized, light-emitting nanostructures — •Stefanie Kietzmann[1], Christian Strelow[1], Andreas Schramm[2], Jussi-Pekka Penttinen[2], Alf Mews[1], and Tobias Kipp[1] — [1]Institut für Physikalische Chemie, Universität Hamburg, Deutschland — [2]Optoelectronics Research Centre, Tampere University of Technolgy, Tampere, Finland

We investigate the interaction of rolled-up AlInP microtubes with colloidal nanoemitters. AlInP is especially interesting, being transparent in the visible spectral range. The thin walls of the microtubes cause evanescent fields, to which the emitters can couple and emit their light into the microtubes' walls where it is confined by total internal reflection. Constructive interference cause the formation of sharp eigenmodes. Their properties sensitively depend on the material and geometry of the microtubes. Lithographic techniques allow for a full control of the three-dimensional light confinement and the resulting eigenspectrum [1]. Easily fabricated by selectively undercutting epitaxally grown strained multilayer systems, AlInP microtubes allow for a variety of applications. As the eigenmode energies sensitively depend on the refractive index of tube's surrounding, they are perfect candidates for micrometer scaled refractive index sensors. Measurements and FDTD simulations of a microtube with varying surrounding materials are presented that demonstrate the refractometer properties of our microtubes [1]. We acknowledge financial support by the DFG via Ki1257/1. [1] Ch. Strelow et.al. Appl. Phys. Lett. 101, 113114 (2012)

HL 33.3 Tue 10:00 POT 006

Study of the disorder effects in Ga(AsBi) single quantum wells — •Mohammad Khaled Shakfa[1], Dimitri Kalincev[1], Alexey Chernikov[1], Sangam Chatterjee[1], Xianfeng Lu[2], Shane R. Johnson[2], Dan A. Beaton[3], Thomas Tiedje[4], and Martin Koch[1] — [1]Department of Physics and Materials Sciences Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]Department of Electrical Engineering, Arizona State University, Tempe, Arizona 85287-6206, United States — [3]Department of Physics and Astronomy, University of British Columbia, Vancouver, British Columbia V6T 1Z4, Canada — [4]Department of Electrical and Computer Engineering, University of Victoria, Victoria, British Columbia V8W 3P6, Canada

Ga(AsBi) semiconductor alloys have attracted increasing interest in recent years due to their special physical properties and potential application in optoelectronic and spintronic devices. These materials typically exhibit a certain degree of disorder due the potential fluctuation associated with the Bi content and to the existence of Bi clusters within the alloy structure. Here, we report on a study to clarify the impact of the Bi content on disorder effects in GaAsBi/GaAs SQWs [1]. The experimental techniques employed are continuous-wave and time resolved photoluminescence. Two theoretical models are used to quantify the disorder parameters. A straightforward model with a single energy scale is based on the carrier dynamics at very low temperatures. Secondly, an excitonic hopping model with two energy scales is based on the features of the PL spectra. [1] J. Appl. Phys. 114, 164306 (2013).

HL 33.4 Tue 10:15 POT 006

Quantum-spectroscopy studies on semiconductor quantum wells — •Martin Mootz[1], Mackillo Kira[1], Stephan W. Koch[1], Andrew E. Hunter[2,3], Hebin Li[2], and Steven T. Cundiff[2,3] — [1]Department of Physics, Philipps-University Marburg, Renthof 5, D-35032 Marburg, Germany — [2]JILA, University of Colorado and National Institute of Standards and Technology, Boulder, CO 80309-0440, USA — [3]Department of Physics, University of Colorado, Boulder, CO 80309-0390, USA

Quantum-optical generalization of laser spectroscopy can characterize many-body states that remain hidden if only classical features of light are applied [1]. We apply quantum-optical spectroscopy by projecting GaAs quantum-well measurements into quantum-optical absorption to light sources with a nonclassical quantum statistics. Our results demonstrate that the quantum-well absorption depends critically on the quantum statistics of the light source. In particular, we find that quantum-optical spectroscopy characterizes the properties of many-body states — ranging from biexcitons to highly correlated electron–hole complexes — with a much higher accuracy than classical spectroscopy does. We also present a general theory [2] that can be applied to compute the energetics of the observed highly correlated many-body states.

[1] M. Kira, S.W. Koch, R.P. Smith, A.E. Hunter, and S.T. Cundiff, Nature Phys. **7**, 799-804 (2011).
[2] M. Mootz, M. Kira, and S.W. Koch, New J. Phys., **15**, 093040

(2013).

HL 33.5 Tue 10:30 POT 006

Terahertz control schemes of semiconductor excitons — •Lukas Schneebeli[1], Christoph N. Boettge[1], Benjamin Breddermann[1], Mackillo Kira[1], Stephan W. Koch[1], Sabine Zybell[2,3], Stephan Winnerl[2], Jayeeta Bhattacharyya[2], Faina Esser[2,3], Harald Schneider[2], Manfred Helm[2,3], William D. Rice[4], and Junichiro Kono[4] — [1]Department of Physics, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, P.O. Box 510119, 01314 Dresden, Germany — [3]Technische Universität Dresden, 01062 Dresden, Germany — [4]Department of Electrical and Computer Engineering, Rice University, Houston, Texas 77005, USA

We analyze recent terahertz (THz) experiments [1] on semiconductor quantum wells with a microscopic theory [2, 3] of THz excitation that systematically includes all relevant many-body interactions. Our results [1] contain an unexpected emission increase to luminescence due to dipole-forbidden intra-excitonic transitions. This many-body effect stems from the Coulomb-interaction induced scattering among excitons. These experimental and theoretical results demonstrate the general manipulation capabilities of THz excitation and the role of Coulomb interaction. We also discuss further control mechanisms of exciton dynamics and present several examples.

[1] W. D. Rice *et al.*, Phys. Rev. Lett. **110**, 137404 (2013).
[2] M. Kira and S. W. Koch, Prog. Quantum Electron. **30**, 155 (2006).
[3] M. Kira and S. W. Koch: *Semiconductor Quantum Optics*, 1st. ed., Cambridge Univ. Press, (2011).

HL 33.6 Tue 10:45 POT 006

Luminescence properties of Silicon nanocrystals excited with femtosecond laser pulses — •Friederike Albrecht[1], Daniel Hiller[2], Margit Zacharias[2], Jürgen Gutowski[1], and Tobias Voss[1] — [1]Institute of Solid State Physics, University of Bremen — [2]Institute for Microsystems Engineering IMTEK, Faculty of Engineering, University of Freiburg

Silicon nanocrystals (Si-NCs) embedded in a SiO_2 matrix have been shown to be rather efficient light emitters as the relaxation of momentum conservation in the nanostructures substantially increases the radiative transition probability of electron-hole pairs compared to bulk silicon. Si-NCs are therefore promising building blocks for all-silicon based optoelectronic applications. Here, we study the luminescence and waveguiding properties of SiO_2-based optical ridge-waveguide structures with embedded Si-NCs as active layer ($2\text{nm} < d_{\text{NC}} < 5\text{nm}$) with the special emphasis on the generation and quantification of net optical gain. Under cw excitation with a HeCd-Laser at room temperature, a luminescence band centered between 700 and 850nm is observed. A blueshift of the photoluminescence is seen for decreasing Si-NC size because of the quantum confinement. To study the transient gain dynamics in the Si-NC waveguides, the samples were excited with the frequency-doubled output of a Ti:Sapphire femtosecond oscillator ($\Delta t < 80\text{fs}$, $\lambda = 375\text{nm}$). We will compare the luminescence spectra of the Si-NCs obtained under pulsed and cw excitation, discuss the excitation and recombination dynamics, and the possibility of achieving optical gain under fs-pulse excitation in the waveguide structures.

HL 34: Invited Talk Elizabeth von Hauff

Time: Tuesday 9:30–10:00 Location: POT 081

Invited Talk HL 34.1 Tue 9:30 POT 081

Influence of molecular structure, conformation and morphology on the performance of polymer solar cells — •Elizabeth von Hauff — Physics of Energy, Department of Physics and Astronomy, Vrije Universiteit Amsterdam, The Netherlands

Organic semiconductors offer vast potential for low cost, flexible energy production. The polymer-fullerene bulk heterojunction solar cell is the most widely investigated type of organic solar cell. The extended donor-acceptor interface facilitates efficient charge transfer while providing pathways for carrier transport for the extraction of photocurrent at the contacts. One major challenge for improving device performance is to understand how key processes at the molecular scale and between material interfaces determine device performance in these complex systems. In this talk, the influence of molecular structure, conformation and morphology on the performance of polymer solar cells is discussed. The photocurrents in these devices are inherently limited by the poor electrical properties of the organic active layer. Strategies to tune carrier transport in the active layer, such as molecular doping and nanomorphological manipulation [1,2], are presented. In operational devices, interfacial phenomena, such as electrical losses between the active layer and contact materials, are significant in determining solar cell performance and solar cell lifetime. Impedance spectroscopy [3,4] is a useful technique to probe the electrical properties of solar cells at different operational points in the current-voltage characteristics, and isolate materials and interfaces which limit performance.

[1] A. V. Tunc, A. De Sio, D. Riedel, F. Deschler, E. Da Como, J. Parisi, E. von Hauff; Org. Electron, 13 (2012) 290-296
[2] A. V. Tunc, A. Giordano, B. Ecker, E. Da Como, B. J. Lear, E. von Hauff, J. Phys. Chem. C, 117 (2013) 22613
[3] B. Ecker, J. Nolasco, J. Pallares, L. Marsal, J. Posdorfer, J. Parisi, E. von Hauff; Adv. Funct. Mat. 21 (2011) 2705-2711
[4] B. Ecker, H.-J. Egelhaaf, R. Steim, J. Parisi, E. von Hauff; J. Phys. Chem. C, 116 (2012) 16333-16337

HL 35: Organic semiconductors: Photovoltaics (with CPP/DS/O)

Time: Tuesday 10:00–12:30 Location: POT 081

HL 35.1 Tue 10:00 POT 081

Analytical transmission electron microscopy on hybrid solar cells based on perovskites — •Diana Nanova[1,2,4], Anne Katrin Kast[1,3,4], Christian Müller[1,4], Rasmus R. Schröder[3,4], Robert Lovrincic[1,4], and Wolfgang Kowalsky[1,4] — [1]Institut für Hochfrequenztechnik, TU Braunschweig — [2]Kirchhoff Insitut für Physik, Universität Heidelberg — [3]Cryo-EM, CellNetworks, Bioquant, Universität Heidelberg — [4]InnovationLab GmbH, Heidelberg

Hybrid solar cells based on metal-organic perovskite absorbers are of major interest due to their remarkable power conversion efficiencies of up to 15%. Recently, it has been shown that the morphology of the perovskite itself as well as the interplay between the absorber and the mesostructured electron acceptor strongly affects the electrical properties of the device. We present a combined study of the structure-function relationship of solution processed solar cells based on mesostructured perovskites. The morphology of the solar cells was studied by analytical transmission electron microscopy (ATEM). In ATEM electron energy loss spectroscopy (EELS) and electron spectroscopic imaging (ESI) are applied in order to obtain material contrast. To be able to classify the TiO2 and the perovskite rich areas in the corss-section of the device a series of monochromatic images in the low-loss regime was acquired. We observed significant changes in pore size, pore filling and pore distribution of the mesostructured layer depending on the annealing conditions of the perovskite. Furthermore, we correlated our results to the I-V characteristics of the solar cells.

HL 35.2 Tue 10:15 POT 081

Alloyed zinc sulfide - copper indium disulfide nanocrystals for application in hybrid photovoltaics — •Björn Kempken, Nikolay Radychev, Christopher Krause, Jie Li, Holger Borchert, Joanna Kolny-Olesiak, and Jürgen Parisi — Carl von Ossietzky University of Oldenburg, 26111 Oldenburg

Semiconductor nanocrystals (NCs) continue to attract immense attention because of their size-dependent optical, physical, and chemical properties which causes them to be a favourable material for

hybrid solar cell applications. A promising candidate for the inorganic/organic active layer is alloys of ZnS and CuInS2 (ZCIS NCs), which on the one hand strongly absorb in the visible range up to 800 nm, and, on the other hand, belongs to the "green" type of semiconductor NCs. In the present work, high quality ZCIS NCs were synthesized and subjected to hexanethiol ligand exchange procedures. Laboratory solar cells based on blends of treated ZCIS NCs and poly[2,6-(4,4-bis-(2-ethylhexyl)-4H-cyclopenta[2,1-b;3,4-b']dithiophene)-alt-4,7(2,1,3-benzothiadiazole)] (PCPDTBT) as active layer were prepared and investigated by current-voltage and electron spin resonance measurements. Hybrid ZCIS/PCPDTBT laboratory solar cells demonstrate well pronounced diode behavior with outstanding characteristics of the open-circuit voltage which reached up to 1.2 V.

HL 35.3 Tue 10:30 POT 081

Improving efficiency of solar power generation by combination of a sensitized mesoscopic solar cell with a thermoelectric generator — •Hans-Fridtjof Pernau, Jana Heuer, Karina Tarantik, Alexandre Jacquot, Jan D. König, Martin Jägle, and Kilian Bartholomé — Fraunhofer IPM, Freiburg, Germany

Standard photovoltaic(PV) solar cells use only about half of the light spectrum provided by the sun. The infrared part is not used for producuction of electrical energy. Even further, the infrared light heats up the pv cell and decreases thereby its efficiency. The basic idea for a combined pv and thermoelectric solar cell has been published in 2008 [1]. The improvements in thermoelectric materials and scientific work on thermoelectrics lead to new ideas for those systems [2] which will be investigated in the EU-FP7-Projekt Globasol. Within the project, a hybrid solar cell made of a sensitized mesoscopic solar cell and a thermoelectric generator (TEG) will being developed. The light of the sun is split at about 800nm. The visible and ultra violet part is transfered to the sensitized mesoscopic solar cell, the infrared part illuminates the TEG cell. With the hybrid solar cell, the full solar spectrum is exploited. We present the first modeling results of the project and the first evaluation version of the hybrid cell.

[1] T.M. Tritt, H. Böttner and L. Chen, *Thermoelectric: Direct Solar Thermal Energy Conversion*, MRS Bulletin, vol.33 (2008) pp. 366-368; [2] D. Kraemer et al., *High-performance flat panel solar thermoelectric generator with high thermal concentration*, Nature materials vol.10 (2011) pp. 532-538.

HL 35.4 Tue 10:45 POT 081

Spin dynamics in organic solar cells measured by pulsed electrically detected magnetic resonance — •Alexander J. Kupijai, Konstantin M. Behringer, Martin Stutzmann, and Martin S. Brandt — Walter Schottky Institut, Technische Universität München, Am Coulombwall 4, 85748 Garching

Organic photovoltaics are of great interest in the development of sustainable energy sources. To investigate the recombination and transport processes in organic solar cells we use the technique of pulsed electrically detected magnetic resonance (EDMR) where we measure the change of the photocurrent caused by resonant X-band microwave pulses in the presence of an external magnetic field. As test devices, we use bulk heterojunction P3HT/PCBM (poly(3-hexylthiophene-2,5-diyl) / [6,6]-phenyl C_{61} butyric acid methyl ester) solar cells. At temperatures of 10K we are able to observe both positively and negatively charged polarons in the pulsed EDMR spectrum and can identify them as partners in a spin-dependent pair process by experiments using two microwave frequencies. Using the time resolution and sensitivity of pulsed EDMR we are able to quantify the spin dynamics of the system and measure the lifetime of parallel spin pairs, the lifetime of antiparallel spin pairs, the spin decoherence time and the coupling strength between the spin partners. All of these microscopic parameters provide valuable information for an optimization of overall solar cell efficiencies.

HL 35.5 Tue 11:00 POT 081

Imaging the origin of S-shaped current-voltage characteristics of organic solar cells by scanning Kelvin probe microscopy — •Christian Müller[1,2,3], Rebecca Saive[1,2,3], Janusz Schinke[1,3], Robert Lovrincic[1,3], and Wolfgang Kowalsky[1,2,3] — [1]InnovationLab GmbH, Heidelberg, Germany — [2]Kirchhoff-Institut für Physik, University Heidelberg, Germany — [3]Institut für Hochfrequenztechnik, Technische Universität Braunschweig, Germany

We investigated organic bilayer solar cells consisting of poly(3-hexylthiophene)/1-(3-methoxycarbonyl)propyl-1-phenyl[6,6]C61 (P3HT/PCBM). Scanning Kelvin probe microscopy (SKPM) was performed on the solar cell cross sections which were exposed with a focused ion beam. We prepared the P3HT/PCBM bilayer solar cells by solution processing. These bilayer solar cells showed normal and anomalous, S-shaped current-voltage characteristics. Using SKPM on the device cross sections, we found that in normal bilayer solar cells the potential dropped at the ITO/PEDOT:PSS contact and over the active area, whereas in S-shaped bilayer solar cells the potential dropped exclusively at the aluminium contact. This behavior confirms the assumption that S-shaped curves are caused by hindered charge transport at electrode interfaces.

Coffee break (15 min.)

HL 35.6 Tue 11:30 POT 081

Improving the Charge Transport Parameters of Near-Infrared Absorbers — •Sebastian Radke[1,2], Frank Ortmann[1,2], Reinhard Scholz[2,3], and Gianaurelio Cuniberti[1,2,4] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany — [2]Dresden Center for Computational Materials Science, TU Dresden, Germany — [3]Institut für Angewandte Photophysik, TU Dresden, Germany — [4]Center for Advancing Electronics Dresden, TU Dresden, Germany

For an improved performance of organic tandem solar cells, efficient organic infrared absorber materials are necessary. A promising class already used successfully in organic solar cells are 4,4'-difluoro-4-bora-3a,4a-diaza-s-indacenes (BODIPYs). Based on a comparative study of the intramolecular electronic properties as well as the intermolecular coupling in the crystal phase of three potential candidates, we find that the benzannulation of the molecular core improves both electron and hole transfer. As the frontier molecular orbitals are delocalized over the entire molecule also by attaching additional functional groups to the molecular core, the intermolecular coupling and especially the performance in amorphous phase can be optimized further. However, an immobilization of these substituents is necessary to regulate an increase in the reorganization energy for hole transfer. Based on these design rules, BODIPYs with optimized charge transfer properties can be synthesized increasing also the performance of the devices.

HL 35.7 Tue 11:45 POT 081

Qualitative und quantitative Auswertung von komplementären bildgebenden Methoden zur Degradationsuntersuchung und Qualitätskontrolle von Polymersolarzellen — •Roland Rösch, Marco Seeland, Daniel Fluhr, Burhan Muhsin, Peter Fischer, Rolf Öttking und Harald Hoppe — Institut für Physik, TU Ilmenau, Deutschland

Wir berichten über beschleunigte Alterungstests an modernen organischen und polymeren Solarzellen, ergänzt durch bildgebenden Methoden, wie z.B. bildgebende Lumineszenz, Lock-in Thermographie und lichtinduziertes Kurzschlussstrommapping. Neben einer qualitativen Interpretation der Daten, ist es durch die Kombination der verschiedenen Methoden möglich, auch eine quatitative Auswertung der Dynamiken der verschiedenen Degradationsmechanismen zu erhalten. Desweiteren vergleichen wir die experimentellen Ergebnisse mit theoretischen Modellen des Ladungsträgerflusses und -Rekombination. Daraus lassen sich intrinsische Paramter der Bauelemente, wie Elektrodenwiderstand und Diodenidealitätsfaktor bestimmen. Die wichtigste Erkenntnis aus diesen Untersuchungen ist, dass die Stabilität von modernen organischen Solarzellen vor allem durch die Elektrodendegradation und die Qualität der Versiegelung begrenzt ist. Diese Arbeit liefert einen Leitfaden für weitere Verbesserungen hin zu stabilen organischen Solarzellen.

HL 35.8 Tue 12:00 POT 081

Visualization of Lateral Phase Separation in Polymer: Fullerene Solar Cells by Quantitative Evaluation of Luminescence Imaging Measurements — •Marco Seeland, Christian Kästner, and Harald Hoppe — Institut für Physik, TU Ilmenau, Ilmenau, Germany

Luminescence imaging has evolved to a versatile characterization method for studying the laterally resolved behavior of polymer solar cells. Especially in degradation studies the use of luminescence imaging is beneficial as it is non-invasive and offers short measurement times. By either electrical or optical excitation separate characterization of the electrical contacts and the active layer is feasible. However, the data analysis so far is mainly qualitative, i.e. interpretation of the

measured luminescence image by comparison with other techniques. In this work we present a quantitative analysis of electroluminescence images of laterally inhomogeneous polymer solar cells. By decoupling the local parameters within an iteration procedure this analysis allows calculation of the local current flow through and the local voltage applied to the active layer. Furthermore quantitative images of the local series resistance and the saturation current-density are achieved. The local saturation current-density contrast was found to correlate perfectly with the strong lateral phase separation occurring in PPE-PPV:PCBM based devices. Further analysis of the lateral difference in the saturation current-densities delivers information on the thermal activation of charge carriers at the donor/acceptor-interface and in the phase separated bulk.

HL 35.9 Tue 12:15 POT 081

The influence of fullerene loading on the photogeneration in intercalated polymer: fullerene bulk heterojunction solar cells — •Andreas Zusan[1], Koen Vandewal[2], Benedikt Allendorf[1], Nis Hauke Hansen[1], Jens Pflaum[1], Martin Heeney[3], Alberto Salleo[2], Vladimir Dyakonov[1,4], and Carsten Deibel[1] — [1]Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [2]Department of Materials Science and Engineering, Stanford University, Stanford, California 94305, USA — [3]Department of Chemistry, Imperial College, London, SW7 2AZ, UK — [4]Bavarian Centre for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg

The conjugated polymer, pBTTT, allows a systematic tuning of the blend morphology by varying the acceptor material and blend ratio, making it a well-suited structural model for studying the fundamental processes in organic BHJ solar cells. To analyze the correlation between photogeneration and intercalation, we have performed time delayed collection field (TDCF) measurements and Fourier-transform photocurrent spectroscopy (FTPS) on pBTTT:PCBM devices in various stoichiometries. An increased PCBM loading resulted in a less field dependent dissociation, which we attribute to enhanced electron delocalization along extended PCBM nanophases and energetically driven spatial separation of polarons due to the presence of pure acceptor domains. The highly efficient transfer of charge carriers from the intercalated phase into the pure phase has been studied further by extending TDCF measurements to include segregated pBTTT:bisPCBM blends.

HL 36: Invited Talk Gary Hodes

Time: Tuesday 12:30–13:00 Location: POT 081

Invited Talk HL 36.1 Tue 12:30 POT 081

Organic-inorganic perovskite solar cells: The new generation of PV — •Gary Hodes — Department of Materials and Interfaces, Weizmann Institute of Science, Rehovot, Israel

The organic-inorganic perovskite solar cells, typified by the most commonly-studied material – methyl ammonium lead iodide – are approaching 16% conversion efficiency in the approximately four years that they have been investigated. Apart from their extraordinarily high efficiencies for such a new type of cell, they also have the advantages of containing no rare elements and can be made with very low energy input (close to room temperature preparation from solution).

In this talk I will discuss the main properties of these perovskites that make them such good photovoltaic materials. The cell operation mechanism – in general they are p-i-n solar cells – will be treated, taking into account that there are several different cell structures. The relatively-high effective diffusion lengths of electrons and holes in the perovskites are one of its favourable properties. Another is the high fraction of the bandgap that can be regained as open circuit photovoltage (typically between 65 and 70%). High voltage cells giving > 1.5 V for a bandgap of 2.3 eV will also be described.

HL 37: Preparation and characterization

Time: Tuesday 9:30–10:30 Location: POT 151

HL 37.1 Tue 9:30 POT 151

Enhanced ferromagnetic coupling in GaMnN/GaN:Mg superlattices — •Laura Tropf[1], Gerd Kunert[1], Richard Wilhelm[2], Sylwia Stefanowicz[3], Rafal Jakiela[3], Stephan Figge[1], Maciej Sawicki[3], Jörg Grenzer[2], Tomasz Dietl[3], and Detlef Hommel[1] — [1]Institut für Festkörperphysik, Universität Bremen — [2]Ionenstrahlzentrum, Helmholtz-Zentrum Dresden-Rossendorf — [3]Institute of Physics, Polish Academy of Science

GaMnN is observed to behave as a dilute magnetic insulator for Mn concentrations of up to [Mn] = 10 %. As the direct incorporation of hole carriers in GaMnN, which is crucial for ferromagnetic coupling at room temperature, shows fundamental difficulties, a different approach was investigated: Superlattices were grown by molecular beam epitaxy, in which the GaMnN layers containing localized spins are separated from the p-doped GaN:Mg layers. An overlap of the hole wave function could enable ferromagnetic p-d-coupling near the interfaces. An extensive characterization gives detailed insight on the impact the variation of the Mg-flux has on the structural and magnetic properties. Superlattices with a maximum Mn concentration of 2.6% in the GaMnN layers and Mg-densities of $4.8 \cdot 10^{20}$ cm^{-3} in the GaN:Mg layers were obtained. This concept leads to ferromagnetic coupling at temperatures of up to 7 K, which is 6 K higher than expected from the magnetic phase diagram for undoped layers. At a certain critical Mg-flux, an abrupt reduction of the Mn- and Mg-incorporation and a deterioration of the layering could be observed and can be explained by polarity inversion from Ga-face to N-face.

HL 37.2 Tue 9:45 POT 151

Optical Anisotropies in Magnetite (110) — •Karsten Fleischer[1], Ruggero Verre[2], Ozhet Mauit[1], John F. McGilp[1], and Igor V. Shvets[1] — [1]School of Physics, Trinity College Dublin, Ireland — [2]Department of Applied Physics, Chalmers University of Technology, 412 96 Göteborg, Sweden

Reflectance anisotropy spectroscopy (RAS) has been used to measure the optical anisotropies of bulk and thin film Fe_3O_4(110). The spectra resemble the derivative of the dielectric function of the samples, indicating that small shifts in energy of the optical transitions, such as those associated with anisotropic strain or electric field gradients, are responsible for the strong signal observed. The RAS response was then measured as a function of temperature. A distinct change in the RAS line shape amplitude was observed in the spectral range from 0.8 to 1.6 eV for temperatures below the metal-insulator Verwey transition of the crystal at T=110K. These changes are discussed in terms of charge ordering models in the crystal.

HL 37.3 Tue 10:00 POT 151

In-situ microscopic investigation of removing native oxide from Si(100) with ambient hydrogen — •Benjamin Borkenhagen, Gerhard Lilienkamp, and Winfried Daum — Institute of Energy Research and Physical Technologies, TU Clausthal, Leibnizstraße 4, 38678 Clausthal-Zellerfeld

This low energy electron microscopy (LEEM) study addresses the technologically important surface deoxidation process of Si(100) wafers. In cleaning processes of Si(100) as applied in vapor phase epitaxy (molecular) hydrogen is present during thermal oxide removal. We therefore mimicked the deoxidation of Si(100) in presence of hydrogen by exposing natively oxidized Si(100) to atomic hydrogen at $p \geq 10^{-7}$ mbar and at $T \sim 700$ °C and imaged the resulting oxide removal with video frequency. Deoxidation of the Si(100) surface was first observed on small localised areas. These areas acted as nuclei for reaction fronts of the deoxidation process and expanded omnidirectionally until the complete surface was oxide-free and probably hydrogen-terminated. Depending on hydrogen pressure, LEEM images of this surface revealed the expected large Si(100) terraces separated by

steps. Typical patterns of the two perpendicularly oriented domains of the well known (2×1) reconstruction were observed with LEEM, and the reconstruction was confirmed by small-area low energy electron diffraction (μLEED) in accordance with previous studies of the clean Si(100) surface. After the deoxidation process, subsequent Auger electron spectroscopy measurements showed an oxygen-free Si.

HL 37.4 Tue 10:15 POT 151

Characteristics of high-quality SnO_2 films deposited on sapphire by IBSD — •Martin Becker, Yinmei Lu, Benedikt Kramm, Angelika Polity, and Bruno K. Meyer — 1st Physics Institute, Justus-Liebig-University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

SnO_2 thin films were grown on (001) (c-cut), (012) (r-cut), (110) (a-cut) and (100) (m-cut) sapphire substrates using ion beam sputter deposition (IBSD) of a pure Sn metallic target at a constant gas mixture of 2.5 sccm argon and 15 sccm oxygen at 550°C substrate temperature. X-ray diffraction in Bragg-Brentano geometry revealed that SnO_2 film deposited on each substrate is grown with preferential orientation. The determined out-of-plane orientation relationships were $SnO_2(100)//Al_2O_3(001)$ (c-cut), $SnO_2(101)//Al_2O_3(012)$ (r-cut), $SnO_2(101)//Al_2O_3(110)$ (a-cut) and $SnO_2(002)//Al_2O_3(100)$ (m-cut). XRD rocking curves indicated close-to-epitaxial growth conditions, perceivable by very small full width at half maximum (FWHM). X-ray pole figure even announced epitaxial in-plane relationships. Energy dispersive X-ray spectroscopy (EDX), X-ray photoelectron spectroscopy (XPS) and secondary ion mass spectroscopy (SIMS) served as procedures to identify composition and stoichiometry. Morphology was studied by scanning electron microscopy (SEM) and atomic force microscopy (AFM), respectively, which reveal smooth and homogeneous surfaces. At room temperature free carrier densities (n-type) range between mid $10^{17}\,cm^{-3}$ to mid $10^{18}\,cm^{-3}$, whereas mobilities are still significantly lower than in bulk SnO_2.

HL 38: Quantum light sources based on solid state systems: Status and visions I (Focus session with TT)

Non-classical quantum light sources with the ability to efficiently generate photon states with tailored properties (e.g. well defined photon-number Fock states, mutually highly indistinguishable photons, or high fidelity quantum entangled states, etc.) are among the fundamental building blocks of numerous proposed applications in the field of quantum information processing – particularly quantum computing and quantum cryptography. The aim of this focus session is to bring together the ideas, concepts and results of leading national and European research groups on semiconductor and solid state-based quantum light sources and to discuss the current status and future goals in this highly topical field of research.

Organizers: Sven Ulrich, Universität Stuttgart, and Christoph Becher, Universität des Saarlandes, Saarbrücken.

Time: Tuesday 9:30–11:15 Location: POT 251

Topical Talk HL 38.1 Tue 9:30 POT 251

Nonclassical light from semiconductor quantum dots — •Gregor Weihs[1,2], Tobias Huber[1], Harishankar Jayakumar[1], Thomas Kauten[1], and Ana Predojević[1] — [1]Institut für Experimentalphysik, Universität Innsbruck, Technikerstr. 25, 6020 Innsbruck, Austria — [2]Institute for Quantum Computing, University of Waterloo, 200 University Ave W, Waterloo, ON N2L 3G1, Canada

For fundamental tests of quantum physics as well as for quantum communications non-classical states of light are an important tool. In our research we focus on developing semiconductor-based and integrated sources of single photons and entangled photon pairs.

In this talk we will present our work on single InAs/GaAs quantum dots. For the highest degree of quantum control we use resonant two-photon excitation to deterministically trigger a biexciton-exciton cascade. We block the pump light from the detectors by using side excitation through the waveguide mode of a planar microcavity. We demonstrate Rabi oscillations, Ramsey interference and all-optical coherent control of the quantum dot resulting in single and paired photons with a high degree of indistinguishability [1]. Using novel quantum optical assessment tools we are then able to show the non-classical and non-Gaussian characteristics of the emitted photons.

This indistinguishability eventually results in time-bin entangled photon pairs through the biexciton-exciton cascade. Time-bin entanglement is a useful variant for long distance communication because it is robust against decoherence in optical fibers. Two successive coherent pulses excite the dot ei-ther in the early or in the late pulse. The emitted photons pass imbalanced interferometers for analy-sis in the energy basis. Through quantum state tomography we are able to demonstrate significant entanglement of the emitted pairs.

This work was supported by the ERC and CIFAR.

[1]H. Jayakumar, A. Predojevic, T. Huber, T. Kauten, G. S. Solomon & G. Weihs, Deterministic Photon Pairs and Coherent Optical Control of a Single Quantum Dot, Phys. Rev. Lett. 110, 135505 (2013).

HL 38.2 Tue 10:00 POT 251

On-demand generation of indistinguishable polarization-entangled photon pairs — •Markus Müller[1], Samir Bounouar[1], Klaus D. Jöns[1], Martin Gläßl[2], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]Institut für Theoretische Physik III, Universität Bayreuth, Universitätsstraße 30, 95440 Bayreuth, Germany

The development of quantum information science using linear optics has made substantial progress in the recent past. This advance is mainly based on the ability to generate high-quality photonic qubits from various kinds of different sources. Furthermore, for practical quantum information operations it is essential to create the qubits deterministically. In this work we show that semiconductor quantum dots (QDs) are suitable to fulfill both of this elementary requirements. To exploit their remarkable properties, a coherent resonant two-photon excitation scheme is applied. Thereby the biexciton state of an InGaAs QD is populated with a near unity preparation efficiency. Because of this individual and coherent addressing, the photons emitted by the biexciton-exciton cascade show enhanced optical and quantum-optical qualities. This is reflected in pure single-photon emission, long coherence times and high indistinguishability visibilities ($V_{HOM} = 0.86 \pm 0.03$ and 0.71 ± 0.04) for the biexcitonic and excitonic emission, respectively. Taking advantage of a QD without fine structure splitting, we can demonstrate the on-demand generation (pair-efficiency = 0.86 ± 0.08) of high fidelity (0.81 ± 0.02) polarization-entangled photon pairs.

HL 38.3 Tue 10:15 POT 251

Feedback-Enhanced Entanglement of Photons from a Biexciton Cascade — •Sven Moritz Hein[1], Franz Schulze[1], Alexander Carmele[2], and Andreas Knorr[1] — [1]Technische Universität Berlin, Institut für theoretische Physik, Nichtlineare Optik und Quantenelektronik, Hardenbergstraße 36, 10623 Berlin, Germany — [2]Institut für Quantenoptik und Quanteninformation, Technikerstraße 21a, 6020 Innsbruck, Austria

Coherent quantum feedback [1] is a method to control and stabilize quantum-mechanical systems by the use of a feedback mechanism that does not rely on measurement, but is completely quantum-mechanical itself. We utilize such a feedback scheme to enhance the entanglement of photons from a biexciton cascade in a quantum dot. The achievable

photon entanglement is usually diminished substantially by exciton fine-structure splitting. We demonstrate that it is possible to increase photon entanglement by feeding the emitted light back into the quantum dot after a certain feedback time, e.g. by using a mirror at a specific distance from the emitter [2]. The complex interplay between original and reflected field modifies the emission spectrum in a way that the achievable entanglement is strongly enhanced. We present a full quantum-mechanical theory of the system, including the feedback-induced modification of the photon mode continuum. We analyze the influence of feedback delay and phase and discuss the involved mechanisms in detail.

[1] S. Lloyd, Phys. Rev. A 62, 022108 (2000).
[2] A. Carmele et al., Phys. Rev. Lett. 110, 013601 (2012).

HL 38.4 Tue 10:30 POT 251

Emission of polarization-entangled photons from biexcitons: two-photon processes and phonon-assisted cavity feeding — •Dirk Heinze, Artur Zrenner, and Stefan Schumacher — Department of Physics and CeOPP, University of Paderborn, Warburger Str. 100, 33098 Paderborn

Semiconductor quantum dots are promising sources for generation of pairs of polarization-entangled photons. In [1] we have shown theoretically that using a direct two-photon emission process inside a high-quality optical microcavity, the degree of achievable polarization-entanglement can be rendered insensitive to exciton fine-structure splitting (in contrast to the usual cascaded emission). The results in [1] were obtained for realistic quantum-dot and cavity parameters but neglecting the influence of phonon-assisted cavity feeding. Here we extend our previous study and include the interaction with a bath of acoustic phonons in a Born-Markov approximation in the master-equation for the system density operator. Our analysis shows the detrimental influence of phonons on the polarization entanglement with increasing temperature. However, it also demonstrates that at low temperature the influence of phonons on the scheme proposed in [1] is strongly suppressed such that high degrees of entanglement can be achieved.

[1] S. Schumacher, J. Förstner, A. Zrenner, M. Florian, C. Gies, P. Gartner, and F. Jahnke. Cavity-assisted emission of polarization-entangled photons from biexcitons in quantum dots with fine-structure splitting. Optics Express, **20**, 5335 (2012).

Topical Talk HL 38.5 Tue 10:45 POT 251

Taming single photons emitted by solid state systems — •Stephan Götzinger — Max Planck Institute for the Science of Light and Friedrich-Alexander-Universitaet Erlangen-Nuernberg (FAU), D-91058 Erlangen, Germany

In the first part of this talk we will discuss single-photon sources with near-unity efficiency. These sources are based on the concept of metallo-dielectric antennas. Then we will present experiments where photons and single solid state emitters strongly interact.

HL 39: Symposium SYSG: Spin properties of graphene

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

Invited Talk HL 39.1 Tue 9:30 HSZ 02

Intrinsic magnetism in graphene — •Irina Grigorieva — School of Physics and Astronomy, University of Manchester, UK

I will review our recent experiments on inducing and controlling magnetic response in graphene via introduction of point defects such as vacancies and adatoms. Graphene is hailed as potentially an ideal material for spintronics due to its weak spin-orbit interaction and the ability to control its electronic properties by the electric field effect. We have demonstrated that point defects in graphene - both vacancies and adatoms - carry magnetic moments, leading to pronounced paramagnetic behaviour that dominates graphene's low-temperature magnetism. Even better, we show that the defect magnetism is itinerant (i.e. due to localisation of conduction electrons) and can be controlled by doping, so that the induced magnetic moments can be switched on and off. This not only adds important functionality to potential graphene devices but also has important implications for spin transport.

Invited Talk HL 39.2 Tue 10:00 HSZ 02

Defect Induced Magnetic Moments in Graphene — •Roland Kawakami — The Ohio State University, Columbus, OH, USA — University of California, Riverside, CA, USA

We utilize non-local spin transport measurements to detect the presence of defect induced magnetic moments in graphene. As shown in this talk, point defects such as hydrogen adatoms and lattice vacancies generate magnetic moments in graphene that have substantial exchange coupling with the conduction electrons. Therefore, this exchange coupling produces spin relaxation in the conduction electrons. Specifically, a characteristic field dependence of the non-local spin transport signal identifies the presence of the magnetic moments. Furthermore, Hanle spin precession measurements indicate the presence of an exchange field generated by the magnetic moments. The entire experiment including spin transport is performed in an ultra-high vacuum chamber, and the characteristic signatures of magnetic moment formation appear only after hydrogen adatoms or lattice vacancies are introduced.

Invited Talk HL 39.3 Tue 10:30 HSZ 02

Role of MgO barriers for spin and charge transport in Co/MgO/graphene spin-valve devices — •Bernd Beschoten — 2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany

We investigate the influence of MgO barriers on spin and charge transport in single (SLG) and bilayer (BLG) graphene spin-valve devices. Similar to previous studies on BLG [1], we observe a $1/\mu$ of the spin lifetime in SLG devices. This general trend is only observed in devices with large contact resistance area products $R_cA > 1\mathrm{k}\Omega\mu\mathrm{m}^2$. In devices with long spin lifetimes, we furthermore observe a second Dirac peak, which results from charge transport underneath the contacts. In contrast, all devices with $R_cA < 1\mathrm{k}\Omega\mu\mathrm{m}^2$ only exhibit a single Dirac peak. Additionally, the spin lifetime is significantly reduced indicating that an additional spin dephasing occurs underneath the electrodes. In the latter devices we achieve a gradual increase of R_cA values by successive oxygen treatments. With this manipulation of the contacts both spin lifetime and amplitude of the spin signal can significantly be increased by a factor of seven in the same device. Finally, we present a new method to fabricate graphene-based lateral spin valves on hexagonal boron nitride yielding spin lifetimes above 3 ns, spin diffusion length above 10 μm and large charge carrier mobilities above 30.000 $\mathrm{cm}^2/\mathrm{Vs}$.

This work was supported by DFG through FOR 912.

[1] T.-Y. Yang *et al.*, Phys. Rev. Lett. 107, 047206 (2011).
[2] F. Volmer *et al.* Phys. Rev. B 88, 161405(R)(2013).

Coffee break (15 min.)

Invited Talk HL 39.4 Tue 11:15 HSZ 02

Defect-Mediated Spin Relaxation and Dephasing in Graphene — Mark Lundeberg[1,2], Silvia Folk[1], and •Joshua Folk[1] — [1]University of British Columbia, Vancouver, Canada — [2]Institute of Photonic Sciences, Barcelona, Spain

This talk will describe a series of transport measurements that disentangle mechanisms of spin and orbital phase relaxation in graphene. The measurements are based on well-known quantum interference phenomena–weak localization and universal conductance fluctuations. We show that a careful analysis of the in-plane magnetic field and temperature dependences of these effects can separately quantify spin-orbit and magnetic scattering rates; this technique works especially well in graphene due to its single-atom thickness. Spin relaxation in exfoliated graphene on SiO_2 is found to be dominated by magnetic scattering (scattering off of magnetic defects), with a smaller contribution from spin-orbit interaction. A similar measurement performed in graphene on SiC suggests that both magnetic scattering and spin-orbit interaction are a factor of 10 stronger than in exfoliated graphene.

Invited Talk HL 39.5 Tue 11:45 HSZ 02

Electron spin relaxation in graphene: resonant scattering off local magnetic moments — •Jaroslav Fabian, Denis Kochan, and Martin Gmitra — Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

Dirac electrons in graphene should have large spin relaxation time, some microseconds, due to the weak spin-orbit coupling of its itinerant electrons. Yet experiments show spin lifetimes as short as 100 ps. Traditional spin relaxation mechanisms, Elliott-Yafet and Dyakonov-Perel, seem incapable to explain such short lifetimes, even though some external influences such as hydrogen adatoms seem to induce giant local spin-orbit coupling [1] and so enhance spin-orbit induced spin flips. We believe that the culprit may instead be local paramagnetic moments due to vacancies and some adatoms. As the local moments sit on resonance sites, the spin flip is resonantly enhanced. These resonant local moments are acting as spatial spin hot spots: they may contribute little to momentum relaxation of graphene, but dominate the spin relaxation. This new mechanism explains the observed 100 ps spin lifetimes with as little as 1 ppm of local moments [2]. We acknowledge support from DFG SFB 689, SPP 1285, GRK 1579, and EC under Graphene Flagship (Contract No. CNECT-ICT-604391). [1] M. Gmitra, D. Kochan, and J. Fabian, Spin-orbit coupling in hydrogenated graphene, Phys. Rev. Lett. 110, 246602 (2013);[2] D. Kochan, M. Gmitra, and J. Fabian, Spin relaxation mechanism in graphene: resonant scattering by magnetic impurities, arXiv:1306.0230.

HL 40: Transport: Spintronics and magnetotransport (organized by TT)

Time: Tuesday 9:30–10:30 Location: BEY 81

HL 40.1 Tue 9:30 BEY 81

Spin-population inversion in Co/Pd heterojunctions — •Torsten Pietsch, Stefan Egle, and Elke Scheer — Department of Physics, Universitätstraße 10, University of Konstanz, 78457 Konstanz, Germany

Herein, we investigate experimentally the magneto-transport properties of nanosized Co/Pd hetero contacts and show that a spin-population inversion can be created by resonantly exciting magnetic heterojunctions with high-frequency waves in the GHz and THz regime. Recently, spin-flip photoemission in such metallic, magnetic heterojunctions was predicted theoretically but has not been observed experimentally. When an external magnetic field is applied the Zeeman splitting in the normal metal lifts the spin-degeneracy. Under a large current bias, hot electrons from the ferromagnet can be injected into the upper Zeeman level, thus creating a spin-population inversion in the normal metal. This non-equilibrium spin-population inversion decays via spin-flip transitions, which results in the creation of magnons, scattering at magnetic impurities and, under certain circumstances, photoemission. In the later, case, the energy of the emitted photon corresponds to the Zeeman energy, which can be tuned by the external magnetic field; typical frequencies are in the range of 0.1GHz to 60GHz. By resonantly exciting the Co/Pd point contacts using an external RF source while monitoring the transport properties, we evaluate the parameter space, where a spin-population inversion can be created at the ferromagnet-normal metal interface.

HL 40.2 Tue 9:45 BEY 81

Tuning the ballistic anisotropic magnetoresistance in single-atom contacts via the apex atom — •Fabian Otte[1], Yuriy Mokrousov[2], and Stefan Heinze[1] — [1]Instiut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Peter Grünberg Institut and Institue for Advanced Simulation, Forschungszentrum Jülich und JARA, D-52425 Jülich, Germany

Recently, the tunneling anisotropic magnetoresistance has been demonstrated at the single-atom limit using scanning tunneling spectroscopy and was explained based on density functional theory calculations of the anisotropy of the vacuum local density of states (LDOS) [1]. In the contact regime the explanation via the LDOS breaks down due to overlap of the wave functions and therefore actual calculations of the conductance are necessary. Here, we report first-principles calculations of ballistic transport in model systems of such single-atom contacts using our recently developed Wannierfunction based approach [2]. We present the ballistic anisotropic magnetoresistance (BAMR) in contact and tunneling regime between two ferromagnetic Ni monowires terminated by single 4*d*- and 5*d*- transition metal apex atoms. We show that the BAMR in the tunneling regime can be enhanced by up to an order of magnitude from 20% for Ni- to 150% for 5*d*-apex atoms. We also observe a change of sign in the BAMR between tunneling and contact regime.
[1] N. Néel *et al.*, PRL **110**, 037202 (2013)
[2] B. Hardrat *et al.*, PRB **85**, 245412 (2012)

HL 40.3 Tue 10:00 BEY 81

Electrical tuning of spin-orbit interaction in InAs nanowires — •Zoltán Scherübl[1], Gergö Fülöp[1], Morten Hannibal Madsen[2], Samuel d'Hollosy[3], Christian Schönenberger[3], Jesper Nygård[2], and Szabolcs Csonka[1] — [1]Departement of Physics, Budapest University of Technology and Economic, Budapest, Hungary — [2]Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark — [3]Departement of Physics, University of Basel, Basel, Switzerland

InAs nanowires are a promising platform to fabricate various quantum electronic devices, for instance they have strong spin-orbit interaction (SOI). The controlled tuning of the SOI is needed in spin based qunatum devices, for example spintronic applications, spin qubits. In this study we investigated the possibility of tuning the SOI by electrostatic field. The sources of the electric field were two sidegates paralel to the wire axis. The strength of the SOI was analyzed by weak-antilocalization. We demonstrated that the SOI can be strongly tuned, by a factor of 3 with the electric field across the nanowire, while the average electron density in the nanowire was kept constant.

HL 40.4 Tue 10:15 BEY 81

Dissipationless spin current between two coupled ferromagnets — •Wei Chen, Peter Horsch, and Dirk Manske — Max Planck Institute for Solid State Research, Stuttgart, Germany

We demonstrate the general principle which states that a dissipationless spin current flows between two coupled ferromagnets if their magnetic orders are misaligned. This principle applies regardless the two ferromagnets are metallic or insulating, and also generally applies to bulk magnetic insulators. On a phenomenological level, this principle is analogous to Josephson effect, and yields a dissipationless spin current that is independent from scattering. The microscopic mechanisms for the dissipationless spin current depend on the systems, which are elaborated in details. A uniform, static magnetic field is further proposed to be an efficient handle to create the misaligned configuration and stabilize the dissipationless spin current.

HL 41: Transport: Graphene (organized by TT)

Time: Tuesday 9:30–13:15 Location: WIL C107

Topical Talk HL 41.1 Tue 9:30 WIL C107

A First-Principles Perspective on Two-Dimensional Transition-Metal Dichalcogenides — •Udo Schwingenschlögl — KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia

Layered transition-metal dichalcogenides recently are attracting great attention, because of the possibility to achieve two-dimensional (2D) materials, similar to the exfoliation of graphene from graphite. Using first-principles calculations, we study prototypical monolayer MoS_2 to obtain insight into the influence of defects and substitutional doping, for a wide range of transition-metal dopants. We also address polar transition-metal dichalcogenide monolayers with respect to their structural stability and the effects of the spin-orbit coupling. Heterojunctions of MoS_2 with unsaturated and saturated MXenes are studied; such hyrid systems are interesting for application in all-2D devices.

[1] Phys. Rev. B 87, 100401(R) (2013)
[2] EPL 102, 57001 (2013)
[3] Phys. Rev. B 87, 245307 (2013)

HL 41.2 Tue 10:00 WIL C107

Ab-initio simulations of local current flows in functionalized graphene flakes and ribbons — •Michael Walz, Alexei Bagrets, and Ferdinand Evers — Institute of Nanotechnology (INT) and Institut für Theorie der Kondensierten Materie (TKM), Karlsruhe Institut of Technologie (KIT), D-76131 Karlsruhe, Germany

Using our DFT-based transport framework AITRANSS [1,2], 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.

As one expects, very wide ribbons (flakes, $W \gg L$) exhibit the bulk conductance $G = \frac{2e^2}{h}\frac{W}{\pi L}$ in the absence of adsorbants. With 20% hydrogen absorbants, we observe very complicated patterns of streamlines with many eddies and a broad distribution of local magnetic fields, $\mathbf{B}(\mathbf{r})$, that are induced by the dc-current flow. We plan to study the statistics of the conductance and $\mathbf{B}(\mathbf{r})$ of such large flakes and its dependency on the impurity concentration. Performing such calculations starting from first principles is challenging because of high computational costs. On this account, we parallelized our transport module AITRANSS using standard MPI and OpenMP techniques, also including Scalapack to treat systems up to 10.000 carbon atoms.

[1] A. Arnold *et al.*, J. Chem. Phys. **126**, 174101 (2007).
[2] J. Wilhelm, MW, *et al.*, Phys. Chem. Chem. Phys. **15**, 6684 (2013).

HL 41.3 Tue 10:15 WIL C107

Quantum transport simulations and Fabry-Perot interference patterns in multiple pn-junctions on graphene — •Fedor Tkatschenko[1], Ming-Hao Liu[1], Klaus Richter[1], Martin Drienovsky[2], Jonathan Eroms[2], and Dieter Weiss[2] — [1]Institut für Theoretische Physik, Universität Regensburg — [2]Institut für Experimentelle und Angewandte Physik, Universität Regensburg

Advancements in experimental techniques have led to an amazing progress towards excellent graphene samples and to graphene devices with fascinating properties, ranging from narrow pnp junctions below 100 nm to large mean free paths up to micron scales. In such devices the charge carriers undergo multiple reflections at pn or np interface leading to interesting Fabry-Perot-type interference patterns in the conductance map[1,2]. We address the peculiar features of Fabry-Perot resonances in graphene. To this end we calculate the potential profiles for typical experimental setups[3] with the quantum capacitance model and perform transport calculations using the recursive Green's function technique. The numerical results are in good agreement with the experimental data. We further show that the leading contribution to the Fabry-Perot resonances in the conductance map originates from the first two pn junctions.

[1] A.F. Young and Ph. Kim, Nat. Phys. **5** (2009)
[2] P. Rickhaus, R. Maurand, M. H. Liu, M. Weiss, K. Richter and C. Schönenberger, Nat. Comm. **4** 2342 (2013)
[3] M. Drienovsky, F.-X. Schrettenbrunner, M. H. Liu, F. Tkatschenko, K.Richter, D. Weiss and J. Eroms, in preparation

HL 41.4 Tue 10:30 WIL C107

Ballistic interferences in suspended graphene — •Ming-Hao Liu[1], Peter Rickhaus[2], Romain Maurand[2], Markus Weiss[2], Klaus Richter[1], and Christian Schönenberger[2] — [1]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany — [2]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

Complex Fabry-Pérot interferences in ultraclean suspended graphene have been recently observed, with the ballistic origin confirmed by transport calculations well agreeing with experiment [1]. The observed conductance oscillations account for quantum interference of electron waves propagating ballistically over distances exceeding 1 μm. The complex interference patterns stem from Fabry-Pérot resonances within different cavities defined by electrically controlled pn junctions and the graphene-contact interfaces. In this talk, the theoretical part of this work [1], namely, the full modeling of the ballistic transport from contact to contact through the suspended graphene, will be illustrated at an appropriate depth.

[1] P. Rickhaus, R. Maurand, M.-H. Liu, M. Weiss, K. Richter, and C. Schönenberger, Nat. Commun. **4**, 2342 (2013)

HL 41.5 Tue 10:45 WIL C107

Ballistic transport in graphene nanoconstrictions — •Danny J. M. Jörger[1,2], Bernat Terrés[1,2], Stephan Engels[1,2], Kenji Watanabe[3], Takashi Taniguchi[3], Slava V. Rotkin[1,4], and Christoph Stampfer[1,2] — [1]JARA-FIT and II. Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan — [4]Physics Department, Lehigh University, Bethlehem, Pennsylvania 18015, USA

Graphene nanodevices, such as for example nanoconstrictions are interesting systems for studying mesoscopic phenomena. Recent developments in the fabrication of graphene devices have revealed a significant increase in carrier mobility (e.g. 200.000 cm^2/Vs in bulk samples), making mean free path in the order of device dimensions accesible. This allows to investigate quantum interference effects and ballistic transport in nanostructured graphene. We discuss the differences in electrostatic coupling ($\alpha \approx 9.4 \times 10^{10}$ $cm^{-2}V^{-1}$) at high and low magnetic fields and the width-dependency of the overall conductance level at zero magentic field. Results confirm the Dirac fermion nature of confined charge carriers in graphene. We report on the observation of quasi one-dimensional subband transport characteristics in graphene nanoconstrictions encapsulated in hexagonal boron nitride. The ballistic nature of the transport in our devices ($l_m \geq 500$ nm) allows to study the interplay between confinement and Landau quantization and its crossover.

15 min. break.

HL 41.6 Tue 11:15 WIL C107

Optical conductivity of graphene — •Julia Link, Peter P. Orth, and Jörg Schmalian — Institute for Theory of Condensed Matter, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

Graphene is a two-dimensional crystal of carbon atoms with a honeycomb structure, which has many fascinating optical and electronical properties. It has a high mobility of electrons at room temperature and a high transparency of light with 97.7%. In the optical domain, the value of the transparency does not depend on the frequency of white light being transmitted and is thus universal. This universality is linked to the fine structure constant $\alpha = 1/137$ and can be derived using non-interacting Dirac fermions.

We aim to understand the correction of the optical transparency due to Coulomb interaction. Since there is a long dispute about this correction in the literature [1-6], we try to resolve this controversy. Therefore we combine two different regularization schemes: dimensional regularization and a deformation of the Coulomb potential. We discuss the physical implication of the choice of the regularization.

[1] Herbut, Juricic, Vafek, Phys. Rev. Lett. **100**,046403 (2008)

[2] Mishchenko, Europhys. Lett. **83**, 17005 (2008)
[3] Sheey, Schmalian, Phys. Rev. B **80**, 193411 (2009)
[4] Juricic, Vafek, Herbut, Phys. Rev. B **82**, 235402 (2010)
[5] Rosenstein et al., Phys. Rev. Lett. **110**, 066602 (2013)
[6] Gazzola, Cherchiglia, Cabral, Nemes, Sampaio, Europhys. Lett. **104**, 27002 (2013)

HL 41.7 Tue 11:30 WIL C107

Polycrystalline graphene: mechanical, electrical and thermal properties — •Thomas Lehmann[1,2], Arezoo Dianat[1,2], Frank Ortmann[1,2], Dmitry Ryndyk[1,2], and Gianaurelio Cuniberti[1,2] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany — [2]Dresden Center for Computational Materials Science, TU Dresden, Germany

Large-area samples of graphene tend to be polycrystalline (PC) on some substrates. Grain boundaries with structural defects are expected to alter the structural and electronical properties of graphene. In this work, the mechanical properties of PC graphene are studied by means of density-functional theory and furthermore the electrical and thermal transport properties are addressed. To construct grain boundaries of zigzag and rotated armchair graphene sheets, molecular dynamics simulations are performed. The critical strain leading to structural failure of PC graphene nanoribbons is only half the value of pristine armchair nanoribbons. However we show that it can be significantly enhanced by the reaction of the chemically active grain boundaries with atmospheric gases. The transport properties of those systems are investigated, both parallel and perpendicular to the grain boundary, using an ab initio based atomistic model combined with Landauer transport theory and recursive Green function method. The electronic part is calculated within a tight-binding model and a force-constant approach has been applied for phonon transport.

HL 41.8 Tue 11:45 WIL C107

Electric field control of spin-polarized electron transport through zigzag graphene nanosheets — •Dirk Wiedmann[1], Marius Bürkle[2], and Fabian Pauly[1] — [1]Department of Physics, University of Konstanz, Germany — [2]National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan

We study the spin-polarized transport through a finite zigzag graphene nanoribbon, contacted by carbon-nanotube electrodes [1]. The electronic structure is determined from density functional theory, and Green's functions are used to compute the phase-coherent electric current within the Landauer scattering theory. We observe antiferromagnetically coupled edge states in the graphene nanosheet, which may lead to spin-polarized currents. We analyze how they depend on the position of the electrodes and on applied transverse electric fields. Our ab-initio results are rationalized with the help of a Hubbard model.
[1] D. Wiedmann, M. Bürkle, and F. Pauly, in preparation.

HL 41.9 Tue 12:00 WIL C107

Radiative damping and synchronization in a graphene-based terahertz emitter — •Andrey Moskalenko and Sergey Mikhailov — Institute of Physics, University of Augsburg, Germany

We investigate the collective electron dynamics in a recently proposed graphene-based terahertz emitter [1] under the influence of the radiative damping effect, which is included self-consistently in a molecular dynamics approach. We show that under appropriate conditions synchronization of the dynamics of single electrons takes place, leading to a rise of the oscillating component of the charge current. The synchronization time depends dramatically on the applied dc electric field and electron scattering rate, and is roughly inversely proportional to the radiative damping rate that is determined by the carrier concentration and the geometrical parameters of the device. The emission spectra in the synchronized state, determined by the oscillating current component, are analyzed. The effective generation of higher harmonics for large values of the radiative damping strength is demonstrated.
[1] S. A. Mikhailov, Phys. Rev. B 87, 115405 (2013)

HL 41.10 Tue 12:15 WIL C107

Non-vanishing Coulomb drag in clean double-layer graphene at the Dirac point — •Sven Aeschlimann[1], Michael Schütt[2], Igor Gornyi[1,2,3], Boris Narozhny[1], and Alexander Mirlin[1,2,4] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institut für Nanotechnologie, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]A. F. Ioffe Physica-Technical Institute, St. Petersburg, Russia — [4]Petersburg Nuclear Physics Institute, St. Petersburg, Russia

Coulomb drag is the frictional effect of simple Coulomb interaction onto two currents driven through two spatially separated conducting layers. Initiating a current through one layer, causes a current or a voltage drop in the other.

Recent experiments revealed a suprising nonvanishing resistance at the Dirac point that was expected to be zero for symmetry considerations. We focus on the possibility of a non-vanishing resistance in clean samples due to third order interaction contributions to drag.

HL 41.11 Tue 12:30 WIL C107

Linear Magnetoresistance in bilayer graphene — •Ferdinand Kisslinger, Christian Heide, Christian Ott, and Heiko B. Weber — Lehrstuhl für Angewandte Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, ferdinand.kisslinger@physik.uni-erlangen.de

We investigate the magnetoresistance in bilayer graphene obtained by hydrogen intercalation of monolayer graphene grown on the SiC(0001) surface. Whereas in monolayer graphene electron-electron-interaction and weak localization can be observed at low temperatures, a strong linear contribution dominates the magnetoresistance for bilayer graphene. It is found to be nearly temperature independent.

A variation of charge carrier density using a bottom gate and the comparison of different samples is carried out. The entity of data agrees well with a theoretical model [1] that describes a resistance network of Van-der-Pauw resistors. Consistency with the experiment is achieved when a network of resistors with different resistances is assumed. There are several possibilities where such inhomogeneities may originate from. We can exclude some of them and propose dislocations recently found in bilayer graphene [2] as a good candidate causing this effect.
[1] M.M. Parish and P.B. Littlewood , Nature 426 (2003) 162
[2] B. Butz, C. Dolle, F. Niekiel, K. Weber, D. Waldmann, H. B. Weber, B. Meyer and E. Spiecker, Nature (2013), accepted, DOI: 10.1038/nature12780

HL 41.12 Tue 12:45 WIL C107

Wigner Crystal phases in bilayer graphene — •Peter Silvestrov and Patrik Recher — Institut für Mathematische Physik, TU Braunschweig, Germany

It is generally believed that Wigner Crystal in single layer graphene can not exist because the magnitudes of the electron interaction and the kinetic energy scale similarly with the decreasing electron density. This scaling argument however does not work for the low energy states in bilayer graphene. We consider the Wigner Crystal in slightly doped bilayer graphene with a gap in spectrum opened by applying a perpendicular electric field. We argue that in this system the formation of the Wigner Crystal is not only possible, but a different phases of the crystal with very peculiar properties may exist here depending on the parameters.

HL 41.13 Tue 13:00 WIL C107

Half-metallic bilayer graphene — •Jie Yuan — Raum 26 A 407 RWTH Aachen Sommerfeldstrasse 26, D-52056, Aachen

Charge neutral bilayer graphene has very likely a gapped ground state, as transport experiments have demonstrated. The nature of the ground state is undertermined yet. One plausible ground state is the layered antiferromagnetic spin density wave (LAF) state, where the spins in the top and bottom layers have the same magnitude with opposite directions. We propose that lightly doped bilayer graphene in an electric field perpendicular to the graphene plane may be a half-metal where only one spin direction lis conducting. By the special properties of the half-metal deriving from the LAF state, the primary source of the gap at charge neutrality may be distinguished from other competing ground states like the quantum spin-Hall state. We study this explicitly by using a mean-field theory on a two-layer Hubbard model.

HL 42: Topological insulators (organized by O)

Time: Tuesday 10:30–13:15 Location: GER 38

HL 42.1 Tue 10:30 GER 38

Topological Insulator goes Elemental: α-Sn on InSb — •M. R. Scholz[1], A. Barfuss[1], L. Dudy[1], A. Fleszar[2], G. Bihlmayer[3], D. Wortmann[3], J. H. Dil[4], G. Landolt[4], M. Radovic[4], G. Li[2], R. Claessen[1], and J. Schäfer[1] — [1]Phys. Inst. and RCCM, Univ. Würzburg — [2]Inst. f. Theo. Physik u. Astronomie, Univ. Würzburg — [3]Peter Grünberg Inst. a. Inst. f. Advanced Simulation, FZ Jülich — [4]Swiss Light Source, Paul-Scherrer-Institut Villigen

We report on the topological insulator phase of epitaxially grown α-Sn on InSb substrates where compressive strain is induced by a slight lattice mismatch. The topological surface state (TSS) forms in the presence of an unusual band order not based on direct spin-orbit coupling, as shown in DFT and GW slab-layer calculations. Angle-resolved photoemission probes how the TSS emerges from the second highest bulk valence band. By means of spin-resolved photoemission we show that the surface state is highly spin-polarized with a counter-clockwise helicity below the Dirac point. The band situation in α-Sn closely resembles that of strained HgTe. Quantum well films of HgTe sandwiched between CdTe are a system where the topological properties have been successfully probed in DC transport [1]. The similarities to HgTe make α-Sn a promising candidate to exhibit the quantum spin Hall effect as well, if the film thickness is reduced to the 2D limit. Particularly, as a nontoxic elemental system, α-Sn is easier to fabricate which opens various pathways to access and manipulate the topological surface state. As a first step, we demonstrate the precise control of the Fermi level by dopants. [1] M. König et al., Science 318, 766 (2007).

HL 42.2 Tue 10:45 GER 38

Temperature effects in soft and hard x-ray photoemission from topological insulators — •Jürgen Braun, Jan Minar, and Hubert Ebert — Dept. Chemie, LMU Universität München, Germany

A brief introduction to the theory of temperature-dependent soft and hard x-ray angle-resolved photo electron spectroscopy (SARPES, HARPES) of solid materials is given with an emphasis on the so-called one-step-model of photoemission. The main aspects of the theory [1,2] and its implementation within the Munich SPR-KKR program package [3] will be reviewed. Our method, which is based on the Coherent Potential Approximation (CPA) alloy theory (alloy analogy model), goes well beyond the simple, but standard Debye-Waller approach to photoemission by including in particular the temperature dependence of the effective photoemission matrix elements as well. This allows among others to reproduce the so called XPS- or density of states limit in angle-resolved photoemission which occurs for high photon energies and/or high temperatures due to a full Brillouin zone averaging caused by phonon scattering. First examples of soft- and hard x-ray ARPES calculations at finite temperature for W(110), Sb_2Te_3 and Bi_2Se_3 will be presented.

1. A. Gray, J. Minár, J. Braun, H. Ebert, C. S. Fadley et al., Nature Materials, **10**, 759 (2011) and Nature Materials **11**, 957 (2012) 2. J. Braun, J. Minár, H. Ebert et al. Phys. Rev. B **88** 005400 (2013) 3. H. Ebert et al., The Munich SPR-KKR package, version 6.3, http://olymp.cup.uni-muenchen.de/ak/ebert/

HL 42.3 Tue 11:00 GER 38

Reorganization of a Topologically Protected Surface State: Theory for Au-Covered Bi_2Te_3(111) — Francisco Muñoz[1,2], •Jürgen Henk[2], and Ingrid Mertig[2] — [1]Facultad de Ciencias, Universidad de Chile, Chile — [2]Martin Luther University Halle-Wittenberg, Halle, Germany

The electronic structure of Au-covered Bi_2Te_3 is investigated by first-principles calculations. The Dirac surface state of the topological insulator Bi_2Te_3 hybridizes with the Au sp states, which gives rise to strong reorganization of the surface electronic structure. Striking features of the modified Dirac surface state are (i) the introduction of new Dirac points within the fundamental band gap of Bi_2Te_3, (ii) an extremely weak dispersion, and (iii) an anisotropic number of conducting channels in the fundamental band gap of Bi_2Te_3 which leads to a complicated Fermi surface. Our findings have impact for spin-dependent surface transport.

HL 42.4 Tue 11:15 GER 38

Barrier-free sub-surface incorporation of magnetic impurities into the Bi(111) surface: Manipulation of the protected surface state - Experiment — •C. Klein[1], P. Zahl[2], N. Vollmers[3], U. Gerstmann[3], D. Lückermann[4], G. Jnawali[1], H. Pfnür[4], C. Tegenkamp[4], W.-G. Schmidt[3], P. Sutter[2], and M. Horn-von Hoegen[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, DE — [2]Center for Functional Nanomaterials, Brookhaven National Laboratory, New York, USA — [3]Department of Physics, University of Paderborn, DE — [4]Institut for Solid State Physics, University of Hannover, DE

Due to the large spin orbit coupling, electron backscattering within the Bi(111) surface states is strongly suppressed. In order to identify possible scattering mechanisms we performed low temperature scanning tunneling microscopy (LT-STM) measurements in which submonolayer amounts of 3d-metals (Fe, Co, Ni, Cu) were deposited at 5K. The metal atoms become immediately embedded in a sub-surface site, as they are not present in STM topography. They only become apparent in STS at tunneling conditions close to the Fermi-energy, as they are surrounded by a pronounced anisotropic threefold electronic scattering pattern with lateral dimensions of more than 10 nm. DFT calculations indeed confirm a barrier free incorporation of the 3d-metal impurities into the first Bi-Bilayer even at such low temperatures. This incorporation effect is limited to 3d-metals, as screening effects of the s- and p- orbitals are of great importance and leads to an effective reduction of the free surface energy of about 5 eV.

HL 42.5 Tue 11:30 GER 38

Efficient full-relativistic DFT calculations for large systems: Application to Bi-related surface states — •Uwe Gerstmann[1], Nora Jenny Vollmers[1], Wolf Gero Schmidt[1], Claudius Klein[2], Michael Horn-von Hoegen[2], Philipp Kröger[3], Daniel Lückermann[3], Herbert Pfnür[3], and Christoph Tegenkamp[3] — [1]Department of Physics, University of Paderborn, Warburger Str. 100, 33098 Paderborn — [2]Center for Nanointegration CENIDE, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg — [3]Institut for Solid State Physics, University of Hannover, Appelstr. 2, 30167 Hannover

Spin-orbit coupling is well-known to be the driving force behind ferromagnetism and can be used to control the functionality of electronic devices in spintronics. In asymmetric quantum wells and at surfaces spin-split electron gases may form and give rise to the Rashba-effect. In some cases, e.g. Bi(111) bilayers, the bandstructures are furthermore affected by k-point dependent shifts in the order of several eV. This effect may become crucial if adatoms are incorporated or adsorbed at the surface, strongly influencing the occupancy of the adatom-induced states and by this the magnetic moments and further magneto-transport properties of the resulting structures. In this work, we present an efficient pseudopotential-based method that allows a full-relativistic description of large systems containing several hundreds of atoms. The approach is used to describe the incorporation of a wide range of atomic species (3d-transition, coin-metal as well as rare-earth ions) into Bi(111) surfaces, where supercells with more than 200 atoms are needed to describe the resulting extended magnetic structures correctly.

HL 42.6 Tue 11:45 GER 38

Magnetic impurities on Bi thin films - Conductivity and surface diffusion — •Philipp Kröger[1], Daniel Lükermann[1], Sergii Sologub[2], Nora Vollmers[3], Uwe Gerstmann[3], Wolf Gero Schmidt[3], Herbert Pfnür[1], and Christoph Tegenkamp[1] — [1]Leibniz Universität Hannover, Inst. für FKP, Appelstr. 2, 30167 Hannover — [2]Inst. of Ph., Nat. Acad. of Sc., Nauky Av. 46, 03028 Kyiv, Ukraine — [3]Universität Paderborn, Theoretische Physik, 33098 Paderborn

The semimetal bismuth has attracted a lot of interest because of its unique electronic properties such as a low carrier concentration and a large mobility. The surface states reveal a pronounced Rashba splitting and the conductivity can be well discriminated from bulk contributions if thin films are grown epitaxially on Si(111) substrates, making surface related effects accessible even in macroscopic conductance measurements.

In this context the adsorption of the magnetic atom Cr (4,8 μ_B) on the Bi(111) surface will be discussed. In comparison to other adsorbates

(Fe, Co, Tb) Cr exhibits the strongest scattering effect, accompanied by a transition from Weak Anti- to Weak Localization. This transition indicates strong impurity scattering, which lifts all spin-dependent selection rules. Furthermore, a significant increase of electron concentration due to hybridization effects has been found. For Tb and Cr surface diffusion of adsorbate-atoms even at T≈10 K needs to be considered.

HL 42.7 Tue 12:00 GER 38

Magnetic interaction and magnetic fluctuations in topological insulators with ordered and disordered magnetic adatoms — •MAIA G. VERGIORY[1,4], LEVAN CHOTORLISHVILI[2], ARTHUR ERNST[1], VITALI DUGAEV[1], ANDREAS KOMNIK[3], MIJAIL OTROKOV[4], EVGUENI CHULKOV[4], and JAMAL BERADKAR[2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [2]Institut fr Physik, Martin-Luther-Universitat Halle-Wittenberg, Germany — [3]Institut fr Theoretische Physik, Universitt Heidelberg, Germany, — [4]Donostia International Physics Center, Donostia - San Sebastian, Spain

Using a first-principles Green's function approach we study magnetic properties of the magnetic binary topological insulators Bi2Se3, Bi2Te23 and Sb2Te3 doped with 3d transition metals. We analyze the magnetic phase for each dopant, the exchange interaction, the Curie temperature and the Bloch spectral function. Furthermore, we observe that the interaction of magnons with surface electrons essentially renormalizes the electron energy spectrum. The renormalized spectrum is nonlinear and can be characterized by a negative effective mass of electrons and holes for any k point different from 0. The electron velocity near the Dirac point depends on the electron-magnon coupling.

HL 42.8 Tue 12:15 GER 38

The edge state at the dark side of the weak topological insulator $Bi_{14}Rh_3I_9$ probed by STM — •Christian Pauly[1], Bertold Rasche[2], Marcus Liebmann[1], Marco Pratzer[1], Klaus Koepernik[3], Manuel Richter[3], Michael Ruck[2], Jeroen van den Brink[3], and Markus Morgenstern[1] — [1]II. Institute of Physics B, RWTH Aachen University and Jara Fit, Germany — [2]Departement of Chemistry and Food Chemistry, TU Dresden, Germany — [3]Institute for Theoretical Solid State Physics, IFW Dresden, Germany

Using scanning tunneling microscopy (STM) and spectroscopy (STS) at 6 K, we probe the local atomic and electronic structure of the weak topological insulator $Bi_{14}Rh_3I_9$ [1]. In [001]-direction, the material is built from stacks of intermetallic planes with non-trivial 2D topology and spacer layers in between. Thus, the surfaces of the intermetallic planes, which are the natural cleaving planes of the material, exhibit a trivial band gap however with topologically protected states at each step edge [1]. $Bi_{14}Rh_3I_9$ is cleaved at a base pressure of 10^{-10} mbar giving rise to several hundreds of nm large terraces of the intermetallic layer interrupted by step edges. Using STS, we identified the band gap on top of the intermetallic layer, which is in agreement with ARPES data, whereas at the step edges we directly mapped the edge state. The edge state appears continuously through the band gap and exhibits a spatial distribution of 0.4 nm FWHM. The observed spatial periodicity along the step edge is in line with the atomic structure confirming the Bloch type of this state. Partially, dispersive features appear which will be discussed. [1] B. Rasche et al., Nature Mater. 12, 422 (2013)

HL 42.9 Tue 12:30 GER 38

Evidence for topological band inversion of the phase change material $Ge_2Sb_2Te_5$ — •Marcus Liebmann[1], Christian Pauly[1], Alessandro Giussani[2], Jens Kellner[1], Sven Just[1], Jaime Sanchez-Barriga[3], Emile Rienks[3], Oliver Rader[3], Raffaella Calarco[2], Gustav Bihlmayer[4], and Markus Morgenstern[1] — [1]II. Inst. Phys. B, RWTH Aachen University — [2]Paul-Drude-Institut für Festkörperelektronik, Berlin — [3]Helmholtz-Zentrum für Materialien und Energie, BESSY, Berlin — [4]Peter-Grünberg-Institut and Institute für Advanced Simulation, Forschungszentrum Jülich

We present an angle-resolved photoemission study of the ternary phase change material $Ge_2Sb_2Te_5$, epitaxially grown on Si(111) in the metastable cubic phase. This material serves, e.g., in DVDs as a fast switchable material (1 ns) between the metallic cubic and an insulating amorphous phase. The observed upper bulk valence band shows a minimum at $\bar{\Gamma}$ being 0.3 eV below the Fermi level E_F and a circular Fermi contour around $\bar{\Gamma}$ with a dispersing diameter of $0.27-0.36$ Å^{-1}. This is in agreement with density functional theory calculations of the Petrov stacking sequence of the cubic phase which is topologically nontrivial. Moreover, the results are in line with all previous calculations of $Ge_2Sb_2Te_5$ exhibiting the valence band maximum at Γ for a trivial $\mathbb{Z}_2$ topology and away from Γ for a non-trivial one. Scanning tunneling spectroscopy exhibits a band gap of 0.4 eV around E_F. Our finding opens the perspective of ns-switching between a topological crystalline and an insulating amorphous phase.

HL 42.10 Tue 12:45 GER 38

Step wise variation of the electrochemical potential at step edges of the Bi_2Se_3 surface — •Christian A. Bobisch, Sebastian Bauer, and Rolf Möller — Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany

Bi_2Se_3 is a 3D topological insulator (TI) whose surface states are protected from direct backscattering by time reversal symmetry [1]. However, step edges on a Bi_2Se_3 surface are predicted to work as an electron scatterer for other scattering angles than 180° backscattering [2]. We studied the electron transport on the surface of a 14.5 QL (quintuple layer) thick Bi_2Se_3 film grown on Si(111). By a distance dependent resistance measurement [3] in the μm range, we found a metallic character of the film with a sheet conductance of $2\times10^{-3}\Omega^{-1}$ which agrees well with recent literature [4]. By scanning tunneling potentiometry (STP) [5], we simultaneously analyzed the topography and the electrochemical potential μ_{ec} under real transport conditions. We observe on the microscopic scale a potential gradient which corresponds well the macroscopic conductance. In the vicinity of step edges we find a step-like variation of μ_{ec} which is a fingerprint of electron scattering at the step edge. For the given sample the electrical conductivity of a 1 QL step could be deduced to $3800\pm500\Omega^{-1}$cm^{-1}.

[1] M. Z. Hasan et al., Rev. Mod. Phys. 82, 3045 (2010). [2] W. Jing et al., Chin Phys. B 22, 067301 (2013). [3] P. Jaschinsky et al., J. Appl. Phys. 104, 094307 (2008). [4] A. A. Taskin et al., Phys. Rev. Lett. 109, 066803 (2012). [5] P. Muralt et al., Appl. Phys. Lett. 48, 514 (1986).

HL 42.11 Tue 13:00 GER 38

Quantum phase transitions of a disordered antiferromagnetic topological insulator — •Paul Baireuther[1], Jonathan M. Edge[1], Ion C. Fulga[1], Carlo W.J. Beenakker[1], and Jakub Tworzydlo[2] — [1]Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands — [2]University of Warsaw, Hoza 69, 00-681 Warsaw, Poland

We have studied the effect of electrostatic disorder on the conductivity of a three-dimensional antiferromagnetic insulator (a stack of quantum anomalous Hall layers with staggered magnetization). The phase diagram contains regions where the increase of disorder first causes the appearance of surface conduction (via a topological phase transition), followed by the appearance of bulk conduction (via a metal-insulator transition). The conducting surface states are stabilized by an effective time-reversal symmetry that is broken locally by the disorder but restored on long length scales. A simple self-consistent Born approximation reliably locates the boundaries of this socalled "statistical" topological phase.

HL 43: Frontiers of electronic structure theory - Non-equilibrium phenomena at the nano-scale III (organized by O)

Time: Tuesday 10:30–13:15 Location: TRE Ma

Topical Talk HL 43.1 Tue 10:30 TRE Ma

Ultrafast relaxation dynamics of Hubbard nanoclusters — •Michael Bonitz[1], Sebastian Hermanns[1], Christopher Hinz[1], and Denis Lacroix[2] — [1]Institut für Theoretische Physik und Astrophysk, CAU Kiel, Leibnizstr. 15, 24098 Kiel — [2]IPN Orsay, 15 Rue Georges Clemenceau, 91406 Orsay

With the growing availability of intense short-pulse radiation sources it becomes possible to drive interacting many-particle or few-particle systems out of equilibrium in a controlled way. The subsequent relaxation and equilibration dynamics is still poorly understood. From a theory point of view these processes are complicated due to the simultaneous dynamics of the occupation functions and of binary correlations. The problem becomes even more complicated when the system has finite size and is spatially inhomogeneous [1]. The Hubbard model is a prototype for treating correlation effects in condensed matter or molecular systems fully including finite size and inhomogeneity effects. We, therefore, concentrate on the relaxation dynamics of small 1D, 2D and 3D Hubbard clusters that contain from a few to several hundred electrons. We observe a complex multi-stage relaxation behavior that depends on the external excitation, on the coupling strength and on the geometry of the system. In this talk we present results from two complementary theoretical approaches: first, from nonequilibrium Green functions where we apply the Generalized Kadanoff Baym ansatz [1] and, second, from a stochastic mean field approach.

[1] K. Balzer, and M. Bonitz, "Nonequilibrium Green's Functions Approach to Inhomogeneous Systems", Lect. Notes Phys. **867** (2013)

HL 43.2 Tue 11:00 TRE Ma

Exact adiabatic approximation in TDDFT — •Jeiran Jokar and Nicole Helbig — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The use of functionals from static density functional theory in an adiabatic way in a time-dependent framework is known to cause various problems due to the resulting exchange-correlation kernel being frequency independent. In order to isolate the effects which are due to the adiabatic approximation we calculate the exact static potential for two electron systems. Before using this potential in an adiabatic way in a time propagation we need to ensure that the potential is well defined also at those parts of space where the density is small as they might become more populated at a later time. We use the exact adiabatic approximation to describe Rabi oscillations, i.e. the oscillation between the ground state and an excited state when a monochromatic laser with a frequency close to the resonance is applied.

HL 43.3 Tue 11:15 TRE Ma

Real-time propagation of coupled Maxwell-Schrödinger and time-dependent Kohn-Sham-Maxwell systems — •René Jestädt[1], Heiko Appel[1], and Angel Rubio[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

Based on the Riemann-Silberstein vector of the electromagnetic field, we formulate Maxwell's equations in a symplectic spinor representation similar to the Dirac equation. This spinor representation allows us to use standard unitary propagation techniques developed for the Schrödinger equation [1] also for Maxwell's equations and simplifies a coupled solution of Maxwell's and Schrödinger's equations. To illustrate our approach, we present the real-time evolution of atomic systems embedded in optical waveguides and dielectric nanostructures. The coupling of Maxwell's equations to the time-dependent Kohn-Sham equations is a basic ingredient for the development of a time-dependent density functional theory formulation of quantum electrodynamics [2]. As an extension of our work on coupled Maxwell-Schrödinger systems, we show first steps of an implementation of Maxwell's equations coupled to the time-dependent Kohn-Sham equations in the first principles real-space real-time code octopus [3].

[1] A. Castro et al., J. Chem. Phys. **121** (2004).
[2] M. Ruggenthaler, F. Mackenroth, and D. Bauer, Phys. Rev. A **84**, 042107 (2011); I. Tolkatly, Phys. Rev. Lett. **110**, 233001 (2013).
[3] X. Andrade et al., J. Phys. Cond. Mat. **24** (2012).

HL 43.4 Tue 11:30 TRE Ma

Nonlinear optics by means of the dynamical Berry phase: Application to second- and third-harmonic generation — •Claudio Attaccalite[1] and Myrta Gruning[2] — [1]Univ. Grenoble Alpes/CNRS, Institut Neel, F-38042 Grenoble, France — [2]School of Mathematics and Physics, Queen's University Belfast, Belfast BT7 1NN, Northern Ireland, UK

We present an real-time approach to study nonlinear optical properties in Condensed Matter systems that is especially suitable for crystalline solids. The equation of motions and the coupling of the electrons with the external electric field are derived from the Berry phase formulation of the dynamical polarization. Many-body effects are introduced by adding single-particle operators to the independent-particle Hamiltonian. Specifically we include crystal local field effects, renormalization of the energy levels and excitonic effects. The approach is validated by calculating the second and third harmonic generation of bulk semiconductors. Finally we present second-harmonic generation spectrum of h-BN or MoS2 monolayers and show that correlation effects double the signal intensity at the excitonic resonances with respect to the contribution from independent electronic transitions.

References: [1] Nonlinear optics from ab-initio by means of the dynamical Berry-phase http://arxiv.org/abs/1309.4012 [2] Second Harmonic Generation in h-BN and MoS2 monolayers: the role of electron-hole interaction http://arxiv.org/abs/1310.7459

15 min. break

HL 43.5 Tue 12:00 TRE Ma

Accurate Correlation Energies from Adiabatic Time-Dependent Density Functional Theory with Renormalized Kernels — •Thomas Olsen[1] and Kristian S. Thygesen[2] — [1]Universidad del Pais Vasco — [2]Center for Atomic-scale Materials Design (CAMD), Technical University of Denmark

We demonstrate the accuracy of electronic correlation energies obtained from the adiabatic connection and Time-Dependent Density Functional Theory (TDDFT) using a non-empirical renormalized gradient-corrected exchange-correlation kernel. The method can be viewed as a natural step beyond the Random Phase Approximation (RPA) and captures the short-range correlation effects which are poorly described in RPA. In particular, we show that for molecules and solids the renormalized kernel gives a four and five fold improvement in binding energies respectively when compared to RPA. We also consider examples of barrier heights in chemical reactions, molecular adsorption and graphene interacting with metal surfaces, which are three examples where RPA has provided highly accurate results. In these cases, our novel kernel provides results that are of equal quality or even slightly better than RPA, with a similar computational cost. We finally note that the renormalization procedure can be applied to any known semi-local exchange-correlation functional and thus defines an entire new class of adiabatic non-local functionals for ground state calculations within TDDFT.

HL 43.6 Tue 12:15 TRE Ma

Low scaling algorithm for the random phase approximation — •Merzuk Kaltak, Jiri Klimeš, and Georg Kresse — University of Vienna, Computational Material Physics

The computationally most expensive step in conventional RPA implementations is the calculation of the independent particle polarizability χ. We present an RPA algorithm that calculates χ using the Green function G in real space and imaginary time. The systematic construction of optimized time and frequency grids for G is obtained by means of solving a fitting problem. Furthermore a non-uniform discrete Fourier transform between the two grids is introduced, which converges exponentially. We show that the usage of the Green function approach in combination with the optimized grids can be used for the calculation of the RPA correlation energy for large systems.

HL 43.7 Tue 12:30 TRE Ma

Long range correlation energy from coupled atomic response functions — •Alberto Ambrosetti and Alexandre Tkatchenko — Fritz Haber Institut der MPG, Faradayweg 4-6 14195 Berlin, Ger-

many

Electron correlation is an elusive and ubiquitous energy contribution that arises from transient collective electron fluctuations. Its reliable (accurate and efficient) modeling is central to the correct description of cohesive, structural, and response properties of molecules and solids. In this regard, the main challenge is to model the long-range correlation energy beyond (semi-)local density-functional approximations. Here we propose a very efficient method to compute the long-range correlation energy for non-metallic molecules and solids within a density functional theory framework, by using coupled atomic response functions (ARF). Extending the recent MBD method [1], we separate the coupling between ARFs into short and long range, allowing for a seamless many-body treatment of weakly and strongly polarizable systems. Thorough benchmarking on large data sets including small molecules (S22, S66x8), large supramolecular complexes (S12L), molecular crystals (X23) and bulk graphite shows consistently good agreement with high level theoretical and experimental reference binding energies (within the order of 6%). The uniform accuracy for molecules and solids represents a strong validation of our method, and further confirms the importance of modeling the truly collective nature of the long-range correlation energy. [1] A. Tkatchenko et al. PRL **108** 236402 (2012).

HL 43.8 Tue 12:45 TRE Ma

The exact Hohenberg-Kohn functional for a lattice model — •Tanja Dimitrov[1], Heiko Appel[1], and Angel Rubio[1,2] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

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 and to gain insight into the behavior of the exact functional, we investigate the exact solution of the many-body Schrödinger equation for a lattice model. Using exact diagonalization, we explicitely construct the exact Hohenberg-Kohn functional and the mapping from densities to wavefunctions. Besides the normal inter-system derivative discontinuity widely discussed in the density-functional theory community, we observe a new feature of the exact functional in the low-density limit. This "intra-system derivative discontinuity" resembles the inter-system derivative discontinuity, but is within the system (work in progress [3]). The description of many physical phenomena linked to charge-transfer processes (both in the static and dynamical regimes) require a proper account of this "intra-system derivative discontinuity".

[1] A. J. Cohen et al. Science **321**, 792 (2008).
[2] P. Mori-Sanchez et al., Phys. Rev. Lett. **100**, 146401 (2008).
[3] T. Dimitrov, H. Appel, A. Rubio to be published

HL 43.9 Tue 13:00 TRE Ma

Incorporating static correlation effects into density functional theory — Nektarios N. Lathiotakis[1], •Nicole Helbig[2], Nikitas I. Gidopoulos[3], and Angel Rubio[4,5] — [1]Theoretical and Physical Chemistry Institute, NHRF Athens, Greece — [2]Peter-Grünberg Institut, Forschungszentrum Jülich, Germany — [3]Department of Physics, Durham University, United Kingdom — [4]Nano-Bio Spectroscopy group, Universidad del Pais Vasco and DIPC, San Sebastian, Spain — [5]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

We present a novel idea that builds on the knowledge acquired in Reduced density matrix functional theory (RDMFT) to construct a density-functional scheme which accurately incorporates static and left-right correlation effects. At the same time, the new scheme preserves the high quality of a density functional description at the equilibrium and keeps the computational costs at an acceptable level comparable to the costs when using hybrid functionals. Within this scheme the natural orbitals, i.e. the eigenfunctions of the one-body density matrix, are constrained to be solutions of a single-particle Schrödinger equation with a local effective potential. This provides a natural way to connect an energy eigenvalue spectrum to the natural orbitals. This energy spectrum is found to reproduce the ionization potentials of different atoms and molecules very well. In addition, the dissociation limit of diatomic molecules is well described without the need to break any spin symmetry, i.e. this attractive feature of RDMFT is preserved. The present scheme can be easily implemented in all first principles codes for electronic structure calculations.

HL 44: ZnO and its relatives: Devices

Time: Tuesday 10:45–12:45 Location: POT 151

HL 44.1 Tue 10:45 POT 151

Energy-selective monolithic multichannel ultraviolet photodiodes based on (Mg,Zn)O thin films — •Zhipeng Zhang, Holger von Wenckstern, Jörg Lenzner, 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 photodiodes employing Schottky contacts based on ternary (Mg,Zn)O thin films in wurtzite modification [1]. We utilize a new concept for forming a continuous composition spread (CCS) [2] within the active layer allowing the design of energy-selective, monolithic and multichannel ultraviolet metal-semiconductor-metal photodiodes [3]. The CCS of (Mg,Zn)O thin film was realized by pulsed-laser deposition on a 2 inch double-sided polished a-plane sapphire wafer using a single segmented target. The Mg-content and with that the bandgap change linearly along the compositional gradient [2].

The photo response of the photodiodes with a defined spectral bandwidth is enabled by an integrated optical filter layer providing a high energy cutoff. Further, we also have fabricated photodiodes from a wafer with separated active and filter layer with lateral graded CCS. By that the onset of absorption was tuned over 330 meV and the bandwidth of the photodiodes can be controlled from 270 meV down to about 30 meV.

[1]: Z. Zhang et al., Appl. Phys. Lett. **99**, 083502 (2011)
[2]: H. von Wenckstern et al., CrystEngComm. **15**, 10020 (2013)
[3]: Z. Zhang et al., Appl. Phys. Lett. **103**, 171111 (2013)

HL 44.2 Tue 11:00 POT 151

MOCVD-growth and characterisation of AZO-contacts for p-doped GaAs nanowire structures — •Christian Koppka[1], Alexander Koch[1], Andreas Nägelein[1], Sana Muhammad Ullah[1], Matthias Steidl[1], Katja Tonisch[1], Peter Kleinschmidt[1,2], Sabine Nieland[2], Uta Stürzebecher[2], Claudia Schmidt[3], Werner Prost[3], and Thomas Hannappel[1,2] — [1]TU Ilmenau, Germany — [2]CiS Forschungsinstitut, Erfurt, Germany — [3]Universität Duisburg-Essen, Germany

A key part in the development of nanowire-based solar cells is based on the production of appropriate front side contacts. In this regard, the application of transparent conductive oxides (TCOs) for the production of tunnel junctions on p-doped III-V semiconductors is investigated. To obtain homogeneous coating of non-planar surfaces, such as core-shell nanowire structures, an ALD type process has been established in a standard MOCVD reactor (Aixtron). Deposition parameters such as growth temperature, carrier gas flow and percursor concentrations were adjusted using planar sapphire and p-GaAs substrates in a first step to achieve highly conductive and transparent films. The deposited films were characterized by scanning electron micrsocopy (SEM), X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS) as well as various methods for determining the optical and electrical properties. Current-voltage measurements reveal an ohmic behaviour of the AZO contact on planar p-doped GaAs. In a next step, this contact system is implemented on nanowire structures.

HL 44.3 Tue 11:15 POT 151

Controlled fabrication of ZnO/ZnS core-shell nanotube arrays prepared on anodic aluminum oxide with enhanced photoluminces and electronic properties — •Samar Tarish[1,2], Chengliang Wang[1], Ahmed Al-Haddad[1,2], Zhijie Wang[1], Zhibing Zhan[1], and Yong Lei[1] — [1]Institute for Physics and IMN Macro-Nano (ZIK), Ilmenau University of Technology, Prof. Schmidt Str. 26, 98693 Ilmenau, Germany. — [2]Department of Physics, College of Science, The University of Mustansiryah, Baghdad, Iraq.

Heterostructured ZnO/ZnS core-shell nanotube arrays on the AAO template were fabricated by a two-step growth process. The ZnO nanotubes were first synthesized by atomic layer deposition ,and the ZnO/ZnS composite arrays can be successfully obtained afterwards through sulfartion reaction. The optical properties of the composite nanotubes change as a function of the ZnS shell thickness , and it was found that the UV emission intensity of ZnO/ZnS core-shell nanotubes is stronger than that of ZnO nanotubes. Besides, ZnO/ZnS core shell shows better electric properties than ZnO nanotubes . With the enhanced electrical conductivity comparing with the bare ZnO arrays the intriguing improvement implies the promising utilization of this special ZnO/ZnS heterstuctured nanotubes array configuration in the applications, such as gas and chemical sensing and optical switching applications.

HL 44.4 Tue 11:30 POT 151

Electrical characteristics of functionalized and bare ZnO nanowire Schottky diodes — •Alejandra Castro-Carranza, Stephanie Bley, Olesea Volciuc, Tobias Voss, and Jürgen Gutowski — Institute of Solid State Physics, University of Bremen, Bremen, Germany

Zinc oxide nanowires (ZnO NW) have shown to be promising 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 nanostructures is to form hybrid assemblies with other materials. Previously, it has been shown that the photoluminescence (PL) spectrum of the ZnO NW arrays is modified when applying other materials, e.g. polymers and metals. This has been attributed to variations of the internal electric field and trap states at the interface. To gain further insight into these physical phenomena, we explore the electrical characteristics by means of Schottky diodes based on bare and coated ZnO NW arrays. Specifically, the internal electric field and charge carrier density of our devices are determined using capacitance-voltage characterization, the quality of the interfaces is examined using current-voltage characteristics, and the density of states is explored using capacitance-frequency characteristics.

HL 44.5 Tue 11:45 POT 151

Influence of antimony doping on optical and structural properties of ZnO nanowires — •Sarah Schlichting[1], Thomas Kure[1], Alexander Franke[1], Emanuele Poliani[1], Eswaran Senthil Kumar[2], Faezeh Mohammadbeigi[2], Simon Watkins[2], and Axel Hoffmann[1] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Berlin, Germany — [2]Simon Fraser University, Department of Physics, Burnaby, Canada

Antimony (Sb) is a canditate to obtain p-conductivity in ZnO. First-principles calculations indicate that a complex with induced Zn vacancies and low formation energy would lead to a shallow acceptor.[1] However, there is also evidence that Sb acts as a shallow donor in ZnO so that the doping mechanism remains controversial.[2]
We investigated the optical and structural properties of Sb-doped ZnO nanowires (NW) by low temperature photoluminescence (PL) under the influence of an external magnetic field, Raman measurements on ensemble and single NW as well as TEM-CL.
We concluded that the Sb emission at 3.3639 eV with a FWHM of approx. 200 μeV originates from a donor bound exciton. Our measurements confirm the observed donor behavior of Sb by the formation of a composed Sb and Zn vacancy complex.

[1] S. Limpijumnong et al., Phys. Rev. Lett. 92, 155504 (2004); [2] E. Senthil Kumar et al., Appl. Phys. Lett. 102, 132105 (2013)

HL 44.6 Tue 12:00 POT 151

XPS investigations of selective surface passivation for highly stable metal oxide TFTs — •Yulia Trostyanskaya, Marlis Ortel, Torsten Balster, and Veit Wagner — Campus Ring 1, 28759 Bremen, Germany

Zinc oxide thin film transistors (TFTs) showing high electron mobilities (7 cm2/Vs in air) were prepared by spray pyrolysis. In air the transistors showed considerable hysteresis and shift in threshold voltage during operation. After selective surface passivation with benzoyl-1,1,1-trifluoroacetone (BTA) the hysteresis and operational stability improved significantly. Analysis of chemical composition and binding properties of the passivation material is crucial to develop a microscopic model of the semiconductor-passivation interaction. By means of X-ray photoelectron spectroscopy (XPS) was found that a monolayer of BTA bond to Zn can be achieved by desorption of weakly bonded multilayers at 30°C only. The BTA-Zn bond withstands high temperatures but decomposition of the compound was observed at 170°C. This is far above the operation temperature of TFTs. The decomposition was monitored by XPS, the F-peak was split from the original one at 688.5 eV to a second one at 685.3eV. This indicates the formation of Zn-F bonds by decomposing the CF3-group. The analysis shows the excellent suitability of BTA as passivation layer due to strong bonding properties of BTA to Zn and high chemical stability under standard operation conditions of TFTs.

HL 44.7 Tue 12:15 POT 151

ZnO nanowires for gas sensing applications — •Manfred Madel, Julian Jakob, Martin Dickel, Florian Huber, Bruno Amann, and Klaus Thonke — Institute of Quantum Matter / Semiconductor Physics Group, University of Ulm

ZnO nanowires with average diameter of $50 - 100\,\mathrm{nm}$ were grown by chemical vapour deposition. Due to the large surface to volume ratio the nanowires show very good sensing behaviour to adsorbed molecules in different gas atmospheres. Besides conventional electrical measurements, micro-photoluminescence (μPL) and photoconductivity read out is used for the detection of oxygen atmosphere.
To adress single nanowires in μPL measurements, these were aligned by the simple and low cost dielectrophoresis method. In our experiments, we find a relationship between sensing behaviour and nanowire form and diameter.
Electrical photoconductivity measurements on dense ensembles of aligned ZnO nanowires on gold contacts show that the decay time of the electrical current after switching off UV illumination depends stronlgy on the ambient gas atmosphere.
For both methods the detection limit for oxygen was found to be in the lower ppm range.

HL 44.8 Tue 12:30 POT 151

Influence of pH and ions on the transistor performance and topography of solution processed ZnO nanoparticles — •Paul Mundt[1,3], Nicole Anderl[2,3], Stefan Vogel[1], and Heinz von Seggern[1] — [1]Electronic Materials Division, Institute of Materials Science, Technische Universität Darmstadt, Alarich-Weiss-Str. 2, 64287 Darmstadt, Germany — [2]Ernst-Berl-Institut für Technische und Makromolekulare Chemie, Technische Universität Darmstadt, Alarich-Weiss-Str. 4, D-64287 Darmstadt, Germany — [3]Merck TU Darmstadt-Lab, Eduard-Zintl-Institut für Anorganische und Physikalische Chemie, Alarich-Weiss-Str. 12, 64287 Darmstadt, Germany

Recently, zinc oxide nanoparticles (ZnO-NP) have become a subject of considerable interest due to their high potential for developing solution processed, low cost, low temperature semiconducting devices. The present work utilizes sol gel processed ZnO-NPs without an additional steric stabilization. Thin ZnO-NP films were produced by spin coating using post-treatment temperatures of 250°C only being therefore suitable for applications on flexible substrates. By using different doping agents, the electronic behaviour of the devices can be influenced in a wide range from semiconducting thin film transistors yielding electron mobilities of 10-2 cm*/Vs up to conducting devices with currents in the order of mA. We investigate these changes in device behaviour for different doping agents using photoelectron spectroscopy and UV/VIS spectroscopy and correlate the results with the change in morphology using scanning electron microscopy and atomic force microscopy.

HL 45: Optical properties II

Time: Tuesday 11:15–12:30 Location: POT 006

HL 45.1 Tue 11:15 POT 006

Photon Echoes from CdTe Quantum Wells in a Magnetic-Field — •Matthias Salewski[1], Lukas Langer[1], Sergey V. Poltavtsev[1,2], Irina A. Yugova[2], Dmitri R. Yakovlev[1,3], Grzegorz Karczewski[4], Tomasz Wojtowicz[4], Ilya A. Akimov[1,3], and Manfred Bayer[1] — [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, Russian Academy of Sciences, 194021 St. Petersburg, Russia — [4]Institute of Physics, Polish Academy of Sciences, PL-02668 Warsaw, Poland

The interaction with a short laser-pulse excites negatively charged excitons (trions) from an ensemble of localized electrons in a n-type CdTe/(Cd,Mg)Te semiconductor quantum well. The resulting polarization undergoes a fast dephasing due to inhomogeneous broadening in the sample. It can be reversed by a delayed laser-pulse that creates a photon echo at exactly twice the delay-time. It is possible to split the second pulse into two single pulses to create a stimulated photon echo. With the different methods one can determine the optical T_1 and T_2 times of the system.

The application of a transverse magnetic-field allows to control the amplitude of the photon echo. Exploiting the Larmor precession of electron spins about the transverse magnetic field we demonstrate transfer of coherence between optically accessible and inaccessible pairs of states. The results are explained in terms of the optical Bloch equations accounting for the spin level structure of electrons and trions.

HL 45.2 Tue 11:30 POT 006

Optical characterization of germanium nanostructures — •Anna-Sophie Pawlik, Jan Beyer, Peter Seidel, Maximilian Geyer, and Johannes Heitmann — Technische Universität Bergakademie Freiberg, Institut für Angewandte Physik

The optical properties of Germanium nanostructures (Ge ns) embedded in a ZrO_2 Matrix were investigated. The samples have been prepared by a co-sputtering-process, at which superlattices consisting of ZrO_2 and Ge/ZrO_2 mixed layers have been deposited on a silicon substrate with and without a silicon nitride (SiN_x) layer. SiN_x was used to prevent a reaction of the ZrO_2 with the native silicon oxide. During rapid thermal processing the formation of Ge ns takes place through a decomposition of the mixed layer. Photoluminescence (PL) measurements have been carried out at temperatures variing from 13 to 300 K. For the visible spectral region, two PL peaks were observed at room temperature, centred at around 2.2 eV and 2.9 eV. These peaks do not correlate with the crystallinity and concentration of the Ge ns. It has been concluded, that these peaks are defect related. Only for samples with a SiN_x layer underneath the superlattices, PL in the infrared wavelength at around 0.83 eV could be observed at low temperatures. Temperature dependent measurements showed a redshift of the PL peak position and a decreasing intensity with increasing temperature. Further investigations indicate that this PL Signal is attributed to the band to band recombination in the Ge ns. This assumption is confirmed by Raman measurements, which show a peak for crystalline Ge at around 300 cm^{-1} for the samples which show PL in the IR region.

HL 45.3 Tue 11:45 POT 006

Investigation of the effective mass in GaAsN — •Faina Esser[1,2], Oleksiy Drachenko[1], Harald Schneider[1], Amalia Patanè[3], Mark Hopkinson[4], and Manfred Helm[1,2] — [1]Institute of Ion Beam Physics and Material Research, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]Technische Universität Dresden, 01062 Dresden, Germany — [3]The University of Nottingham, Nottingham, United Kingdom — [4]The University of Sheffield, Sheffield, United Kingdom

As a member of diluted nitrides, GaAsN is a highly interesting material system for many application purposes such as LEDs, lasers, solar cells, and infrared photodetectors because of the tuning possibility of these devices by the variation of the nitrogen content. For an accurate description of this material system, a profound knowledge of the band structure and in particular the effective mass (EM) is crucial. Because of the inconsistency of previous results, which can be traced down to the particular investigation method, we apply several methods on one sample series of GaAsN containing samples with 0.1 - 1 percent of nitrogen. Cyclotron resonance spectroscopy, beeing the most direct method, reveals that the EM is not significantly affected by the nitrogen doping. Photoluminescence, on the other hand, stems from several transitions, which are not resolved spectrally, but identified in time-resolved measurements. We discuss the different behaviour of the involved transitions in magnetic fields up to 7 T (static) and 41 T (pulsed).

HL 45.4 Tue 12:00 POT 006

Determination of Raman tensor components in α-GaN — •Christian Röder, Gert Irmer, Cameliu Himcinschi, and Jens Kortus — TU Bergakademie Freiberg, Institute of Theoretical Physics, Leipziger Str. 23, D-09599 Freiberg, Germany

In order to specify charge carrier concentration and mobility in GaN by Raman spectroscopy the value of the Faust-Henry coefficient is required but it is still debated. According to the symmetry of wurtzite-type GaN three different Faust-Henry coefficients are implied which can be related to the peak ratios of LO- and TO-phonon of the corresponding polar Raman active modes and the Raman scattering efficiency of phonon-polaritons [1]. In this work the Raman tensor components of α-GaN single crystals were determined by Raman intensity measurements using various scattering geometries. The obtained values of the Faust-Henry coefficients are compared with Raman scattering efficiency results on phonon-polaritons in wurtzite-type GaN.
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] Irmer, G. *et al.*: Phys. Rev. B **88**, 104303 (2013)

HL 45.5 Tue 12:15 POT 006

Optimizing the optical properties of elliptically-shaped micropillars — •Tim Schönfeld[1], Stephan Figge[1], Kathrin Sebald[2], Thorsten Klein[1], Elahe Zakizadeh[1], and Detlef Hommel[1] — [1]Institute of Solid State Physics, Semiconductor Epitaxy, University of Bremen, P.O. Box 330440, 28334 Bremen, Germany — [2]Institute of Solid State Physics, Semiconductor Optics, University of Bremen, P.O. Box 330440, 28334 Bremen, Germnay

The optical confinement in microcavities of different geometries opens new possibilities to control the light-matter interaction. Structures like photonic molecules, waveguides and elliptically shaped micropillars can be realized by focused ion-beam etching.

The quality of these structures, especially the smoothness of the sidewalls strongly depends on the etching parameters but also on the software structuring routine. Conventionally, bitmap files are used to define the pattern. In this case the fixed line or column scanning direction of the ion beam leads to shiftings at the sidewalls and consequently to a deteriorated quality. In order to overcome this problem we used stream files to be able to control the beam direction along the contour of pattern. In this contribution we comparatively study the properties of elliptically shaped micropillars generated by conventional bitmap and stream file routines. The sidewall quality of these structures is investigated by scanning electron microscopy as well as micro photoluminescence in order to compare the deduced quality factors of both microcavities.

HL 46: Nitrides: mostly structural characterization

Time: Tuesday 11:45–12:45 Location: POT 051

HL 46.1 Tue 11:45 POT 051

Aberration-corrected STEM investigation of epitaxial GaN thin films — •David Poppitz, Andriy Lotnyk, Jürgen W. Gerlach, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstr. 15, D-04318 Leipzig

The semiconductor material GaN is widely used in photonics applications. To improve emission efficiency it is necessary to minimize density of defects in GaN thin films. In this study epitaxial GaN thin films with different thicknesses and a high crystalline quality were produced by ion-beam assisted molecular-beam epitaxy (IBA-MBE) on 6H-SiC substrates. These thin films were characterized by advanced transmission electron microscopy at the atomic scale. A FEI Titan G2 60-300 probe aberration corrected scanning transmission electron microscope (S/TEM) was used to perform the experiments. Annular bright field (ABF) STEM imaging was applied for imaging of carbon and nitrogen elements at the GaN-SiC interface. To identify strain in the thin films nano-beam diffraction (NBD) experiments were done.

High-resolution STEM investigations showed a high density of defects in regions close to the GaN-SiC interface. The defects were identified as grain and antiphase boundaries, stacking faults as well as dislocations at the boundaries. It was also found that the thin films consist of hexagonal and cubic GaN. ABF-STEM studies of the GaN-SiC interface revealed local polarity of GaN structure at the interface as Ga-polar. Above a certain thickness, the thin films grow as hexagonal GaN and with highly reduced defect densities.

HL 46.2 Tue 12:00 POT 051

Emission properties of coupled asymmetric cubic AlGaN/GaN quantum wells — •Florian Hörich[1], Marcus Prier[1], Jürgen Bläsing[1], Tobias Wecker[2], Donat J. As[2], Martin Feneberg[1], and Rüdiger Goldhahn[1] — [1]Otto-von-Guericke University, Magdeburg, Germany — [2]University of Paderborn, Germany

Cubic AlGaN/GaN double QWs with different quantum well thicknesses and barrier compositions were grown by plasma-assisted MBE. HRXRD and ellipsometry were performed to determine the composition and barrier heights. The coupling between the QWs was studied by temperature depended photoluminescence spectroscopy. Measured transition energies were compared to theoretical values obtained by transfermatrix method taking the varying exciton binding energy for single QWs into account. Current results suggest a conduction band offset of 64% of the band-gap differences between GaN and AlGaN.

HL 46.3 Tue 12:15 POT 051

Influence of substrate material on InN island nucleation during double-pulsed PAMBE — •Andreas Kraus, Christopher Hein, Heiko Bremers, Uwe Rossow, and Andreas Hangleiter — Institut für Angewandte Physik, Technische Universität Braunschweig

Using pulsed and alternating source fluxes with In pulses less than one monolayer, we are able to grow huge and atomically flat InN islands. However, after a critical island diameter only partial coalescence takes place and In droplet formation occurs. In this contribution we present our investigations on InN island growth on different substrates. The influence of strain, sticking coefficient and surface morphology was studied by growing InN on pure c-oriented sapphire, nitridated sapphire (AlN/Al_2O_3) and MOVPE grown (0001) GaN/Al_2O_3 templates. Furthermore, the influence of dislocation densities was investigated by comparing growth on MOVPE GaN templates with dislocation densities of approximately $10^9\,cm^{-2}$ and pseudo-bulk GaN with only $10^7\,cm^{-2}$. The samples were characterized by AFM, SEM, RHEED and HRXRD. The results show the largest island aspect ratio for growth on Al_2O_3 a smaller one on AlN/Al_2O_3 and the smallest on GaN/Al_2O_3. The island density follows an opposite trend. Growth on (0001) GaN/Al_2O_3 templates leads to two different kinds of island shapes which are very smooth islands and spiral hillocks. The density of the latter one is much less on pseudo-bulk GaN substrates. Spiral hillocks and dendritic features at their rims are correlated with the hindered coalescence with adjoining islands. Therefore, using pseudo-bulk GaN is promising to achieve coalesced InN layers.

HL 46.4 Tue 12:30 POT 051

Structural and optical properties of MBE grown asymmetric cubic AlGaN/GaN double quantum well structures — •Tobias Wecker[1], Florian Hörich[2], Martin Feneberg[2], Rüdiger Goldhahn[2], Dirk Reuter[1], and Donat J. As[1] — [1]University of Paderborn, Germany — [2]Otto-von-Guericke University, Magdeburg

Asymmetric double quantum wells based on group III nitrides are in the focus of interest for the design of quantum cascade lasers and fountain lasers, which emit in the 1.55 μm infrared spectral region. Thus they are important for future devices in the telecommunication. The design of low dimensional optoelectronic devices in hexagonal group III nitrides is complicated by spontaneous polarization fields along the c-axis. By growing cubic group III nitrides in the (001) direction this harmful effect could be avoided. Asymmetric cubic $Al_xGa_{1-x}N/GaN$ double hetero-structures with different Al content were grown on 3C-SiC(001) substrates by radio-frequency plasma-assisted molecular beam epitaxy. For in-situ monitoring of the growth process reflection high energy electron diffraction (RHEED) was used. Clear RHEED oscillations were observed permitting an adjustment of the growth parameters to achieve good sample qualities. Furthermore ex-situ characterization was done by high resolution X-Ray diffraction and inter-band photoluminescence measurements taken at low temperature. The photoluminescence spectra provide four spectral separated emission bands, which clearly could be assigned to the specific layers. A partial stress in the barriers was measured, employing X-Ray diffraction reciprocal space maps (RSM) in the (113) direction.

HL 47: Spintronics (organized by MA)

Time: Tuesday 13:45–16:00 Location: HSZ 401

HL 47.1 Tue 13:45 HSZ 401

Sound Waves in a Magnon Bose Einstein Condensate — •Patryk Nowik-Boltyk[1], Oleksandr Dzyapko[1], Vladislav E. Demidov[1], Sergej O. Demokritov[1], Vasyl Tyberkevych[2], and Andrej N. Slavin[2] — [1]Institute of Applied Physics, University of Muenster, Muenster, Germany — [2]Department of Physics, Oakland University, Rochester, USA

Magnon Bose-Einstein condensation (mBEC) in Yttrium-Iron-Garnet films is a spectacular room-temperature macroscopic quantum phenomenon, which is under investigation since recently [1]. Although the basic properties of mBEC such as temporal [2] and spatial [3] coherence have extensively been studied during the last 5 years, the perturbed dynamics of the condensate have not been addressed so far. Here we report an experimental study of sound waves in a magnon gas, above and below the threshold for mBEC, performed using a space- and time-resolved Brillouin light scattering technique. The magnon gas was prepared using microwave pumping of magnons, while the sound waves were excited by, an additional, localized, oscillating, RF magnetic field. We show that at small wave vectors sound waves exhibit a linear dispersion law with a density independent group velocity, while at large wave vectors the dispersion changes from a linear dependence into a quadratic one at the threshold for mBEC. We demonstrate that this sudden change is due to an additional scattering mechanism that arises when an mBEC is formed. [1] S.O. Demokritov et al. Nature 443, 430 (2006) [2] V.E. Demidov et al. Phys. Rev. Lett. 100, 047205 (2008) [3] P. Nowik-Boltyk et al. Nature Sci. Rep. 2, 482 (2012)

HL 47.2 Tue 14:00 HSZ 401

Antiferromagnetic spintronics — •I. Fina[1,2], X. Marti[3,4,5], D. Yi[3], C. Rayan-Serrao[3], J. Liu[3], J.-H. Chu[3], S.J. Suresha[3], J. Zelezny[5], T. Jungwirth[5,6], J. Fontcuberta[3], and R. Ramesh[3] — [1]Max Planck Institute of Microstructure Physics, Weinberg 2, Halle Germany — [2]Institut de Ciencia de Materials de Barcelona, ICMAB-CSIC, 08193 Bellaterra, Spain — [3]Department of Materials Science and Engineering, University of California, Berkeley, CA 94720, USA

— [4]Dept. Condensed Matter Physics Charles University in Prague — [5]Institute of Physics ASCR, v.v.i., Cukrovarnick 10, 162 53 Praha 6, Czech Republic — [6]School of Physics and Astronomy, University of Nottingham, Nottingham NG7 2RD, United Kingdom

Magnetic semiconductors entwine two of the most successful concepts in both fundamental physics and industrial applications. Recently antiferromagnets have been proposed as new and atractive material systems. Antiferromagnetic spintronics have been demonstrated by the fabrication of tunnel devices, atomic-size proof-of concepts, even devices without auxiliary ferromagnetic layers. Here we present the control of the electrical conductivity of an antiferromagnetic semiconductor by manipulating the magnetic state of a contiguous ferromagnetic.

We present an oxide-based fully epitaxial heterostructure, its structural characterization and the electrical measurements showing a direct link between state of the ferromagnetic gate and ohmic resistance of the semiconductor, even displaying distinct remnant resistance states. We will also show that distinct remnant states can also been obtained at room temperature, promising potential applicability.

HL 47.3 Tue 14:15 HSZ 401

Calculating spin transport and magnetization dynamics parameters in textured magnetic materials — •Zhe Yuan — Faculty of Science and Technology, University of Twente, Enschede, The Netherlands — Institute of Physics, Johannes Gutenberg-University Mainz, Mainz, Germany

First-principles calculations allow us to understand the electronic and magnetic properties of real materials in terms of their chemical composition, atomic structure and magnetic configuration by numerically solving the quantum mechanical equations that describe the motion of the electrons. We have developed a unique first-principles formalism of scattering theory that can be used to calculate quantities such as the resistivity, Gilbert damping, and spin-transfer torque for a wide variety of material systems. In this talk, I will focus on how magnetic domain walls (DWs) modify the above transport and magnetization dynamics properties in real materials. Taking the technologically important Ni80Fe20 magnetic alloy, as an example, we have studied the change in its resistance due to the presence of a DW. The Gilbert damping in a DW is found to be anisotropic and drastically enhanced by the magnetization gradient, which has significant effects on field- and/or current-driven DW motion.

HL 47.4 Tue 14:30 HSZ 401

Spin Solar Cell for Spin Injection into Semiconductors. — Bernhard Endres, Mariusz Ciorga, Maximilian Schmid, Martin Utz, Dominique Bougeard, Dieter Weiss, Christian Back, and •Günther Bayreuther — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D-93040 Regensburg

Optical spin pumping allows to create spin-polarized carriers in III-V semiconductors, but requires circularly polarized light of a well-defined wavelength. Here we describe a spin-generating solar cell without such limitations [1,2]. The device consists of a p-n junction with highly n-doped GaAs at the n-side and ferromagnetic (Ga,Mn)As at the p-side. Illuminating this junction creates a photo-voltage causing electrons to tunnel across the narrow barrier from the n-GaAs into the (Ga,Mn)As. Due to the spin-dependent tunneling probability a spin accumulation occurs in the n-GaAs. This spin solar cell effect is demonstrated with a laser beam generating electron-hole pairs and detecting the spin accumulation via the polar magneto-optic Kerr effect and by measuring non-local voltages. On applying a large negative bias the sign of the photo-induced spin polarization is reversed as expected due to the suppression of the tunneling current through a wider barrier. This mode of operation corresponds to a spin photodiode. The spin solar cell effect should equally work for metallic ferromagnets with a high Curie temperature and allow to convert unpolarized light into a spin current also in semiconductors without a direct band gap like Si and Ge.

[1] B. Endres et al., Nature Commun. 4, 2068 (2013).
[2] R. Jansen, Nature Mater. 12, 779 (2013)

HL 47.5 Tue 14:45 HSZ 401

Magnetic anisotropy in CoFe/MgO/CoFe magnetic tunnel junctions with ultrathin electrode layers and its composition dependence — •Jia Zhang, Christian Franz, Michael Czerner, and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University, Giessen, Germany

MgO based magnetic tunnel junctions (MTJs) with ultrathin CoFeB magnetic electrodes can have perpendicular magnetic anisotropy and a low switching current. In addition, MgO-MTJs with perpendicular anisotropy may also be easier to switch by thermal spin transfer torque and may pave its potential application in Spincaloritronics. In this talk, the magnetic anisotropy in CoFe/MgO/CoFe-MTJs on different substrates for instance Cu, Au, MgO etc. and different CoFe alloy composition are discussed using full relativistic Korringa-Kohn-Rostoker and coherent potential approximation (CPA) first-principles calculations. The magnetic anisotropy energy (MAE) in CoFe/MgO/CoFe-MTJs was calculated by employing magnetic force theory. The calculated MAE in Co_xFe_{1-x}/MgO/Co_xFe_{1-x}-MTJs decreased with the increasing of Co composition. The $d_{zx}(d_{yz})$ and $d_{xy}(d_{x^2-y^2})$ orbital and its evolution in the spin down channel was found to be responsible for the rise of magnetic anisotropy and the composition dependence. The shape anisotropy energy was also calculated and thus the phase diagram with perpendicular anisotropy versus composition and thickness was determined. Finally, we will give a brief discussion on magneto resistance and spin-transfer torque in CoFe/MgO/CoFe-MTJs with perpendicular easy axis.

HL 47.6 Tue 15:00 HSZ 401

Magnetic and electronic properties of $Ni_2S_2O_2N_6C_{57}H_{78}P^+$ on Au(111) — •Kai Trepte, Claudia Martin, and Jens Kortus — Institute of Theoretical Physics, TU Bergakademie Freiberg, Germany

The electronic and magnetic properties of a Ni^{2+} dimer including a PPh_3- ligand in contact with a Au(111) surface have been measured [1]. We will present theoretical calculations using DFT (with and without van der Waals interactions) including only the PPh_3- ligand binding on the Au(111) surface in order to determine the magnetic exchange and anisotropy. We will discuss charge transfer and the bonding situation for the favored binding position in more detail. Finally we will compare these results with a calculation of the dimer on the surface including geometry changes and charge transfer.

[1] M. Golecki et al. Chemisorption of exchange-coupled $[Ni_2L(dppba)]^+$ complexes on gold by using ambidentate 4-(diphenylphosphino)benzoate co-ligands. *Chemistry - A European Journal*, 19(24):7787-7801, 2013.

HL 47.7 Tue 15:15 HSZ 401

Manipulating the coupling between metal and molecule in hybrid structures by changing of organic anchor groups — •Simon Liebing, Torsten Hahn, and Jens Kortus — Institut of Theoretical Physics, TU Bergakademie Freiberg, 09599 Freiberg

There are theoretical and experimental works which propose to the use of amino anchor groups [1] instead of the more often used thiol [2] ones. So far there is no systematic study comparing the properties of different anchor groups. The present study investigates the properties of amino, cyano, furan, hydroxyl, pyrol thiol and thiophen in a break junction like geometry. The anchor groups are attached to a novel molecular system based on an anthraquinone-core with conjugated spacers to form a model system. These anchor groups include also some that could form π-like bonds and allow fully and cross-conjugated electron systems.

The molecular structures are constructed with Avogadro [3] and optimized by all-electron DFT-code NRLMOL [4]. The device structures are than optimized with the GPAW program package [5] an plane wave augmented wave again. The same software is used for the calculation of the transport properties by means of the NEGF-formalism.

References

1 Angela. D. et. al. Nano Letters 10, no. 7 (2010), 2 Markussen, T. et al. JCP 132 , 224104 (2010), 3 Hanwell, M. D. et al. Journal of Cheminformatics 4, 17 (2012), 4 Pederson, M. et. al. Phys. Status Solidi b 217, 197. (2000), 5 Enkovaara, J. et al. Journal of Physics: Condensed Matter 22, 253202 (2010)

HL 47.8 Tue 15:30 HSZ 401

Barrier dependent tunneling magnetoresistance in carbon nanotubes — •Carola Meyer[1,2], Cate Morgan[1,2], Dominik Metten[3], Sebastian Heedt[1,2], Thomas Schäpers[1,2], and Claus M. Schneider[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA - Fundamentals of Future Information Technologies — [3]Institut de Physique et Chimie des Matériaux de Strasbourg and NIE, UMR 7504, Université de Strasbourg and CNRS, France

Carbon nanotubes (CNTs) are a material of interest in spintronics, because in addition to exhibiting ballistic transport, the low atomic number and low abundance of ^{13}C nuclei in CNTs is expected to lead

to low spin orbit coupling and hyperfine interaction indicating a long spin relaxation time. However, the size of the magnetoresistance (MR) observed depends strongly on the current regime and on the type of CNT device measured. In the single-electron-tunneling regime, typically only a few percent MR can be reached. MR in multiwalled CNTs with a large diameter has shown to be as large as 60% for contacts with high polarization [1].

We present a way to compare the MR of different devices from single-wall and multiwalled CNTs with respect to the current regime. Temperature dependent data confirm tunneling MR as the main effect. The size of the MR measured depends on the strength of the tunnel barrier and follows the Slonczewski model. Finally, the presence of the Hanle effect proves successful spin injection.

[1] L. E. Hueso et al., Nature 445, 410 (07)

HL 47.9 Tue 15:45 HSZ 401

Transport properties of multiferroic tunnel junctions in an embedded Green-function approach — •Andera Neroni, Daniel Wortmann, Ersoy Sasioglu, Stefan Blügel, and Marjana Ležaić — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Multiferroics tunnel junctions are promising structures for spintronic devices due to their transport properties. From the theoretical point of view the study of transport in Metal/Ferroelectric/Metal needs to deal with several degrees of freedom. Structural distortions at the interface, polarization and magnetization directions, presence of oxides at the interface and strong correlations must be taken into account. We focus on the tunneling properties of a Fe/BTO/Fe barrier obtained in an embedded Green-function approach [1] implemented with the framework of the full-potential linearized augmented plane-wave (FLAPW) method `FLEUR` [2]. Electronic charge self-consistency is achieved in the same approach. Strong correlations are taken into account employing the LDA+U approach within the framework of the density functional theory (DFT) with a Hubbard U parameter determined by constrained random phase approximation (cRPA) [3].

Work is supported by Helmholtz Young Investigators Group Program VH-NG-409.

[1] www.flapw.de
[2] D. Wortmann, H. Ishida, and S. Blügel, PRB **65**, 165103 (2002)
[3] E. Şaşıoğlu, C. Friedrich, and S. Blügel, PRB **83**, 121101(R) (2011)

HL 48: Transport

Time: Tuesday 14:00–16:00 Location: POT 006

HL 48.1 Tue 14:00 POT 006

Fermi liquid theory of the strongly interacting quantum RC circuit — •Michele Filippone — Dahlem Center for Complex Quantum Systems - Freie Universitat Berlin

The quantum coherence effects between electrons in nanodevices lead to a rich variety of phenomena in quantum transport. One of these is the violation of Kirchhoff's laws in the quantum RC-circuit. In this system, a metallic lead exchanges electrons coherently with a quantum dot driven dynamically by a top metallic gate. In the non interacting case, the charge relaxation resistance of the system differs from the usual dc-transport resistance given by the Landauer formula. The charge relaxation resistance is universally fixed to $h/(2e^2)$ for a single mode conductor, regardless of the transmission of the mode. We show that the Fermi liquid behavior of these systems at low energy explains this universality even in the presence of strong interactions in the dot. Moreover, we discuss the emergence of a giant dissipation regime associated to the breaking of the Kondo singlet for Zeeman energies of the order of the Kondo temperature. We provide a comprehensive analytical description of the peak of the charge relaxation resistance associated to this giant dissipation and demonstrate its persistence out of the Kondo regime.

HL 48.2 Tue 14:15 POT 006

Weak Localization and Antilocalization in Two-Dimensional Hole Gases — •Paul Wenk[1], Tobias Dollinger[1], Andreas Scholz[1], Roland Winkler[2], John Schliemann[1], and Klaus Richter[1] — [1]Institut I - Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany — [2]Department of Physics, Northern Illinois University, IL 60115 DeKalb, USA

We investigate the appearance of persistent spin states in two-dimensional hole gases including both Rashba and Dresselhaus spin-orbit coupling. To this end, we extend previous models for III-V semiconductors by going beyond the axial approximation. Using an effective 2×2 heavy-hole model, we find persistent and long persisting spin states by analyzing the crossover from weak localization to weak antilocalization. The findings are derived using both Landauer-Büttiker framework and diagrammatic perturbation theory by exact diagonalization of the Cooperon.

[1] T. Dollinger *et al.*, `arXiv:1304.7747` (2013)
[2] J. Schliemann *et al.*, Phys. Rev. Lett. **90** 146801 (2003)
[3] S. Kettemann, Phys. Rev. Lett. **98** 176808 (2007)
[4] P. Wenk, S. Kettemann, Phys. Rev. B **81** 125309 (2010)

HL 48.3 Tue 14:30 POT 006

Magneto-Oscillations in GaAs/InAs Core/Shell Nanowires — •Fabian Haas[1,2], Tobias Wenz[1,2], Patrick Zellekens[1,2], Natalia 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 Institute - 9, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA - Fundamentals of Future Information Technology

In GaAs/InAs core/shell nanowires the electrons are confined in the hollow cylindrical conductive InAs shell. The ring geometry of this InAs nanotube allows flux periodic modulation of the electron concentration in magneto-transport measurements, if a magnetic field is aligned alongside the nanowire axis. Magneto-oscillations with h/e periodicity are expected due to one-dimensional transport through angular momentum states, which are solutions to the Schrödinger equation for a radially confined system.

In this contribution, we present magneto-transport measurements of several GaAs/InAs core/shell nanowires of different dimensions. Pronounced oscillations with h/e periodicity are found in the magneto-conductance of all the wires. By variation of external parameters such as temperature, gate voltage and tilt angle with the magnetic field the underlying energetic spectrum is analyzed.

HL 48.4 Tue 14:45 POT 006

Electronic transport through nano sized GaAs pillars — Thorben Bartsch, Christian Heyn, and •Wolfgang Hansen — Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Jungiusstraße 11, 20355 Hamburg, Germany

We perform magneto-transport experiments on GaAs nanopillars embedded in an AlGaAs matrix. The nanopillars are about 10 nm long, 100 nm in diameter and are epitaxially grown with perfect lattice match to n-doped, three-dimensional GaAs contact areas. Current-voltage characteristics and the magneto-conductance are investigated and compared to two reference samples containing undoped pillars and no pillars, respectively. A pronounced conductance peak observed in a magnetic field oriented along the pillar axis is discussed in terms of Chambers breakdown. In the voltage dependence of the differential conductance distinctive resonances are found that are not present in undoped pillars and the sample without pillars. These peaks slightly change with magnetic field. So far, the origin of the resonances is not clear. A possible mechanism leading to such oscillations will be discussed.

HL 48.5 Tue 15:00 POT 006

Microscopics of Disordered Quantum Hall Systems with Rashba Spin-Orbit Interaction: Spectral Properties and Transport in the Hydrodynamic Regime — •Daniel Hernangomez-Perez[1], Jascha Ulrich[2,3], Serge Florens[3], and Thierry Champel[1] — [1]Laboratoire de Physique et Modélisation des Milieux Condensés, CNRS and Université Joseph Fourier, Grenoble, France — [2]Institute of Physics and JARA-FIT, RWTH Aachen University, Aachen, Germany — [3]Institut Néel, CNRS and Université Joseph Fourier, Grenoble, France

We develop a semicoherent state Green's function formalism to study disordered two-dimensional electron gases (2DEG) in the quantum Hall regime with random Rashba interaction and Zeeman coupling. As a

first step, we calculate the energy spectrum in weakly curved smooth disorder potentials with fluctuating Rashba fields and compute a microscopic non-perturbative expression for the local density of states (LDoS). The expression, valid in different temperature regimes, is used to interpret recent experimental data through the study of the spatial dispersion and linewidth of the LDoS peaks. Next, we discuss transport properties of these systems in the hydrodynamic regime. We compute analytical expressions for the edge and bulk current densities and show that, in the semiclassical limit, the Hall conductance presents robust (quantized) Hall plateaux even in the presence of Rashba interaction. Finally, we discuss the dissipationless transport of angular momentum in the 2DEG and show that the semiclassical spin Hall conductance is free of resonances, contrary to previous predictions in the literature.

HL 48.6 Tue 15:15 POT 006

In-plane Magnetic Field Effects in Antidot Lattices in High Mobility Heterostructures — •Jakob Schluck[1], Mihai Cerchez[1], Thomas Heinzel[1], Dimitris Kazazis[2], Klaus Pierz[3], and Hans Werner Schumacher[3] — [1]Solid State Physics Laboratory, Heinrich-Heine University Düsseldorf, Universitätsstr. 1, D-40225 Düsseldorf — [2]Route de Nozay CNRS-LPN F-91960 Marcoussis — [3]PTB Braunschweig, Bundesallee 100 D-38116 Braunschweig

Antidot lattices in two-dimensional electron gases are known to cause peaks in the magnetoresistance whenever the cyclotron radius of the electrons is commensurate with the superlattice. Furthermore, phase coherent oscillations can be observed at low temperatures in hexagonal lattices.

We report the effects of a strong in-plane magnetic field on those two phenomena in large-period hexagonal antidot lattices (superlattice constant between 750 nm and 1.5 μm), defined in high-mobility Ga[Al]As based two-dimensional electron gases at temperatures below 1 K. We observe modifications of the magnetoresistivity which can be traced back to magnetic mass effects.

HL 48.7 Tue 15:30 POT 006

Magnetoresistance studies in GaAs/AlGaAs quantum wells with additional impurity — •Eddy P. Rugeramigabo[1,2], Lina Bockhorn[1], and Rolf J. Haug[1] — [1]Institute for Solid State Physics, Dep. Nanostructures, Leibniz Universität Hannover — [2]QUEST Centre for Quantum Engineering and Space-Time Research, Leibniz Universität Hannover

GaAs/AlGaAs heterostructures, with the two-dimensional electron gas being located in GaAs single quantum wells, were grown using the molecular beam epitaxy technique. Beside the modulation-doping, additional homogeneous Si-doping of the quantum well was performed, the Si-atoms in the quantum well acting as impurity scattering sites. The samples differ by the density of the incorporated Si-atoms. The quantum well of the reference sample was left undoped, reflecting the unintentional background impurity. Transport measurements were performed on the samples for a wide range of temperatures. For the reference sample we found a high mobility $\mu = 2 \times 10^6$ cm^2/Vs. For increasing additional impurity density we found a drastic decrease of the mobility down to 1×10^4 cm^2/Vs. All samples exhibit parabolic magnetic field dependence at low magnetic fields and low temperatures, attributed to electron-electron interaction. A narrow peak around zero magnetic field in the samples with additional impurity is attributed to weak localization. The differences in the magnetoresistance curves are analyzed in detail in order to study the direct influence of the impurity density on the magnetotransport in 2DEG systems

HL 48.8 Tue 15:45 POT 006

Study of the doping of crystalline silicon nanoparticle films with TCNQ molecules — •Willi Aigner[1], Stanislav Abramov[1], Hartmut Wiggers[2], Rui N. Pereira[1,3], and Martin Stutzmann[1] — [1]Walter Schottky Institut, Technische Universität München, Germany — [2]Institute for Combustion and Gasdynamics - Reactive Fluids, Universität Duisburg-Essen, Germany — [3]Institute for Nanostructures, Nanomodelling and Nanofabrication, Department of Physics, University of Aveiro, Portugal

Electronic devices incorporating solution-processable, semiconducting nanocrystals have been the subject of many studies in the last years. Recently, a significant enhancement of the electron conduction in silicon nanocrystal (Si-NC) thin films has been found by simply doping the films with a small amount of tetrafluorotetracyanoquinodimethane (F4-TCNQ) [1]. The F4-TCNQ molecules provide empty electronic states within the free space between the Si-NCs, which are close to the lowest unoccupied states of the NCs and, in this way a more efficient charge transport in the Si-NC network is achieved. In this work, we carried out a comprehensive study of doping Si-NC thin films with tetracyanoquinodimethane and compare the results with those obtained with F4-TCNQ. For a deeper understanding of the physics governing the molecule-induced electrical activation, films made of p- and n-type Si-NCs were also studied. According to theory [1], the electronic states introduced by the small molecules are solely accessible to electrons, implying that they are not expected to lead to an enhancement of hole conduction. [1] R. N. Pereira, J. Coutinho, et al. submitted, (2013)

HL 49: Energy materials: Thermoelectrics

Time: Tuesday 14:00–16:00 Location: POT 051

HL 49.1 Tue 14:00 POT 051

Silicene: A Promising Thermoelectric Material — •Xiaoliang Zhang[1] and Ming Hu[1,2] — [1]Institute of Mineral Engineering, Division of Materials Science and Engineering, Faculty of Georesources and Materials Engineering, RWTH Aachen University, 52064 Aachen, Germany — [2]Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University, 52062 Aachen, Germany

Thermoelectric materials can directly convert waste heat to electricity for improving the efficiency of energy utilization. Silicene, the silicon-based counterpart of graphene, has shown its great potential for thermoelectric applications. First of all, from electronic structure point of view ab initio calculations suggest that silicene is equivalent to graphene, i.e., the electrical conductivity of silicene is as high as that of graphene. Second, in contrast to graphene, silicene has a buckled atomic structure, leading to non-zero energy gap and enhanced Seebeck coefficient. Third, by conducting molecular dynamics simulations, we confirm that the thermal conductivity of silicene is extremely low, suggesting silicene as a potential candidate of high efficiency thermoelectric materials. Moreover, our molecular dynamics simulation results suggest that the thermal conductivity of silicene can be further reduced by hydrogenation and oxidation implying enhanced thermoelectric performance. Compared with pristine silicene, the hydrogenated and oxidized silicene structures are more stable and thus can be used for energy conversion at high temperatures.

HL 49.2 Tue 14:15 POT 051

Resonant tunneling energy harvesters — Andrew N. Jordan[1], Björn Sothmann[2], •Rafael Sánchez[3], and Markus Büttiker[2] — [1]Department of Physics and Astronomy, University of Rochester, Rochester, U. S. A — [2]Département de Physique Théorique, Université de Genève, Genève, Switzerland — [3]Instituto de Ciencia de Materiales de Madrid, CSIC, 28049, Madrid, Spain

An important task in condensed matter physics is to find new ways to harvest ambient thermal energy, particularly at the smallest length scales where electronics operate. To achieve this goal, there is on one hand the miniaturizing of electrical devices, and on the other, the maximization of either efficiency or power the devices produce. We present the theory of nano heat engines able to efficiently convert heat into electrical power. We propose a resonant tunneling quantum dot engine that can be operated either in the Carnot efficient mode, or maximal power mode. The ability to scale the power by putting many such engines in a "Swiss cheese sandwich" geometry gives a paradigmatic system for harvesting thermal energy at the nanoscale[1].

Alternative configurations based on resonant tunneling through quantum wells provide a comparable thermoelectric performance with the advantage of being easier to construct[2].

[1] A. N. Jordan, B. Sothmann, R. Sánchez, M. Büttiker, Phys. Rev. B 87 (2013) 075312.

[2] B. Sothmann, R. Sánchez, A. N. Jordan, M. Büttiker, New J. Phys. 15 (2013) 095021.

HL 49.3 Tue 14:30 POT 051

Hybrid Si/AlO$_x$ thin films of the electron crystal-phonon glass type — •Markus Trutschel[1,2], Jens Glenneberg[2], Stefan Ebbinghaus[2], Peter Werner[1], and Hartmut S. Leipner[2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle (Saale) — [2]Martin-Luther-Universität, Halle (Saale)

Heat in modern integrated circuits is produced concentrated in small areas. Active cooling may enhance the performance of such devices. Materials for thermoelectric cooling require a high electrical conductivity and Seebeck coefficient together with a low thermal conductivity. Thus, suitable materials are those of the electron crystal-phonon glass type. Composites may provide nontoxic, cheap and available materials with a good thermoelectric performance to be integrated in silicon technology.

We studied structural, electrical and thermoelectric properties of silicon particles formed in an aluminum oxide matrix. The samples were synthesized by means of a physicochemical process. Thin films of aluminum were deposited on silicon oxide layers followed by a thermal annealing step in argon atmosphere. The silicon oxide was reduced to silicon during the heat treatment, whereas the aluminum was oxidized. For annealing temperatures between 540°C and 600°C, the size, shape and distribution of the silicon particles formed was found to be interesting for technical applications. We present the structural characterization of hybrid Si/AlO$_x$ films along with the results of the electrical and thermoelectric properties.

HL 49.4 Tue 14:45 POT 051

Phononic thermal transport in nanostructured silicon membranes — •Sanghamitra Neogi, Luiz F. C. Pereira, and Davide Donadio — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

The interest in energy harvesting using thermoelectric devices and thermal management in nanostructures has heightened the necessity of understanding the phononic thermal transport in nanoscale materials. Nanostructuring can result in the reduction of the thermal conductivity of crystalline semiconductors while preserving their electronic properties, leading to an improved TE efficiency in these systems [1].

We use harmonic lattice dynamics and classical molecular dynamics to investigate the nature of phononic thermal transport in ultra-thin silicon membranes, with thicknesses up to 20 nm. We show that dimensionality reduction has a significant effect on the phonons of the membranes and leads to a 4-fold reduction in the thermal conductivity of the membranes. Nanostructuring Si membranes by means of pattern formation and surface oxidation, in combination with dimensionality reduction, results in a 25-fold reduction in the thermal conductivity of the membranes with respect to the bulk, implying a 25-fold enhancement of the thermoelectric figure of merit at room temperature. Such figures make nanostructured silicon membranes viable materials for thermoelectric units.

[1] M. S. Dresselhaus et al, Adv. Mater., 22, 3970 (2010).

Acknowledgment: This project is funded by the program FP7-ENERGY-2012-1-2STAGE under contract number 309150.

HL 49.5 Tue 15:00 POT 051

Thermoelectric transverse voltage by Joule heating — a Boltzmann equation approach beyond quasi-equilibrium — •Stephan Rojek, Alfred Hucht, and Jürgen König — Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany

We consider structures within a two-dimensional electron gas where a thermoelectric transverse voltage is measured perpendicular to an input current. The latter gives rise to Joule heating. An external potential induced by surface gates breaks the transverse symmetry. To realize tunable rectification devices [1] or to get insight into thermoelectric transport properties of the electron gas [2] are two of various applications. Heat diffusion and finite size effects lead to a non-trivial temperature profile, which have to be taken into account if the device's dimensions are of the order of the energy diffusion length.

We employ a Boltzmann equation approach beyond the quasi-equilibrium description with an effective chemical potential and temperature. An expansion in moments of the distribution function allows for a systematic calculation of all non-equilibrium contributions.

[1] A. Ganczarczyk, S. Rojek, A. Quindeau, M. Geller, A. Hucht, C. Notthoff, J. König, A. Lorke, D. Reuter, and A. D. Wieck, Phys. Rev. B **86**, 085309 (2012).

[2] W. E. Chickering, J. P. Eisenstein, and J. L. Reno, Phys. Rev. Lett. **103**, 046807 (2009).

HL 49.6 Tue 15:15 POT 051

Thermoelectric Coefficients from First Principles — •Karsten Rasim, Christian Carbogno, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

In spite of significant efforts, an accurate assessment of the electronic transport coefficients, i.e., the electrical conductivity σ, the Seebeck coefficient S and the electronic heat conductivity κ_{el}, still constitutes an open challenge for first-principles theory. Even the most involved approaches [1] treat the nuclear dynamics in the harmonic approximation and thus become inaccurate at elevated temperatures. To overcome this limitation, we use the *Kubo-Greenwood formalism* [2] to assess σ, S, and κ_{el} from the thermodynamic equilibrium fluctuations of the electronic structure and of its dipole transition matrix elements. Anharmonic effects in the nuclear motion are fully incorporated by the means of *ab initio* molecular dynamics. We discuss the details of our implementation and validate our approach by investigating various direct and indirect band gap semiconductors. Furthermore, we compute the temperature dependent electronic transport coefficients of borcarbides, a material class regarded as promising for thermoelectric applications. We demonstrate that in this case anharmonic effects are crucial to achieve a correct description of the transport coefficients.

[1] P. Boulet and M. J. Verstraete, Comp. Mat.Sci. **50**, 3 (2001)

[2] B. Holst, M. French, and R. Redmer, Phys. Rev. B **83**, 235120 (2011).

HL 49.7 Tue 15:30 POT 051

First-principles Study of Vacancies in Thermoelectric Clathrates — •Amrita Bhattacharya, Christian Carbogno, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

For the development of improved thermoelectrics, one promising material class may be clathrates, i.e., semiconducting host lattices that can encapsulate guest atoms. Even in the simplest clathrates, such as Si_{46} and Ge_{46}, the introduction of guests can result in surprising electronic and structural changes: In the case of Si, the addition of K results in a K_8Si_{46} clathrate that exhibits metallic behavior due to the electrons donated by the guests [1]. Conversely, Ge-based clathrates remain semiconducting, since two spontaneously generated vacancies balance the donated electrons in K_8Ge_{44}. But even more intriguingly, filling the Ge-clathrate with Ba does not generate *four*, but *three* vacancies, whereby the resulting Ba_8Ge_{43} exhibits a metal-semiconductor transition at $\sim$ 280 K [2]. In this work, we use density-functional theory to investigate these effects and to unravel their puzzling mechanism. We compute the formation energies for vacancies and vacancy complexes in Si- and Ge-hosts as function of the filling with K and Ba, whereby we take into account structural disorder as well as geometric and lattice relaxations. Furthermore, we study the dynamics in these compounds (also analyzing *non-harmonic effects*) to clarify the role the vacancies play for the thermodynamic properties.

[1] G. K. Ramachandran, *et al.*, *J. Sol. St. Chem.* **154**, 626 (2000)

[2] U. Aydemir *et al.*, *Dalton Trans.* **39**, 1078 (2010).

HL 49.8 Tue 15:45 POT 051

Thermoelectric power factor of ternary single-crystalline Sb_2Te_3- and Bi_2Te_3-based nanowires — •Svenja Bässler[1], Tim Böhnert[1], Johannes Gooth[1], Christian Schumacher[1], Eckhard Pippel[2], and Kornelius Nielsch[1] — [1]Institute of Applied Physics, Universität Hamburg, Jungiusstrasse 11, 20355 Hamburg, Germany — [2]Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany

Nanowires of bismuth antimony telluride and bismuth telluride selenide ($Bi_{15}Sb_{29}Te_{56}$ and $Bi_{38}Te_{55}Se_7$) are grown by template-based pulsed electrodeposition. The composition and the crystallinity of the nanowires are determined by high resolution transmission electron microscopy. The thermoelectric properties (Seebeck coefficient and electrical conductivity) of single p- and n-type nanowires with a diameter of 80 nm and 200 nm, respectively, are determined as a function of temperature before and during heating in helium atmosphere up to 300 K along the growth direction of the nanowires. After additional annealing in Te atmosphere at 525 K, significantly enhanced transport properties are observed. Bulk-like power-factors are achieved. In $Bi_{38}Te_{55}Se_7$ nanowires the Seebeck coefficients increase up to -115 μV K^{-1} and the thermoelectric power factors up to 2820 μW K^{-2} m^{-1} at room temperature. In $Bi_{15}Sb_{29}Te_{56}$ nanowires Seebeck coefficients

of up to +156 μV K^{-1} and power factors of up to 1750 μW K^{-2} m^{-1} are obtained at room temperature.

Reference:
S. Bäßler *et al.* Nanotechnology 24 (2013) 495402

HL 50: Organic semiconductors: Transistors and OLEDs (with CPP/DS)

Time: Tuesday 14:00–15:45 Location: POT 081

HL 50.1 Tue 14:00 POT 081

Solution-gated organic field effect transistors: small-molecule versus polymeric materials — •Hannah Schamoni[1], Rossella Porrazzo[1,2], Jose A. Garrido[1], and Maria Rosa Antognazza[2] — [1]Walter Schottky Institut, Technische Universität München, Deutschland — [2]Center for Nanoscience Technology (CNST) of IIT@Polimi, via Pascoli 70/3, 20133 Milano, Italy

Solution-gated organic field effect transistors (SGOFETs) are promising devices for biosensing applications featuring, amongst others, low production costs. For the organic semiconductor, two different kinds of materials are typically used, namely polymers like poly(2,5-bis(3-hexadecylthiophen-2-yl)thieno[3,2-b]thiophene) (pBTTT) and small molecules like α-sexithiophene (6T). In this work, we have investigated devices of both types regarding their performance, stability, and pH and ion sensitivity. A comparison of the two approaches is presented, taking also into account the differences in processing: While polymers can be spin-coated onto the substrate, small molecules are grown using organic molecular beam deposition. Finally, we will discuss the potential of SGOFETs as light sensors to stimulate nerve cells, which can pave the way towards the development of a new generation of retinal implants.

HL 50.2 Tue 14:15 POT 081

Light-induced switching mechanism of porphyrin-coated Si nanowire field effect transistors — •Eunhye Baek[1], Sebastian Pregl[1,2], Mehrdad Shaygan[3], Lotta Röhmhildt[1], Dmitry Ryndyk[1,2], Larysa Baraban[1], and Gianaurelio Cuniberti[1,2] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany — [2]Center for Advancing Electronics Dresden, TU Dresden, Germany — [3]Division of IT Convergence Engineering, Pohang University of Science and Technology, Pohang, Korea

We present light-induced switching mechanism of porphyrin-coated Si nanowire field effect transistors (Si NW FETs). Si NW FETs were fabricated by bottom-up methods and show ambipolar characteristics due to thermally annealed Schottky barrier on the contact between the electrode and NW channel. Si NW FETs are functionalized by porphyrin, a key dye molecule in photosynthetic process, to have photo-sensitive operation. Porphyrin-coated devices show clear current switching under light illumination that is not shown in bare devices. Switching time and switching current ratio depend on the concentration of porphyrin. Under light irradiation, electrical properties of molecular layer are changed; increased mobile charges by photo-excitation screen electrical field from the applied bias. In addition, molecules are polarized by charge separation that build vertical field towards the NWs. The electrical charge of porphyrin layer modifies the total applied field in NW, which induces current switching according to the concentration of porphyrin.

HL 50.3 Tue 14:30 POT 081

Lithographically processed vertical organic thin-film transistors (VOTFTs) — •Alrun Aline Günther[1], Hans Kleemann[2], Björn Lüssem[3], Daniel Kasemann[1], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, TU Dresden, George-Bähr-Str. 1, 01069 Dresden Germany — [2]Novaled AG, Tatzberg 49, 01307Dresden, Germany — [3]Department of Physics, Kent State University, Kent, OH 44242, USA

Vertical organic transistors are a novel type of organic semiconductor devices, the first of such devices having been presented by Ma et al. in 2004[1]. The idea of this novel device concept is to overcome the limitations often faced in conventional organic thin-film transistors (OTFTs), where performance parameters (e.g. cut-off frequency or transconductance) are limited by the channel length of the OTFT. The VOTFT concept developed at IAPP[2] allows for downscaling of this channel length to the order of nanometres, while using a novel photolithography approach[3] to achieve patterning of the source electrode. In the present work, the effects of semiconductor film morphology and addition of dopant molecules are investigated for pentacene VOTFTs. It is expected that knowledge of such effects will give a more detailed insight into the fundamental functional principles of the device, as these are not yet well understood.

References [1] L. Ma et al, Appl. Phys. Lett. 85, 21 (2004) [2] H. Kleemann et al, Small, Epub ahead of print (2013) [3] H. Kleemann et al, Org. Elec. 13, 3 (2012)

HL 50.4 Tue 14:45 POT 081

Controlling morphology of a Vertical Organic Transistor for enhanced current gain and very low operation voltages — •Felix Kaschura, Axel Fischer, Björn Lüssem, Daniel Kasemann, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden

Vertical Organic Triodes represent a novel transistor technology enabling high current densities without the need for expensive structuring techniques. These devices require a permeable base for highly efficient operation. Therefore, we place a morphology modifying gold layer underneath the organic semiconductor, which enhances charge carrier transmission and thus the current gain. We have further studied a geometry optimization of the device structure allowing to tune the built-in field of the device. This results in an increased transmission as the built-in field at the collector actively gathers charge carriers, as well as a very low minimum operation voltage - both desirable characteristics for practical applications.

HL 50.5 Tue 15:00 POT 081

Contact Resistance Adjustment in Top-Contact Organic Field Effect Transistors by Localized Doping — •Ji-Ling Hou, Björn Lüssem, Daniel Kasemann, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Str. 1, 01069 Dresden, Germany

The contact resistance between metal and organic interface is a key challenge for Organic Field-Effect Transistors (OFETs) when short channel lengths are used to achieve low-cost and high-frequency. In this study, bottom-gate top-contact organic field effect transistors (OFETs) with different thickness of the p-dopant 2,2-(perfluoronaphthalene-2,6-diylidene) (F6-TCNNQ) under Au electrodes were fabricated by orthogonal photolithography to further investigate their impact on contact resistance. Extracted by the transmission line method (TLM), contact resistance was found to be significantly reduced from 50 kOhm*cm to 10 kOhm*cm by adding a 1nm thin dopant layer. Doping leads to an improved injection at low gate voltages, while the contact resistance is also reduced in the undoped reference device due to the applied field at higher gate voltages. Finally, we conducted temperature dependent I-V measurement to study the change of contact resistance at lower temperature. The result shows an abrupt transition in the linear region between 220K and 240K, which gives a direct evidence and link between contact resistance and doping effect.

HL 50.6 Tue 15:15 POT 081

IR spectroscopic investigation of charge transfer in organic semiconductors I: Doped layers — •Tobias Glaser[1,2], Sebastian Beck[1,2], David Gerbert[1,2], Johannes Zimmermann[1,2], and Annemarie Pucci[1,2,3] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg — [2]InnovationLab GmbH, Heidelberg — [3]Centre for Advanced Materials, Universität Heidelberg

Electrochemical doping of amorphous organic semiconductors is a frequently used technique in order to increase the amount of free charge carriers and thereby the conductivity of the doped layers. But for organic semiconductors, in general very low doping efficiencies in the range of only a few percent have been reported.

We performed infrared (IR) spectroscopy under ultrahigh vacuum conditions in order to investigate the process of charge transfer in various p-doped material systems. The charge transfer in doped layers can be determined with IR spectroscopy, as the new electronic structure of the charged molecules leads to a change in bond length and bond strength within the charged molecules that therefore exhibit a different vibrational spectrum compared to the neutral molecules. The

appearance of broad electronic excitations in these systems shows the formation of new electronic states due to hybridization. We investigated the behavior of these electronic states after annealing as well as after degradation of the doped layers.

Financial support from the BMBF via the MESOMERIE Project (FKZ 13N10724) is gratefully acknowledged.

HL 50.7 Tue 15:30 POT 081

IR spectroscopic investigation of charge transfer in organic semiconductors II: Interfaces — •Sebastian Beck[1,2], David Gerbert[1,2], Tobias Glaser[1,2], and Annemarie Pucci[1,2,3] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg — [2]InnovationLab GmbH, Heidelberg — [3]Centre for Advanced Materials, Universität Heidelberg

In organic semiconductors charge transfer (CT) is crucial for all kinds of applications but its basic mechanisms are still under severe discussion. Especially a better knowledge of CT at organic/organic and inorganic/organic interfaces is essential for the design of new electronic devices with improved performance.

In this study we want to introduce a new approach to investigate CT at interfaces by means of in situ infrared (IR) spectroscopy. We investigated the system 4,4'-bis(N-carbazolyl)-1,1'-biphenyl (CBP)/MoO_3, as a prototypical example, and spectroscopically identified charged and non-charged species of CBP molecules, that were deposited onto MoO_3. Both species can be distinguished by their specific vibrational modes in the mid IR range. The inverted layer structure with MoO_3 deposited onto CBP shows a significantly different behavior that is attributed to the diffusion of MoO_3 into the organic film.

Financial support by BMBF (project MESOMERIE) is gratefully acknowledged.

HL 51: Invited Talk Gregor Koblmüller

Time: Tuesday 14:00–14:30 Location: POT 112

Invited Talk HL 51.1 Tue 14:00 POT 112

Advanced optical properties of (In,Ga)As nanowire heterostructures — •Gregor Koblmueller — Walter Schottky Institut, Technische Universität München, Garching, Germany

In this talk, we focus on our most recent results on the growth and fundamental understanding of the physical properties of (In,Ga)As-based NWs as fabricated on Si, and further highlight advanced optical emitters tunable from the infrared to the THz regime. First, I will describe routes for completely catalyst-free (In,Ga)As NWs on Si (111), grown via (i) self-assembled and (ii) more sophisticated selective-area epitaxy (SAE) schemes. Based on the growth, several unique structural properties (such as wurtzite phase in the commonly cubic arsenides) will be highlighted and distinct structure-electronic function relationships (such as crystal-phase dependent band gap, radial quantum confinement, etc.) elucidated. In the second part, the optical emission characteristics will be explored based on advanced core-shell NW concepts of InAs-InAsP and GaAs-AlGaAs core-shell NWs. For both core-shell NW systems we demonstrate significant enhancements (˜100-1000-fold) in the photoluminescence efficiency via suppression of surface states and carrier confinement. Furthermore, based on the GaAs-AlGaAs core-shell NW heterostructures we report very efficient resonators that enable even lasing operation at room-temperature. Finally, we show that InAs NWs can be also utilized as very strong THz emitters with record high THz radiation efficiencies that are >3x stronger than p-type bulk InAs, currently the best semiconductor THz emitter.

HL 52: Quantum wires: Optical properties (with TT)

Time: Tuesday 14:30–16:15 Location: POT 112

HL 52.1 Tue 14:30 POT 112

Continuous Wave Lasing in Sn:CdS Nanowires — •Marcel Wille[1,2], Robert Röder[2], Sebastian Geburt[2], Carsten Ronning[2], Mengyao Zhang[3], and Jia Grace Lu[3] — [1]Institut für Experimentelle Physik II/Halbleiterphysik, Universität Leipzig — [2]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena — [3]Department of Physics and Electrical Engineering, University of Southern California

Semiconductor nanowires (NWs) are promising candidates for future optoelectronic applications due to their possibility of light generation, optical waveguiding and light amplification. The controlled modification of their electrical and optical properties by doping will continue the consequent progress in NW research. In a modified VLS growth process using tin (Sn) as catalyst the in-situ doping of cadmium sulphide (CdS) NWs was demonstrated. Optical investigations using temperature dependent photoluminescence and cathodoluminescence technique were correlated with electrical transport measurements in field-effect-transistor geometry [1]. Furthermore, these NWs exhibit ideal Fabry-Pérot resonator morphology necessary for the occurrence of laser oscillations under continuous wave excitation. The continuous wave lasing mode is proven by the evolution of the emitted power and spectrum with increasing pump intensity [2]. The high temperature stability up to 120 K at given pumping power is determined by the decreasing optical gain necessary for lasing in an electron hole plasma. [1] Zhang, M., Wille, M. et al., Submitted to Nano Letters, 09.2013 [2] Röder, R., Wille, M. et al., Nano Letters 2013, 13, 3602-3606

HL 52.2 Tue 14:45 POT 112

Phonon-assisted lasing in ZnO microwires — •Stefan Lange, Tom Michalsky, Christof P. Dietrich, 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 lasing properties of ZnO microwires. The spectral distribution of the lasing modes reveals a strong exciton-phonon interaction as the main lasing mechanism. These findings are supported by former results measuring a strong exciton-phonon interaction in ZnO [1,2] and showing indications for an increase of the coupling strength with reduced structure size [2]. Photoluminescence and coherence measurements under varying excitation density prove the transition from spontaneous to stimulated emission.

[1] D.C. Reynolds et al., J. Appl. Phys. 89, 6189 (2001)
[2] H.C. Hsu et al., J. Crystal Growth 261, 520 (2004)

HL 52.3 Tue 15:00 POT 112

Phonons in PbSe nanostructures — •Efterpi Kalesaki and Ludger Wirtz — Physics and Materials Science Research unit, University of Luxembourg, Luxembourg

The prospect of efficient utilization of lead chalcogenides in optoelectronic, photovoltaic and thermoelectric devices has brought PbSe into the spotlight of scientific research. Bulk PbSe exhibits a plethora of intriguing characteristics, in terms of structural, electronic and vibrational properties, which have been the subject of intense investigation. In particular, the phonon dispersion displays a near-Kohn anomaly of the LO mode at Γ [1]. However, attempts to understand the vibrational properties of corresponding nanostructures are limited.

We present results of ab-initio calculations on the phonon dispersions of <001> - oriented PbSe slabs of various thicknesses. The latter are correlated with the phonon modes of bulk PbSe via the quantum confinement model [2]. Quantum confinement and strain effects are identified as parameters critically affecting the lattice dynamics of PbSe nanostructures. In contrast to most nanocrystalline materials, where the Raman active phonon modes shift down in frequency, a blueshift of the longitudinal optical mode with decreasing layer thickness is recorded for PbSe nanostructures, validating recent experimental results of Raman spectra for lead selenide nanocrystals [2]. Softening of the TO mode in the slabs is an indication of near-ferroelectric behaviour in PbSe nanostructures.

[1] O. Kilian et al., Phys. Rev. B 80, 245208 (2009)
[2] J. Habinshuti et al., Phys. Rev. B 88, 115313 (2013)

HL 52.4 Tue 15:15 POT 112

Picosecond time-resolved photocurrents in single semiconductor nanowires — •Stefan Zenger[1,2], Nadine Erhard[1], and Alexander Holleitner[1] — [1]Walter Schottky Institute and Physik-Department, Technische Universität München, Germany — [2]stefan.zenger@wsi.tum.de

Conventional scanning photocurrent microscopy experiments on semiconductor nanowires are typically limited to timescales exceeding several tens of picoseconds. Yet, it is known from optical experiments that carrier relaxation and transport processes can occur on much faster timescales in semiconducting nanowires. We apply a recently developed pump-probe photocurrent spectroscopy to investigate the photocurrent dynamics in single nanowires made out semiconductors, such as InAs, GaAs, and InGaN, with an on-chip THz-time domain spectroscopy [1]. Hereby, the ultrafast photocurrent response of the nanowire is sampled at a field probe in a stripline circuit a picosecond time-resolution. We discuss ultrafast thermoelectric, displacement, and carrier lifetime limited currents as well as the time-resolved transport of photogenerated holes.

[1] N. Erhard, P. Seifert, L. Prechtel, S. Hertenberger, H. Karl, G. Abstreiter, G. Kobelmueller,and A. Holleitner, Ann. Phys. (Berlin) 525, 180 (2013).

We gratefully acknowledge financial support from the ERC-grant NanoREAL.

HL 52.5 Tue 15:30 POT 112

Combined optical and electrical characterization of single AlGaN/GaN nanowire heterostructures — •Jan Müssener, Pascal Becker, Svenja van Heesvijk, Markus Schäfer, Pascal Hille, Jörg Schörmann, Jörg Teubert, and Martin Eickhoff — I. Physikalisches Institut, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

We report on the photoluminescence characterization of single GaN nanowires (NWs) with embedded AlGaN/GaN heterostructures under the influence of an external electric field. Group III-nitrides exhibit strong internal polarization-induced electric fields which influence the optical properties via the quantum confined Stark effect (QCSE). While the presence of the QCSE in NWs has been proven, a controlled modification of the QCSE via external axial electric fields on a single NW basis has not been achieved up to now. NWs were grown along $[000\bar{1}]$ by plasma assisted molecular beam epitaxy on a Si(111) substrate. Their geometry consists of a single ND embedded in AlGaN barriers and surrounded by Ge-doped GaN contacts. We performed numerical simulations of the three dimensional quantum confinement to optimize the sample structure with respect to its opto-electrical properties. Single NWs were isolated for μ-PL measurements and contacts were formed using electron beam lithography to allow application of external axial electric fields. The effect of current induced heating on the low temperature μ-PL spectra was investigated. The application of axial electric fields leads to a suppression or an enhancement of the QCSE which corresponds to the polarity of the NWs.

HL 52.6 Tue 15:45 POT 112

Nanospectroscopic imaging of twinning superlattices in individual Beryllium-doped GaAs/AlGaAs core-shell nanowires — •Alexander Senichev[1], Igor Shtrom[2], Vadim Talalaev[1,3], George Cirlin[2,4], Christoph Lienau[5], Jörg Schilling[3], and Peter Werner[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [2]St. Petersburg Academic University RAS, St. Petersburg, Russia — [3]Martin-Luther-Universität, ZIK "SiLi-nano", Halle, Germany — [4]Ioffe Physico-Technical Institute, St. Petersburg, Russia — [5]Institut für Physik, Carl von Ossietzky University, Oldenburg, Germany

We report on subwavelength-resolution near-field photoluminescence (PL) spectra and transmission electron microscopy (TEM) images taken from the very same single p-GaAs/AlGaAs core-shell nanowire grown on silicon.By correlation with the TEM images, we distinguish between the emission spectra of pure ZB-type regions and those of periodic twinning plane superlattices (TSL). Emission from the ZB region is governed by direct interband recombination whereas the TSL spectra are split into two peaks, separated in energy by the hole confinement at a single WZ-type quantum disk. Blue-shifts of the local emission spectra reveal electron quantum confinement in twinning superlattices and allow us to trace spatial variations of the TSL period by all-optical means. Our results provide direct and quantitative insight into the correlations between morphology and optics of TSL nanowire and hence present an important step towards band gap engineering of GaAs nanowires by controlled crystal phase formation.

HL 52.7 Tue 16:00 POT 112

Optical characterization and enhanced luminescence properties of InAs-InAsP core-shell nanowires — •Thomas Stettner[1], Julian Treu[1], Michael Bormann[1], Hannes Schmeiduch[1], Stefanie Morkötter[1], Markus Döblinger[2], Sonja Matich[1], Peter Wiecha[1], Kai Saller[1], Benedikt Mayer[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

Using optical spectroscopy InAs nanowires (NW) grown by molecular beam epitaxy (MBE) and subsequently overgrown and passivated with an $InAs_{1-x}P_x$-shell by a hybrid metal-organic vapor phase epitaxy (MOVPE) process are studied in detail. With a microphotoluminescence (PL) setup designed for the mid infrared spectral range we demonstrate up to 100x enhancement of the InAs core signal [1]. By systematically varying both the shell thickness and the phosphorus content x(P) we show that it is possible to further tune the emission energy >100meV for comparatively low x(P) due to strain effects, which is confirmed by numerical simulation. For even higher P-content an asymmetric shell growth leads to a drastic reduction in PL efficiency/blueshift due to an onset of plastic relaxation which proves the importance to engineer a high quality InAs-InAsP core-shell interface for future use in photonic and optoelectronic devices like solar cells.

[1] J. Treu, et al., Nano Lett.2013, dx.doi.org/10.1021/nl403341x

HL 53: Nitrides: Preparation of nonpolar and semipolar orientations

Time: Tuesday 14:00–16:15 Location: POT 151

HL 53.1 Tue 14:00 POT 151

Analytic solutions of kp-Hamiltonian for III-nitride semiconductors with arbitrary strain situation — •Michael Winkler, Rüdiger Goldhahn, and Martin Feneberg — Otto-von-Guericke-Universität, Magdeburg, Germany

Calculation of transition energies and optical polarization degrees in semi- and nonpolar wurtzite semiconductors demand new analysis schemes within **kp**-theory. We demonstrate that the Bir-Pikus Hamiltonian for nonpolar or semipolar material with *arbitrary strain situation*, following Hooke's law, is analytically solvable for eigenenergies and eigenvectors. These results contribute to an in-depth understanding of valence band distances and relative oscillator strengths. We discuss valence band crossing and anticrossing behavior under symmetry not preserving strain at the Γ-Point.

The fully analytical parametrization of eigenvalues for semipolar wurtzite layers allows finally for a quick qualitative analysis of oscillator strengths and band order. The methodology allows for an easy expansion to pressure-dependent optical experiments. Calculational results are put in relation to experimental data. We find that valence band crossings are exotic events occuring under special conditions only, which is discussed in detail.

HL 53.2 Tue 14:15 POT 151

The impact of silicon doping on the optical properties of the stacking fault emission in a-plane GaN — •Gordon Schmidt, Christopher Karbaum, Sebastian Metzner, Frank Bertram, Peter Veit, Matthias Wieneke, Hartmut Witte, Armin Dadgar, Martin Feneberg, Rüdiger Goldhahn, Alois Krost, and Jürgen Christen — Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Germany

In GaN the basal plane stacking fault (BSF) type I_1 is a two dimen-

sional defect characterized by a cubic inclusion within the wurtzite structure. Excitons are bound at the BSF I_1 similar to the localization in a quantum well heterostructure leading to an efficient radiative recombination.

We present a study of the BSF I_1 emission from a-plane GaN layers with a systematic variation of the silicon doping level. Using metal-organic vapor phase epitaxy the a-plane GaN layers were grown on r-plane sapphire substrates with an AlGaN seeding layer. Varying the silane flow rate the electron concentration (n_e) was changed between nominally undoped and $3{\cdot}10^{19}$ cm^{-3}.

In cathodoluminescence (CL) experiments at 5 K the BSF I_1 emission is the most intense recombination whose peak energy exhibits a strong blueshift from 3.423 eV to 3.473 eV with increasing n_e. The recombination kinetics of the dominant CL show a monoexponential decay with initial lifetimes of the BSF I_1 emission decreasing with higher n_e from 2.9 ns to 470 ps. Our results will be discussed in terms of reduction of the quantum confined Stark effect within the BSF I_1.

HL 53.3 Tue 14:30 POT 151

In-situ analysis of the surface electronic properties of polar and nonpolar InN and GaN films — •Marcel Himmerlich, Anja Eisenhardt, and Stefan Krischok — Institut für Physik and Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, PF 100565, 98684 Ilmenau, Germany

Intrinsic surface electronic properties of nitrides are still under debate especially due to a lack of in-situ analyses that allow the characterization of clean surfaces commonly considered in electronic structure calculations. Here we present in-situ studies on the surface properties of polar and nonpolar configurations of GaN and InN thin films prepared by plasma-assisted molecular beam epitaxy utilizing ultraviolet and X-ray photoelectron spectroscopy [1,2]. It will be shown that especially surface reconstructions or relaxations are responsible for the existence of occupied and unoccupied electron states that determine the band alignment at surfaces and interfaces. For both group III nitrides, GaN and InN, the metal-polar surface exhibits different band bending V_{bb} compared to the N-polar, m-plane and a-plane surface. Thereby V_{bb} depends on the position of surface states that induce a pinning of the Fermi level. Furthermore, the GaN and InN surface states are easily saturated by adsorbates due to exposure to reactive gases like oxygen or water, partly combined with strong changes in the surface band bending.

[1] M. Himmerlich et al., Phys. Rev. B 88 (2013), 125304.
[2] A. Eisenhardt et al., Appl. Phys. Lett. 102 (2013), 231602.

HL 53.4 Tue 14:45 POT 151

Luminescence characteristics of pyramidal InGaN/GaN light emitter — •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 green spectral range is an important topic for the field of semiconductor light emitters nowadays. The lack of efficient InGaN/GaN green emitters due to the Quantum Confined Stark Effect (QCSE) limits the use of semiconductors in optical devices. The QCSE reduces the recombination efficiency for electrons and holes in these emitter drastically by shifting the wavefunctions away from each other. To overcome this we grow semipolar InGaN quantum wells on top of three dimensional GaN pyramids. The use of semipolar facets instead of c-plane GaN as growth surface reduces the QCSE by a large amount and should increase the efficiency of green InGaN/GaN emitter. Since up to now semipolar and nonpolar GaN substrates are not widely available we use the method of epitaxial lateral overgrowth (ELO) to force a three-dimensional growth of the GaN. This provides us with easy accessible semipolar growth surfaces for the InGaN quantum well. In this contribution we would like to show our latest results in the control and growth of pyramidal GaN structures as well as the optical characteristics and the dynamics of the charge carriers of these structures.

HL 53.5 Tue 15:00 POT 151

Determination of polarisation fields in group III-nitride heterostructures by capacitance-voltage-measurements — •Monir Rychetsky[1], Ingrid Koslow[1], Jens Rass[1,2], Tim Wernicke[1], Konrad Bellmann[1], Veit Hoffmann[2], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Germany — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Berlin, Germany

InGaN/GaN heterostructures exhibit strong piezoelectric and spontanous polarisation fields and sheet charges resulting in band bending. This leads to a reduction in the radiative recombination rate in light-emitting diodes (LEDs) and a red shift in the emission wavelength, due to the quantum-confined Stark effect.

There are several methods by which the magnitude and orientation of these polarisation fields have been measured. However, no exact values for the polarisation fields in semipolar planes have been reported.

In this contribution we propose a new approach to determine polarisation fields by using capacitance-voltage measurements. The sheet charges at the heterointerface influence the charge distribution in a PIN (positive intrinsic negative) junction and therefore the depletion width and the capacitance. In order to improve the accuracy of the method we compare the depletion width of two PIN junctions, one with an embedded InGaN layer and therefore influenced by the internal polarisation fields and one without it. First results of an $In_{0.08}Ga_{0.92}N$ quantum well on (0001) show an internal field strength in the range of 0.95 - 1.25 MV/cm in $[000\bar{1}]$ direction.

HL 53.6 Tue 15:15 POT 151

Optical and structural nano-characterization of GaN based LED structures with semipolar sub-μm patterned InGaN QWs — •Sebastian Metzner[1], Marcus Müller[1], Gordon Schmidt[1], Benjamin Max[1], Peter Veit[1], Silke Petzold[1], Frank Bertram[1], Robert Leute[2], Dominik Heinz[2], Junjun Wang[2], Ferdinand Scholz[2], and Jürgen Christen[1] — [1]Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg — [2]Institute of Optoelectronics, University of Ulm

We present the nano-scale correlation of optical and structural properties of an LED structure with sub-μm semipolar InGaN quantum wells (QWs) using liquid helium temperature scanning (transmission) electron microscope cathodoluminescence (SEM/STEM-CL). The semipolar n-doped GaN structures were selectively grown on a SiN mask consisting of stripes with a period of 260 nm on top of a c-plane GaN/sapphire template using metalorganic vapour phase epitaxy. The $\{10\bar{1}1\}$ side facets were subsequently covered by InGaN and finally completely filled up and planarized by p-doped GaN. The InGaN QWs on top of the $\{10\bar{1}1\}$ GaN stripes are clearly resolvable in cross-section STEM images in high-angle annular dark field contrast and can directly be correlated to intense CL emitting at $\sim$ 440 nm. We will discuss the impact of e.g. systematic thickness changes of the QW on the luminescence properties as well as the effect of the mask patterning process and selective growth on the planarization during p-doped GaN growth.

HL 53.7 Tue 15:30 POT 151

Cathodoluminescence mapping on differently inclined semipolar InGaN facets — •Matthias Hocker[1], Ingo Tischer[1], Benjamin Neuschl[1], Jeffrey Helbing[1], Junjun Wang[2], Ferdinand Scholz[2], and Klaus Thonke[1] — [1]Institute of Quantum Matter / Semiconductor Physics Group, University of Ulm, D-89081 Ulm, Germany — [2]Institute of Optoelectronics, University of Ulm, D-89081 Ulm, Germany

Indium gallium nitride (InGaN) based converter structures are promising candidates for optical devices emitting in the green spectral range. They are realized by epitaxial overgrowth of three-dimensional semipolar gallium nitride (GaN) by InGaN multiple quantum wells. Besides structural deficiencies, differently inclined facets incorporate different amounts of indium, resulting in a broadening of the integral light output spectrum. To overcome these deficiencies, such converter structures were investigated in detail by spatially and spectrally resolved low-temperature cathodoluminescence (SEM-CL), which offers the possibility to distinguish the origin of the different spectral contributions locally. In the CL maps, dark areas and subfacets with blue shifted emission patterns were found. These emission features correlate with undesirable subfacets of the GaN templates. By suppressing these subfacets, it is possible to achieve a more homogenous luminescence distribution, resulting in a better performance of the final device.

HL 53.8 Tue 15:45 POT 151

Generalized ellipsometry of semipolar AlGaN — •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

We present generalized spectroscopic ellipsometry data obtained from the anisotropic semiconductor material system aluminum gallium ni-

tride (AlGaN). The several micrometer thick AlGaN layers were grown by metal-organic vapor phase epitaxy on m-plane sapphire substrates. The samples cover the whole composition range between GaN and AlN. The (11-22) orientation of the AlGaN surface allows for alignment of the optical axis parallel to the plane of incidence, no perpendicular alignment is possible. The optical axis of the as well anisotropic sapphire substrate is pointing in a different direction. This challenging sample geometry requires careful measurement of the main and the secondary elements of the Jones matrix. As result of the evaluation of the measurements we present the successfully separated ordinary and extraordinary tensor components of the dielectric function. We not only succeeded in fitting model dielectric functions to experimental data but also present point-by-point fitted dielectric functions of several AlGaN samples. The valence band structure of AlGaN governing optical selection rules and thus the dielectric function is expected to show a crossing at certain but unknown Al concentration. Our study experimentally narrows the possible band crossing range in AlGaN.

HL 53.9 Tue 16:00 POT 151

Direct identification of luminescence from I1 type basal plane stacking faults in semipolar AlGaN layer with low Al content — •Ingo Tischer[1], Manuel Frey[1], Matthias Hocker[1], Robert A.R. Leute[2], Ferdinand Scholz[2], Heiko Groiss[3], Erich Müller[3], Dagmar Gerthsen[3], Willem van Mierlo[4], Johannes Biskupek[4], Ute Kaiser[4], and Klaus Thonke[1] — [1]Institut für Quantenmaterie, Gruppe Halbleiterphysik, Universität Ulm, 89081 Ulm — [2]Institut für Optoelektronik, Universität Ulm, 89081 Ulm — [3]Laboratorium für Elektronenmikrokopie, Karlsruhe Institute of Technology, 76131 Karlsruhe — [4]Materialwissenschaftliche Elektronenmikroskopie, Universität Ulm, 89081 Ulm

For nitride-based laser diodes and LEDs high quality AlGaN electron blocking layers are required. Due to the lattice mismatch of AlGaN and GaN, the occurance of structural defects increases strongly, especially on semipolar surfaces. In this study, we assign distinct spectral luminescence features to structural defects of AlGaN layers on a semipolar GaN template. Spatially resolved cathodoluminescence (CL) recorded at temperatures below 10K using a scanning electron microscope, performed on the cross section and on the $\{10\bar{1}1\}$ side facet surface, allows to determine the spatial and spectral distribution of luminescence features. High resolution STEM investigations at the same sample area allow the direct assignment of optical bands to distinct structural features like basal plane stacking faults and regions with different Al content.

HL 54: Quantum light sources based on solid state systems: Status and visions II (Focus session with TT)

Continuation of 'Quantum light sources based on solid state systems: Status and visions I'

Organizers: Sven Ulrich, Universität Stuttgart, and Christoph Becher, Universität des Saarlandes, Saarbrücken.

Time: Tuesday 14:00–15:45 Location: POT 251

Topical Talk HL 54.1 Tue 14:00 POT 251

Quantum network challenges for solid-state spins and photons — •Mete Atature — University of Cambridge, Cambridge, United Kingdom

Spins confined in solids, such as quantum dots and atomic impurities provide interesting and rich physical systems. Their inherently mesoscopic nature leads to a multitude of interesting interaction mechanisms of confined spins with the solid state environment of spins, charges, vibrations and light. Implementing a high level of control on these constituents and their interactions with each other creates exciting opportunities for realizing stationary and flying qubits within the context of spin-based quantum information science. I will provide a snapshot of the progress and challenges for optically interconnected spins, as well as first steps towards hybrid distributed quantum networks.

HL 54.2 Tue 14:30 POT 251

Indistinguishable single photons from quasi-resonantly pumped quantum dots in adiabatic micropillar cavities — •Sebastian Unsleber[1], Michael Dambach[1], Matthias Lermer[1], Sven Höfling[1,2], 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

Single, indistinguishable photons are very important for applications in quantum networks and communication as well as linear optical quantum computing. Due to their atom-like emission properties quantum dots are promising candidates for photon sources matching this characteristics. Furthermore quantum dots can be implemented in nanostructured waveguides and microcavities leading to higher emission rates of single, indistinguishable photons.

We report on the emission of single and indistinguishable photons generated from quantum dots under quasi-resonant excitaion. The quantum dots are implemented in a adiabatic cavity design where we applied Bloch-wave engeneering to realize submicron diameter high quality factor GaAs/AlAs micropillars. Single photons emission with $g^{(2)}(0)$-values as low as 0.036 are observed and quantum interference of the quantum dots leads to visibility as high as 76%. Furthermore we studied the influence of the quantum dot cavity detuning on the indistinguishability of the emitted photons.

HL 54.3 Tue 14:45 POT 251

Indistinguishable photons generated from deterministic quantum light sources fabricated by in-situ electron-beam lithography — •Tobias Heindel, Luzy Krüger, Elisabeth Schlottmann, Manuel Gschrey, Marc Seifried, Ronny Schmidt, Jan-Hindrik Schulze, Sven Rodt, André Strittmatter, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, D-10623, Germany

Quantum communication technology relies vitally on efficient nonclassical light sources emitting single indistinguishable photons on demand. A promising approach to realize such light sources is based on single self-assembled semiconductor quantum dots (QDs) embedded into microcavity systems. The main challenge of this approach is the precise control of the coupling between the statistically grown QD and the optical mode of the microcavity. In this work we tackle this issue by using in-situ electron-beam lithography to embed target QDs deterministically into sub-μm mesa structures [1] as well as microlenses with enhanced photon extraction efficiency. The huge potential of this device technology is demonstrated by quantum optical studies which reveal distinct excitonic emission lines with resolution limited linewidths below 10 μeV and a strong suppression of multiphoton emission events associated with $g^{(2)}(0) < 0.04$. Furthermore, Hong-Ou-Mandel type two-photon interference experiments are used to analyze the indistinguishability of the emitted photons.

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

HL 54.4 Tue 15:00 POT 251

Bright quantum dot single photon source based on a low Q defect cavity — •Sebastian Maier[1], Peter Gold[1], Alfred Forchel[1], Niels Gregersen[2], Sven Höfling[1,3], Christian Schneider[1], and Martin Kamp[1] — [1]Technische Physik, Physikalisches Institut and Wilhelm Conrad Röntgen-Research Center for Complex Material Systems, Universität Würzburg, Am Hubland, D-97074, Würzburg, Germany — [2]DTU Fotonik, Department of Photonics Engineering, Technical University of Denmark, Building 343, DK-2800 Kongens Lyngby, Denmark — [3]present address: SUPA, University of St Andrews, St Andrews, KY16 9SS, United Kingdom

Efficient light outcoupling in quantum dot single photon sources is critical and usually complicated resonator geometries, lithographic steps and spatial alignment are necessary. In this paper we demonstrate a quantum dot based quasi-planar single photon source with a high

extraction efficiency of 42% measured with a numerical aperture of 0.7. Our sample was fabricated via molecular beam epitaxy (MBE) and contains a λ-thick cavity which is sandwiched between two distributed Bragg reflector (DBRs), consisting of 18 (5) bottom (top) layers of AlAs/GaAs mirror pairs. The high efficiency is caused by the self-aligned formation of oval defects on top of the quantum dots which is interesting for a possible scalable sample layout. Besides the high extraction efficiency the sample shows a high purity with a g2(0) value of 0.023. Due to the absence of any etched and exposed lateral semiconductor-air interfaces, such cavities are nearly ideal for spin manipulation and readout experiments.

HL 54.5 Tue 15:15 POT 251

On-demand single-photon emission from electrically pumped, site-controlled quantum dots based on buried stressors — •Alexander Schlehahn, Waldemar Unrau, David Quandt, Jan-Hindrik Schulze, Tobias Heindel, Tim D. Germann, Ole Hitzemann, Udo W. Pohl, Dieter Bimberg, André Strittmatter, and Stephan Reitzenstein — Institut für Festkörperphysik, TU Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

Single photons, emitted on demand, is one of the most basic needs in quantum information technology. We present pulsed operation of a lately introduced electrically driven source based on single quantum dots, deterministically aligned to a strain-inducing and current-path-restricting oxide aperture. The aperture is formed by oxidation of an AlAs/AlGaAs sandwich structure. The modification of its crystalline structure leads to geometry dependent strain in the topping GaAs-layer. Due to this strain modulation at the surface, an accumulation of quantum dots occurs above the aperture when depositing InGaAs. These QDs show excellent optical properties regarding the emission linewidth ($FWHM < 25\mu$eV) and the single photon purity ($g^{(2)}(0) < 0.05$), and outclass the reported characteristics of QDs grown by other prepositioning methods. The sample characterization is facilitated by an automatized micro-electroluminescence setup which includes a He-flow cryostat with an internal high-frequency probe in combination with a precise x-y-z-stage. This system allows for efficient sample testing without the need for wire bonding.

HL 54.6 Tue 15:30 POT 251

Integrated quantum optics in coupled quantum-dot micropillar cavities — •Pierce Munnelly — Institut für Festkörperphysik, Technische Universität Berlin

The development of novel concepts for integrated photonics has become an area of intensive research in the field of semiconductor nanotechnology. The overall goal is to integrate light sources, waveguides, non-linear optical elements and detectors into compact and externally controllable optical networks. Up till now, most approaches for integrated nanophotonics have relied on planar waveguide structures and photonic crystal membranes, where the integration of active and passive areas on the same chip or the definition of electrical contacts is challenging. In an alternative approach for 'free space' integrated optics we take advantage of the fact that electrically contacted micropillar cavities allow for efficient in-plane emission of light via whispering gallery modes. Using this very appealing feature, we demonstrate that electrically driven micropillar lasers can act as integrated light sources to perform cavity quantum electrodynamics experiments in laterally coupled micropillar cavities. Moreover, electrical contacts at the coupled micropillars allow for resonance tuning using the quantum confined Stark effect and for integrated light detection via on-chip photocurrent measurements.

HL 55: Transport: Topological insulators I (organized by TT)

Time: Tuesday 14:00–16:00 Location: HSZ 304

HL 55.1 Tue 14:00 HSZ 304

All in-ultra-high-vacuum study of thin film topological insulators: Bi_2Te_3 — •Katharina Hoefer, Diana Rata, Christoph Becker, and Liu Hao Tjeng — Max Planck Institute for Chemical Physics of Solids

Thin films of topological insulators offer the possibility for the experimental study of the expected specular phenomena occurring at the surface or interface with these materials due to the increased surface to bulk ratio in comparison to bulk crystals. Bulk materials are always defective which leads to extra contributions in conductance.

To protect the surface integrity an all in- ultra-high-vacuum study is crucial. High quality thin films of Bi_2Te_3 were grown on well lattice matched $BaF_2(111)$ substrates using Molecular Beam Epitaxy. The preparation, characterization by RHEED, LEED, XPS and ARPES and especially transport measurements, were performed all in-situ under ultra-high-vacuum conditions.

Results of this study and the effect of air exposure on the electronic structure and transport properties will be presented.

HL 55.2 Tue 14:15 HSZ 304

Finite width effect on weak antilocalization in MBE grown Bi_2Te_3 thin films — •Christian Weyrich[1,2], Tobias Merzenich[1,2], Igor E. Batov[3], Gregor Mussler[1,2], Jörn Kampmeier[1,2], Jürgen Schubert[1], Thomas Schäpers[1,2], and Detlev Grützmacher[1,2] — [1]Peter Grünberg Institute (PGI-9) and JARA-Fundamentals of Future Information Technology, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Virtual Institute for Topological Insulators (VITI), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [3]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, 142432, Moscow Distr., Russia

The weak antilocalization effect is measured in Bi_2Te_3 layers under various tilt angles of the magnetic field with respect to the layer surface. The investigated Bi_2Te_3 layer was prepared by molecular beam epitaxy. For a magnetic field oriented perpendicularly to the layer the weak antilocalization effect at different temperatures can be well-fitted by the Hikami-Larkin-Nagaoka model. From the fit a phase coherence length of about 200 nm is obtained at a temperature of 2 K. A clear signature of weak antilocalization is also observed when the magnetic field is oriented parallel to the Bi_2Te_3 layer. This effect is compared to classical models as well as a recently developed theory, which takes into account the finite penetration depth of the surface or interface states into the bulk.

HL 55.3 Tue 14:30 HSZ 304

Band structure and magnetotransport in strained HgTe — •Jan Böttcher and Ewelina M. Hankiewicz — Universität Würzburg, Faculty for Physics and Astronomy, Am Hubland, D-97074 Würzburg

Strained mercury telluride is a 3D topological insulator with negligible bulk conductivity [1]. Here we report on band structure calculations using a six-band Kane model with a self-consistent Poisson solver. We find that while the surface states lie within the band gap, the Dirac point lies deep in the heavy hole subbands. We study this system as a function of gate voltage and give possible explanations of exciting experimental observations of the Landau level structures in high magnetic fields as well as oscillations in the Shubnikov-de Hass data at low magnetic fields.

We acknowledge financial support via grant HA 5893/4-1 within SPP 1666.

[1] C. Brüne, C. X. Liu, E. G. Novik, E. M. Hankiewicz, H. Buhmann, Y. L. Chen, X. L. Qi, Z. X. Shen, S. C. Zhang, and L. W. Molenkamp, Phys. Rev. Lett. 106, 126803 (2011)

HL 55.4 Tue 14:45 HSZ 304

Photoemission investigation of the predicted topological Kondo insulator behavior of SmB_6 — •Peter Hlawenka[1], Emile Rienks[1], Konrad Siemensmeyer[1], Eugen Weschke[1], Andrei Varykhalov[1], Natalya Shitsevalova[2], Slavomir Gabani[3], Karol Flachbart[3], and Oliver Rader[1] — [1]Helmholtz-Zentrum Berlin — [2]Institute for Problems of Material Science, Kiev, Ukraine — [3]IEP, Slovak Academy of Science, Kosice

The system SmB_6 is known for its unusual resistivity which increases exponentially with decreasing temperature and saturates below 3 K [1]. This has recently been attributed to topological-Kondo-insulator behavior where a topological surface state is created by Sm4f-5d hybridization and is responsible for the transport [2]. The local-density-approximation + Gutzwiller calculations of the (100) surface predict the appearance of three Dirac cones in the surface Brillouin zone [2].

We perform angle-resolved photoemission (ARPES) below 1 K and do not observe the predicted Dirac cones at $\overline{\Gamma}$ or $\overline{X}$. Moreover, the Fermi surface is made up of steeply dispersing bulk Sm5d states. The Sm^{2+} 4f band and the hybridization gaps where the surface states are expected [2] are too far ($\sim$ 20 meV) below the Fermi energy in order to contribute to the transport. These results will be discussed in comparison to other ARPES studies.

[1] J. C. Cooley, M. C. Aronson, Z. Fisk, P. C. Canfield, Phys. Rev. Lett. 74, 1629 (1995)
[2] F. Lu, J. Zhao, H. Weng, Z. Fang, Xi Dai, Phys. Rev. Lett. 110, 096401 (2013)

HL 55.5 Tue 15:00 HSZ 304

Excitations of surface and bulk states in spin orbit dominated materials — •Peter Lemmens[1], Vladimir Gnezdilov[1,2], Dirk Wulferding[3], Patrik Recher[4], Helmuth Berger[5], Yoichi Ando[6], R Sankar[7], and Fang-Cheng Chou[7] — [1]IPKM, TU-BS, Braunschweig — [2]ILTPE, Kharkov, Ukraine — [3]POSTECH, Korea — [4]IMAPH, TU-BS, Braunschweig — [5]EPFL, Lausanne, Switzerland — [6]ISIR, Osaka, Japan — [7]CCMS, National Taiwan Univ., Taipei, Taiwan

Using Raman scattering experiments we probe inelastic processes in the giant Rashba material BiTeI, the topological semimetal Cd_3As_2 and several topological insulators. By comparing surface with bulk scattering processes we notice the dominance of quantum well states. With exception to Cd_3As_2 all materials show pronounced resonances in the Raman scattering cross section.

HL 55.6 Tue 15:15 HSZ 304

Josephson Effect in Topological Insulator Planar, Nanostep and Edge Junctions — •Jennifer Nussbaum, Rakesh Tiwari, Thomas Schmidt, and Christoph Bruder — University of Basel, Switzerland

Topological insulators are states of quantum matter which are characterized by a full insulating gap in the bulk and gapless surface states which are protected by time-reversal symmetry. By using the superconducting proximity effect on a Bi_2Se_3 topological insulator, a topological superconductor - topological insulator - topological superconductor (SIS) junction can be engineered. By solving the Dirac-Bogoliubov-De-Gennes equation in such a junction the maximal supercurrent that can flow through the surface of the Bi_2Se_3 topological insulator with heavily doped superconducting electrodes is calculated. In this manner, short and wide nanostep Josephson junctions involving different side surfaces of the 3D topological insulator are investigated. The results are compared to the Josephson response of a junction involving only one side surface. The comparison reveals, for example, that a step setup leads to a non-trivial scaling of the Josephson current.

HL 55.7 Tue 15:30 HSZ 304

Parity measurement in topological Josephson junctions — •François Crépin and Björn Trauzettel — Institute for Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany

We study the properties of a topological Josephson junction made of both edges of a 2D topological insulator. We show that, due to fermion parity pumping across the bulk, the global parity of the junction has a clear signature in the periodicity and critical value of the Josephson current. In particular, we find that the periodicity with the flux changes from 4π in a junction with an even number of quasi-particles to 2π in the odd sector. In the case of long junctions, we exhibit a rigorous mathematical connection between the spectrum of Andreev bound-states and the fermion parity anomaly, through bosonization. Additionally, we discuss the rather quantitative effects of Coulomb interactions on the Josephson current.

HL 55.8 Tue 15:45 HSZ 304

PN junctions of Topological Insulators — •Sourin Das[1] and Disha Wadhawan[2] — [1]MPIPKS, Dresden, Germany & University of Delhi, India — [2]University of Delhi, India

Spin textures of surface states of topological insulators (TI) open up possibilities for designing ultra fast electrically controllable spin transistor. In this context I will discuss spin-valve effect associated with a gating induced PN junction designed on the surface state of 2D and 3D TI. I will show that *conduction to conduction* and *conduction to valence* band transport in a PN junction is topologically distinct resulting in asymmetric electrical transport. The topological distinction is shown to be quantifiable in term of the Pancharatnam geometric phase.

HL 56: Invited Talk Xavier Blase

Time: Wednesday 9:30–10:00 Location: POT 006

Invited Talk HL 56.1 Wed 9:30 POT 006

Ab initio many-body perturbation theory for organic photovoltaics — •Xavier Blase — Institut Néel, CNRS and UJF, Grenoble, France

Initially developed in the mid-eighties at the ab initio level for inorganic semiconductors, a family of many-body perturbation theories, the so-called GW and Bethe-Salpeter (BSE) formalisms, have been shown recently to yield electronic and optical (excitonic) properties of bulk and gas phase organic systems with a remarkable accuracy. After introducing some of the important limitations associated with organic photovoltaic cells, we will show that key features, such as band gaps and offsets, bands dispersion, electron-phonon coupling strength, and donor-to-acceptor charge-transfer excitations, can be described with unprecedented accuracy by such techniques that are parameter-free and allow the study of systems comprising up to a few hundred atoms. Upcoming challenges, such as the development of specific embedding techniques that may account for dynamical long range screening in disordered dense organic phases, will conclude this presentation. The selected calculations have been performed with a recently developed Gaussian-basis GW and BSE package, the Fiesta code.

Selected references: I. Duchemin and X. Blase, Phys. Rev. B 87, 245412 (2013); I. Duchemin, T. Deutsch, X. Blase, Phys. Rev. Lett. 109, 167801 (2012); S. Ciuchi et al., Phys. Rev. Lett. 108, 256401 (2012); C. Faber et al., Phys. Rev. B, 86, 155315 (2012); C. Faber et al., Phys. Rev. B 84, 155104 (2011).

HL 57: Graphene: Transport (with MA/O/TT)

Time: Wednesday 9:30–12:15 Location: POT 051

HL 57.1 Wed 9:30 POT 051

Ratchet effects in graphene with a lateral potential — •Josef Kamann[1], Leonid Golub[2], Matthias König[1], Jonathan Eroms[1], Felix Fromm[3], Thomas Seyller[3], Dieter Weiss[1], and Sergey Ganichev[1] — [1]University of Regensburg, Germany — [2]Ioffe Physical-Technical Institute of the RAS, St. Petersburg, Russia — [3]Technical University of Chemnitz, Germany

We report on the observation of terahertz radiation induced ratchet effects in graphene with a lateral periodic potential. These effects generate a dc electric current from an ac electric field. To probe ratchet effects, a metal grating has been deposited on top of epitaxially grown graphene. This lattice contains periodically deposited stripes with different widths and spaces and, therefore, has no inversion symmetry.

We demonstrate that the ratchet effect is generated only in the modulated area and does not arise in unpatterned graphene. This proves the symmetry breaking induced by the asymmetric lateral potential. Additional effects like edge currents or the circular ac Hall effect are excluded by the geometry of the samples and by illumination under normal incidence. The ratchet signal is studied with respect to the polarization and the wavelength of the radiation. We show that the ratchet effect is sensitive to both linear and circular polarization and conducted calculations for different elastic-scattering processes to compare them to our experimental findings.

HL 57.2 Wed 9:45 POT 051

Magnetic quantum ratchet effect in graphene — •Christoph Drexler[1], Sergey Tarasenko[2], Peter Olbrich[1], Johannes Karch[1], Marion Hirmer[1], Florian Müller[1], Martin Gmitra[1], Jaroslav Fabian[1], Rositza Yakimova[3], Samuel Lara-Avila[4], Sergey Kubatkin[4], Minjie Wang[5], Junichiro Kono[5], and Sergey Ganichev[5] — [1]THz Center, University of Regensburg, Germany — [2]Ioffe Physical-Technical Institute, St. Petersburg, Russia — [3]Linköping University, Sweden — [4]Chalmers University, Göteborg, Sweden — [5]Rice University, Houston, USA

We report on the experimental observation of the magnetic quantum ratchet effect in epitaxial- and CVD- grown graphene layers excited by pulsed terahertz (THz) - laser radiation [1]. Our experimental findings can be well understood in terms of asymmetric carrier scattering in graphene in presence of an in-plane magnetic field yielding strong structure inversion asymmetry (SIA) in graphene. The SIA stems from the fact that graphene is deposited on a substrate and/or is sensitive to chemical bonding of adatoms on the surface. Considering hydrogen atoms on top of carbon we calculated the magnitude of the photocurrent being in good agreement with the data obtained from the experiments. The amplitudes of the current differ significantly for the used material systems whereas its sign can be influenced by the post-groth treatment of the samples. The ratchet current can be calibrated to measure the strength of the SIA, which plays an important role in graphene ferromagnetism and spintronics.

[1] C. Drexler et al, Nat. Nano. 8 104-107, 2013.

HL 57.3 Wed 10:00 POT 051

Spin transport in arrays of graphene nanoribbons — Matthias Berl, Bastian Birkner, Andreas Sandner, Silvia Minke, Dieter Weiss, and •Jonathan Eroms — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany

We performed non-local spin valve and Hanle measurements in arrays of graphene nanoribbons in both single and bilayer graphene. Nanoribbons were patterned by electron beam lithography and oxygen-based reactive ion etching. By fabricating several sets of electrodes, we can compare spin transport data in bulk and nanoribbons on the same graphene flake. Due to band-gap opening in the nanoribbons at low temperatures, spin transport measurements were only possible at 200 Kelvin. For single layer graphene we observe that while nanopatterning decreases the electron mobility, the spin lifetime increases from 200 ps to 500 ps. This is consistent with a Dyakonov-Perel-like contribution to spin relaxation. In bilayer graphene, we observe a low electron mobility and high spin lifetimes of about 1 ns in both bulk and nanoribbons, again consistent with Dyakonov-Perel-like spin relaxation. Attempting to see an influence of possible magnetic moments at the sample edges, no clear signature was detected in the Hanle data at 200 Kelvin.

HL 57.4 Wed 10:15 POT 051

THz radiation interacting with epitaxial graphene — •Christian Sorger, Sascha Preu, and Heiko B. Weber — Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

We investigate the interaction between terahertz (THz) radiation and periodically doped graphene ribbons. We find a remarkable polarization dependence. The Drude response of graphene can be probed with THz electric fields parallel to the ribbons. This results in a high-pass filter-like behavior with a 3dB-frequency in the THz range. The exact value depends on carrier mobility and carrier concentration. For THz electric field perpendicular to the ribbons we detect rather high transmission as the response is dominated by plasmonic effects. Utilizing the material system epitaxial graphene on silicon carbide (SiC) we show that no lithographic patterning is required to couple light into the two-dimensional electron gas (2DEG). As the interaction strength depends on the geometry of the 2DEG and its electronic properties, respectively, this strategy allows for a characterization of the AC conductivity in epitaxial graphene.

HL 57.5 Wed 10:30 POT 051

Numerically exact approach to transport properties of disordered two-dimensional materials — •Stefan Barthel[1,2], Malte Rösner[1,2], Fernando Gargiulo[3], Oleg V. Yazyev[3], and Tim O. Wehling[1,2] — [1]Institut für Theoretische Physik, Universität Bremen, Germany — [2]Bremen Center for Computational Materials Science, Universität Bremen, Germany — [3]Institute of Theoretical Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland

We present a numerical method for modeling electron transport in disordered two-dimensional materials such as graphene with resonant impurities. Covalently bonded adatoms, such as hydrogen, modify the electronic structure and transport properties of graphene in the diffusive as well as localized regime in which quantum corrections become important. The electronic structure is described using a tight-binding model involving pz-orbitals on a honeycomb lattice, whereas the transport properties are evaluated in the linear response approximation (Kubo-Greenwood) using the kernel polynomial method as a solver. By combining these methods we gain access to large systems containing up to 10ˆ6 atoms. These results are compared to the ones obtained using the Landauer-Büttiker approach in the above-mentioned transport regimes.

HL 57.6 Wed 10:45 POT 051

Quantum Hall Effect in Chemically Functionalized Graphene: Defect-Induced Critical States and Breakdown of Electron-Hole Symmetry — •Nicolas Leconte[1,2], Jean-Christophe Charlier[2], and Stephan Roche[1] — [1]ICN2 - Institut Catala de Nanociencia i Nanotecnologia, Campus UAB, 08193 Bellaterra (Barcelona), Spain — [2]Université catholique de Louvain (UCL), Institute of Condensed Matter and Nanoscience (IMCN), Chemin des étoiles 8, 1348 Louvain-la-Neuve, Belgium

Unconventional magneto-transport fingerprints in the quantum Hall regime (with applied magnetic field from one to several tens of Tesla) in chemically functionnalized graphene are reported. Upon chemical adsorption of monoatomic oxygen (from 0.5% to few percents), the electron-hole symmetry of Landau levels is broken, while a double-peaked conductivity develops at low-energy, resulting from the formation of critical states conveyed by the random network of defects-induced impurity states. Scaling analysis suggests an additional zero-energy quantized Hall conductance plateau, which is here not connected to degeneracy lifting of Landau levels by sublattice symmetry breakage. This singularly contrasts with usual interpretation, and unveils a new playground for tailoring the fundamental characteristics of the quantum Hall effect. The study on oxygen is complemented with a study on a simplified divacancy model, confirming the percolation of impurity states leading to delocalized states.

Coffee break (15 min.)

HL 57.7 Wed 11:15 POT 051

Ultra long spin decoherence times in graphene quantum dots with a small number of nuclear spins — •Moritz Fuchs[1], John

Schliemann[2], and Björn Trauzettel[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg — [2]Institut für Theoretische Physik, Universität Regensburg, 93053 Regensburg

We study the dynamics of an electron spin in a graphene quantum dot, which is interacting with a bath of less than ten nuclear spins via the anisotropic hyperfine interaction. Due to substantial progress in the fabrication of graphene quantum dots, the consideration of such a small number of nuclear spins is experimentally relevant. This choice allows us to use exact diagonalization to calculate the longtime average of the electron spin as well as its decoherence time. We investigate the dependence of spin observables on the initial states of nuclear spins and on the position of nuclear spins in the quantum dot. Moreover, we analyze the effects of the anisotropy of the hyperfine interaction for different orientations of the spin quantization axis with respect to the graphene plane. Interestingly, we then predict remarkable long decoherence times of more than 10ms in the limit of few nuclear spins.

HL 57.8 Wed 11:30 POT 051

Carrier dynamics in graphene under Landau quantization — •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 ultrafast dynamics of low-energetic Dirac electrons in graphene under Landau quantization [1]. In a joint experiment-theory study, we provide calculations based on the density matrix formalism [2] as well as measurements of the relaxation dynamics via differential transmission spectroscopy.

As a consequence of the linear dispersion at the Dirac points, graphene exhibits a non-equidistant Landau level spectrum which allows to address specific transitions by optical pumping. Exploiting this to selectively excite the energetically lowest Landau levels, we employ pump-probe spectroscopy to explore the carrier dynamics in this regime. A surprising sign reversal in differential transmission spectra is observed both in experiment and theory and provides evidence for strong Auger scattering on a picosecond timescale. Our calculations even predict the occurrence of a substantial carrier multiplication in Landau quantized graphene [3].

[1] M. Mittendorff et al., (in preparation).

[2] E. Malic, A. Knorr, Graphene and Carbon Nanotubes: Ultrafast Optics and Relaxation Dynamics, (Wiley-VCH, Berlin, 2013).

[3] F. Wendler, A. Knorr, and E. Malic, (submitted).

HL 57.9 Wed 11:45 POT 051

Polarization dependence of optical carrier excitation in graphene — •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, P.O. Box 510119, 01314 Dresden, Germany — [2]Technische Universität Dresden, 01062 Dresden, Germany — [3]Technische Universität Berlin, Hardenbergstraße 36 10623 Berlin, Germany

We present near-infrared pump-probe measurements to investigate the polarization dependence of optical carrier excitation in graphene. Excitation with linearly polarized radiation leads to an anisotropic distribution of the nonequilibrium carriers in momentum space. This anisotropy can be revealed by the comparison of pump-probe signals for different polarization configurations. In parallel configuration the probe beam has the same polarization with respect to the pump beam, for the perpendicular configuration the polarization of the probe beam is rotated by 90°. The signal amplitude of the parallel configuration is about twice as large as compared to the perpendicular configuration. The initial relaxation process is faster for the parallel polarized probe beam, which leads to identical signals about 150 fs after excitation. At this time delay an isotropic carrier distribution is reached by electron-phonon scattering. These findings are confirmed by microscopic calculations.

HL 57.10 Wed 12:00 POT 051

Anisotropic photoinduced current injection in graphene — •Julien Rioux[1], John Sipe[2], and Guido Burkard[1] — [1]University of Konstanz — [2]University of Toronto

Quantum-mechanical interference effects are considered in carrier and charge current excitation in gapless semiconductors using coherent optical field components at frequencies ω and 2ω. Due to the absence of a bandgap, excitation scenarios outside of the typical operation regime are considered; we calculate the polarization and spectral dependence of these all-optical effects for single- and bilayer graphene. For linearly-polarized light and with one-photon absorption at ω interfering with 2ω absorption and ω emission, the resulting current injection is five times stronger for perpendicular polarization axes compared to parallel polarization axes. This additional process results in an anisotropic current as a function of the angle between polarization axes, in stark contrast with the isotropic current resulting from the typical interference term in graphene [Rioux et al., PRB 83, 195406 (2011)]. Varying the Fermi level allows to tune the disparity parameter $d = \eta_I^{xyyx}/\eta_I^{xxxx}$ closer to typical values in GaAs [$|d| \approx 0.2$, Rioux and Sipe, Physica E 45, 1 (2012)]: from -1, when the additional process is fully Pauli-blocked, to $-3/7$, when it is fully accessible, thus facilitating polarization sensitive applications.

HL 58: Emerging oxide semiconductors I (Focus session with DS)

Oxides are increasingly explored for their semiconducting properties. This session sets a focus to the physics, material and surface science of oxides that have recently been considered as active material for *n*-type and *p*-type semiconductor devices. Besides the classical use in gas sensorsand as transparent contactsfor optoelectronics devices, novel applications of semiconducting oxides in power electronics, UV sensors, photovoltaics, and solar water splitting devicesare addressed.

Organizers: Oliver Bierwagen, Paul-Drude-Institut für Festkörperelektronik, Berlin, Norber Esser, Leibniz-Institut für Analytische Wissenschaften ISAS, Berlin, Rüdiger Goldhahn, Otto von-Guericke-Universität Magdeburg, and Marius Grundmann, Universität Leipzig.

Time: Wednesday 9:30–13:00 Location: POT 081

Topical Talk HL 58.1 Wed 9:30 POT 081

Computational design of oxide semiconductors — •Stephan Lany — National Renewable Energy Lab, Golden, CO, 80401

Traditional semiconductors are the group-V, III-V, and II-VI systems as well as their isovalent and isostructural alloys. Within the field of oxide semiconductors, there is a continuing interest in n-type wide gap compounds, such as ZnO, In2O3 and related materials, but there is also growing interest in oxide semiconductors for novel applications, e.g., for oxide photovoltaics or solar water splitting. This background leads us to explore the range of possible semiconducting properties within the realm of oxide semiconductor alloys. From a computational materials design perspective, this includes modeling of the alloy structure and energetics, prediction of band-structures, optical properties, and electrical properties (doping and defects). We will discuss two recent examples of this materials design effort, i.e., the realization of tetrahedral MnO alloys, and the optimization of the photovoltaic properties of Cu2O by aliovalent alloying through ultrahigh doping.

Work in collaboration with H. Peng, V. Stevanovic, and funded by the U.S. Dept. of Energy.

HL 58.2 Wed 10:00 POT 081

Phonon properties of Copper-Oxide phases from first principles — •Marcel Giar, Markus Heinemann, and Christian Heiliger — I. Physikalisches Institut, Justus-Liebig-University, D-35392 Giessen, Germany

We present *ab initio* investigations on phonon properties of the copper-oxide phases Cu_2O, CuO, and Cu_4O_3. Phonon bandstructure and density of states for all three phases are derived from a supercell small displacement method. This method relies on displacing atom(s) within a supercell and calculating resulting forces on all other atoms. As copper-oxides exhibit polar bonding the splitting of the LO and TO modes at the Γ point must be properly taken into account. We derive these splittings from Born effective charges and the dielectric tensor which enter the non-analytical contributions to the dynamical matrix in the limit $\mathbf{q} \to 0$.

HL 58.3 Wed 10:15 POT 081

Intrinsic point defects in Cu_2O - Lifting of Raman selection rules — •Thomas Sander, Christian T. Reindl, and Peter J. Klar — I. Physikalisches Institut, Justus-Liebig-Universität Gießen

The copper oxide system Cu_2O receives currently a renewed interest due to its potential photovoltaic applications. Its natural p-type conductivity is due to intrinsic defects. Understanding the formation and properties of such point defects is of major relevance for tuning the material for optoelectronic applications.

Crystalline cubic Cu_2O exhibits a very unusual feature which is up to now unexplained in the literature. Instead of showing just one optical mode expected for cubic symmetry, Raman spectra of Cu_2O are dominated by Raman forbidden phonons independent of the method used for growth. A group theoretical analysis will be presented showing that the forbidden phonons will become Raman allowed when the symmetry is lowered due to the formation of point defects. Furthermore, it will be shown that of all possible intrinsic defects the copper split vacancies cause the lifting of the Raman selection rules. The results are experimentally confirmed by making use of the full angle and polarization dependence called rotational Raman spectroscopy (RoRa). Low temperature Raman studies further reveal that the degeneracy of phonon modes is lifted which is in accordance with the results of the group theoretical analysis.

Thus the detailed Raman study of Cu_2O in combination with the group theoretical analysis yields much more insight than just a proof of selection rules or identification of lattice modes.

HL 58.4 Wed 10:30 POT 081

Effect of Chemical Precursors On the Optical and Electrical Propertiesof p-Type Transparent Conducting Cr_2O_3:(Mg,N) — Elisabetta Arca, •Karsten Fleischer, Sergey A. Krasnikov, and Igor V. Shvets — School of Physics, Trinity College Dublin, Ireland

Cr_2O_3:(Mg,N) has been reported as a p-type transparent conducting oxide. In this contribution the effect of each precursor used for deposition by spray-pyrolysis will be explored and their role in determining the optical and electrical properties of Cr_2O_3 will be outlined. A correlation between the structural, electrical, and optical properties upon introducing nitrogen precursors has been established. In particular it has been shown that the presence of ammonium salts in the deposition environment results in less absorbing films. By combining optical measurements and NEXAFS studies, a mechanism is proposed to explain the change in the optical properties. Moreover, it is shown that the presence of the nitrate moiety in the reaction environment is necessary to improve the electrical conductivity of the deposited films. The reaction of the nitrate moiety with the ammonium moiety has been proposed as the mechanism to explain the boost in conductivity.

HL 58.5 Wed 10:45 POT 081

Tailoring the electronic and magnetic structure of doped rutile-TiO_2 using p-elements (C,N); A Hybrid DFT study. — •Jacqueline Atanelov, Christoph Gruber, and Peter Mohn — Vienna University of Technology, Center for Computational Materials Science

We study the electronic and magnetic structure of carbon and nitrogen impurities and interstitials in rutile TiO_2. To this end we perform *ab-initio* calculations of a 48-atom supercell employing the VASP code. In order to obtain a realistic description of the electronic and magnetic structure, exchange and correlation are treated with the HSE06 hybrid functional. Substitutional carbon and nitrogen are found to have a magnetic moment of 2 and $1\mu_B$, respectively, with a tendency for anti-ferromagnetic long range order. For C/N on interstitial sites we find that carbon is non-magnetic while nitrogen always possesses a magnetic moment of $1\mu_B$. We find that these interstitial positions are on a saddle point of the total energy. The stable configuration is reached when both carbon and nitrogen form a C-O and N-O dimer with a bond length close to the double bond for CO and NO. This result is in agreement with earlier experimental investigations detecting such N-O entities from XPS measurements. The frequencies of the symmetric streching mode are calculated for these dimers, which could provide a means for expermental verification. For all configurations investigated both C and N states are found inside the TiO_2 gap. These new electronic states are discussed with respect to tuning doped TiO_2 for the application in photocatalysis.

HL 58.6 Wed 11:00 POT 081

Magneto-optical characterization of thin films of magnetic oxides prepared via aqueous solution processing — •Peter Richter[1], Michael Fronk[1], Paul N. Plassmeyer[2], Catherine J. Page[2], Dietrich R.T. Zahn[1], and Georgeta Salvan[1] — [1]Semiconductor Physics, Technische Universität Chemnitz, 09107 Chemnitz, Germany — [2]Department of Chemistry, University of Oregon, Eugene, Oregon 97403, USA

Ferromagnetic oxides are of great interest for a wide variety of applications. In spintronics, LaMnO3 and La1-xSrxMnO3 are now among the most commonly used materials for electrodes. Other oxides like the ferrites can show multiferroic properties and can be fabricated to be transparent and are therefore useful for optical and photovoltaic applications. However, the deposition of such magnetic oxide layers usually requires sophisticated instrumentation and may be expensive. We present a new approach to effectively prepare smooth thin films of metal oxides by spin coating them from aqueous precursor solutions. The full dielectric tensor (including the Voigt constant) of the obtained layers is determined from spectroscopic ellipsometry and magneto-optical Kerr effect (MOKE) spectroscopy measurements for a spectral range of 1.7 to 5.0 eV. The magnetic properties are investigated by MOKE magnetometry. Of particular interest, the ferrites $CoFe_2O_4$ and $NiFe_2O_4$ show characteristic spectral features and a ferromagnetic hysteresis at room temperature. We observe a variation of the optical and magnetic properties depending on the temperatures at which the samples were annealed after spin coating.

Coffee break (15 min.)

Topical Talk HL 58.7 Wed 11:30 POT 081

Beta-Ga2O3: Single crystal growth and semiconductor applications — •Encarnacion G. Villora[1], Daisuke Inomata[3], Stelian Arjoca[1,2], Kazuo Aoki[3], and Kiyoshi Shimamura[1,2] — [1]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan — [2]Graduate School of Advanced Science and Engineering, Waseda University, 3-4-1 Okubo, Shinjuku, Tokyo 176-0022, Japan — [3]Koha Co., Ltd., Nerima, Tokyo 176-0022, Japan

β-Ga_2O_3 is a unique transparent conductive oxide, which is attracting an increasing attention in the recent years. It possesses two major features. The first is its very wide bandgap Eg=4.8 eV, which leads to a high transparency (>260 nm) and to a Baliga's figure of merit over three times that of GaN and SiC counterparts. The second feature is the capability to grow crystals from the melt, which makes possible the mass production of large substrates at low cost.

High quality 2 inch single crystals are grown by the EFG technique, and 4 inch are already in progress. N-type carrier concentration is controlled by Si- or Sn-doping. Conductive wafers are used as transparent conductive substrates for high-brightness vertically structured LEDs based on InGaN multi-quantum wells. Schottky barrier diodes and transistors have been demonstrated.

Additionally, a new phosphor concept for high-brightness white LEDs and LDs is presented. In contrast to currently used powder phosphors embedded in resins, single-crystal phosphors exhibit outstanding internal quantum efficiencies and do not degrade either under light irradiation or the increase of temperature.

HL 58.8 Wed 12:00 POT 081

MOCVD grown homo and heteroepitaxial β-Ga_2O_3 layer studied by transmission electron microscopy — •Robert Schewski, Martin Albrecht, Günter Wagner, Michele Baldini, Zbigniew Galazka, and Reinhard Uecker — Leibniz-Institut für Kristallzüchtung, Max-Born-Strasse 2, 12489 Berlin, Germany

We report on the structural properties of β-Ga_2O_3 layers, grown by MOCVD for various growth conditions. In detail, the influence of different precursors, namely pure oxygen, water, and CO_2 on the crystalline film quality has been investigated. Our studies were carried out for hetero- as well as homoepitaxially grown samples on (0001)

sapphire and melt grown (100) β-Ga_2O_3 substrates, respectively. The conclusions are mainly based on transmission electron microscopy and x-ray data.

As main results, we found that pure oxygen in the growth ambient leads to the formation of nano-crystals in form of wires or agglomerates for both hetero- and homoepitaxial growth. However, by using water as oxygen precursor, smooth (rms: 6.5 nm) single crystalline layers can be achieved for homoepitaxial growth. Still, the structural quality of these thin films suffers from a substantial amount of stacking faults, which can be evidenced by TEM and x-ray data. However, annealing in oxidizing atmosphere at (900°C) leads to a reduction these stacking faults and thus improves the crystalline quality of the film. Another interesting observation is the formation of a pseudomorphic, 3 monolayers thick Ga_2O_3 layer in the alpha phase, directly at the interface between the sapphire substrate and the film.

Topical Talk HL 58.9 Wed 12:15 POT 081

Combinatorial approach to group-III sesquioxides — •Holger von Wenckstern — Universität Leipzig, Fakultät für Physik und Geowissenschaften, Institut für Experimentelle Physik II, Halbleiterphysik

Semiconducting group-III sesquioxides find potential application as chemical/biological sensors, deep-UV photo-detectors, and within transparent and high-power electronics. Technology for bulk growth of binary Me_2O_3 (Me=Al, Ga, In) exists and first promising devices on homoepitaxial layers have been demonstrated. For the exploration of ternary or quarternary systems thin film technology is required. In this contribution we introduce a facile approach to create lateral continuous composition spread(s) (CCS) within thin films on 2 inch wafers by pulsed-laser deposition (PLD) [1]. We ablate from a single, segmented, rotating target keeping the growth rate is for this approach as high as for conventional PLD. We will illustrate the potential of our CCS-technique and discuss structural, optical and electronic properties of $(In,Ga,Al)_2O_3$ thin films and their utilization in device demonstrations like rectifiers or photo-detectors.

[1] H. von Wenckstern *et al.*, CrystEngComm **15**, 10020 (2013)

HL 58.10 Wed 12:45 POT 081

Schottky contacts on β-Ga_2O_3 and In_2O_3 thin films — •Daniel Splith[1], Stefan Müller[1], Holger von Wenckstern[1], Oliver Bierwagen[2,3], James S. Speck[3], and Marius Grundmann[1] — [1]Universität Leipzig, Institut für Experimentelle Physik II, Leipzig, Germany — [2]Paul Drude Institut, Berlin, Germany — [3]Materials Department, University of California, Santa Barbara, USA

Oxide semiconductors like β-Ga_2O_3 or In_2O_3 are promising materials for a new generation of transparent electronic devices. Oxide field-effect transistors but also the electrical characterization of these oxides by capacitance-voltage measurements or deep-level transient spectroscopy rely on Schottky contacts (SCs). For our study we fabricated SCs on β-Ga_2O_3 and In_2O_3 thin films and investigated their electrical properties. The β-Ga_2O_3 thin films were grown by pulsed laser deposition on highly conducting (00.1) oriented ZnO:Ga acting as a back contact layer. The In_2O_3 thin films were grown by molecular beam epitaxy on yttria-stabilized zirconia substrates. We prepared SCs by dc sputtering of different metals. On β-Ga_2O_3 the I-V characteristics of Cu SCs exhibit high rectification ratios up to 7 orders of magnitude. Temperature dependent measurements between 110 and 320 K yield a mean barrier height of 1.32 eV, which is in accordance to the effective barrier height at a temperature of 550 K, where the ideality factor decreases to 1.03. Due to surface electron accumulation, the realization of SCs on In_2O_3 is challenging. In a proof of principle experiment we fabricated SCs on In_2O_3 by reactive sputtering of Au, Pt and Pd with rectification ratios up to 3 orders of magnitude.

HL 59: Topological insulators: Theory (with MA/O/TT)

Time: Wednesday 9:30–11:15 Location: POT 151

HL 59.1 Wed 9:30 POT 151

Stabilizing Chern and fractional Chern insulators — •Adolfo G. Grushin, Johannes Motruk, and Frank Pollmann — Max Planck Institute for the Physics of Complex Systems, Dresden

The experimental realization of Chern insulators (CI) and fractional Chern insulators (FCI), zero field lattice analogues of the integer and fractional Hall effects respectively, is still a major open problem in condensed matter. For the former, it was proposed that short range interactions at the mean-field level can drive a trivial insulator into a CI. For the latter, the effect of band dispersion and sizes of the single-particle gaps with respect to the interaction strength have been argued to be important to stabilize an FCI state. In this talk we will examine the robustness and fate of these statements both with exact diagonalization and infinite density matrix renormalization group (iDMRG).

HL 59.2 Wed 9:45 POT 151

Point contacts and localization in generic helical liquids — •Christoph P. Orth, Grégory Strübi, and Thomas L. Schmidt — University of Basel, Switzerland

We consider two helical liquids on opposite edges of a two-dimensional topological insulator, which are connected by one or several local tunnel junctions. In the presence of spatially inhomogeneous Rashba spin-orbit coupling, the spin of the helical edge states is momentum dependent, and this spin texture can be different on opposite edges. We demonstrate that this has a strong impact on the electron transport between the edges. In particular, in the case of many random tunnel contacts, the localization length depends strongly on the spin textures of the edge states.

HL 59.3 Wed 10:00 POT 151

***ab-initio* investigation of topological states and symmetry inversion in HgTe-CdTe Quantum wells** — •Sebastian Kuefner, Juergen Furthmueller, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany

Topological insulators (TIs) recently attracted a high level of attention in solid state physics due to their unique physical properties. Generally, a TI is a material that is insulating in the bulk but exhibits metallic surface or edge states. These states are topologically protected which means that they are independent of surface orientation and passivation. The edge states usually have linear band dispersion forming Dirac cones.

The electromagnetic properties of the edge states might be used for the realisation of topological superconducting phases. In two dimensions the edge states build the quantum spin Hall state (QSH). In 2006, Bernevig et al. predicted the occurence of the QSH in HgTe-CdTe superlattices theoretically by an **kp**-approch which was later verified by König et al. experimentally.

However, these results have not yet been discussed in the framework of a reasonable electronic structure theory based on *ab-initio* methods but account for quasiparticle effects and spin-orbit coupling. Using density-functional theory together with the Tran-Blaha approximation we discuss the occurence of topological quantum-well states and investigate the topological transition in atomic structures.

HL 59.4 Wed 10:15 POT 151

Nontrivial Interface States Confined Between Two Topological Insulators — •Tomáš Rauch[1], Markus Flieger[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

By *ab initio*-based tight-binding calculations, we show that nontrivial electronic states exist at an interface of a $\mathcal{Z}_2$ topological insulator and a topological crystalline insulator. At the exemplary (111) interface between Bi_2Te_3 and SnTe, the two Dirac surface states at the Brillouin zone center $\overline{\Gamma}$ annihilate upon approaching the semi-infinite subsystems but one topologically protected Dirac surface state remains at each time-reversal invariant momentum $\overline{\mathrm{M}}$. This leads to a highly conducting spin-momentum-locked channel at the interface but insulating bulk regions. For the Sb_2Te_3/Bi_2Te_3 interface we find complete annihilation of Dirac states because both subsystems belong to the same topology class.

HL 59.5 Wed 10:30 POT 151

Natural three-dimensional topological insulators in Tl_4PbTe_3 and Tl_4SnTe_3 — •Chengwang Niu[1,2], Ying Dai[1], Baibiao Huang[1], Gustav Bihlmayer[2], Yuriy Mokrousov[2], Daniel Wortmann[2], and Stefan Blügel[2] — [1]School of Physics, Shandong University, Jinan, China — [2]Peter Grünberg Institut (PGI-1) & Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The recently discovered three-dimensional topological insulators have attracted much interest due to their exceptional properties of possessing insulating bulk but time-reversal symmetry protected metallic surfaces with Dirac-like band structure [1,2]. The search for new topological insulators is critical for both fundamental and practical interests. Based on first-principles calculations, we reveal that both Tl_4PbTe_3 and Tl_4SnTe_3 are strong topological insulators with different band inversion behaviors at Γ point [3]. The mechanisms of band inversion in Tl_4PbTe_3 and Tl_4SnTe_3, as well as in Bi_2Se_3 and Sb_2Se_3, are investigated and classified. The Z_2 topological invariants and topological surface states are investigated to confirm the topologically non-trivial phase. Our calculations further indicate that the electron- or hole-type Dirac fermion can be effectively engineered by hole doping, which is necessary for device applications of topological insulators.

[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] C. Niu et al., in preparation.

HL 59.6 Wed 10:45 POT 151

Electronic properties of the topological crystalline insulator SnTe and its (001) and (111) surfaces: an ab-initio study — •Matthias Drüppel, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster

The insulator SnTe belongs to the recently discovered class of materials in which a crystalline symmetry ensures the existence of topologically protected surface states. We report on the properties of these states at the (001) and (111) surfaces. To this end, we have employed density-functional theory.

The bulk band structure of SnTe is characterized by inversion at the four equivalent L points giving rise to a mirror Chern number $n_m = -2$. The (001) surface exhibits two mirror planes and shows four Dirac cones at non-time-reversal-invariant points along the $\pm\bar{\Gamma}\bar{X}$ and $\pm\bar{\Gamma}\bar{X}'$ lines, respectively. Here we explore the influence of lattice deformations on the stability of the surface states. Our results reveal that distortions of the topmost layers which break a mirror symmetry locally at the surface do *not* lead to an opening of the surface band gap. We find that only *bulk* lattice deformations, e.g. rhombohedrial distortions, that break one or both mirror symmetries also in the bulk part of the system give rise to a surface band gap. Our calculations show that the Sn terminated (111) surface exhibits Dirac cones centered at $\bar{\Gamma}$ and $\bar{M}$. In particular at the $\bar{M}$ point, these topologically protected states are distinctly extended into the bulk. Interestingly, we observe for the Te terminated (111) surface a gap-closing Dirac state only at the $\bar{\Gamma}$ point

HL 59.7 Wed 11:00 POT 151

Adsorbate- and vacancy-induced band bending in Bi_2Se_3: ab-initio calculations — •Tobias Förster, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

Bi_2Se_3 is one of the first topological insulators ever discovered. It has been widely studied both experimentally und theoretically, due to its simple electronic structure with only one Dirac point at $\bar{\Gamma}$. In experiments, a downward band bending and an ageing effect are frequently observed. This has been attributed to an intrinsic n-doping and to coverage with adsorbates. Models for the band bending mostly focussed on the intrinsic doping.

Using DFT calculations, we show that a long-ranged potential also occurs for an adsorbate-covered surface, even without intrinsic doping. As a prototype adsorbate, we have investigated potassium at various coverages. The resulting changes in the charge density, the potential, and the band structure can be attributed to two distinct origins: short-ranged adsorbate-specific changes and the formation of a long-ranged potential (which is independent of the specific adatom). We will explain how the band bending is related to the layered structure of Bi_2Se_3. Similar effects result from our calculations for different types of adsorbates as well as for selenium vacancies in the surface layer.

HL 60: Quantum dots: Optical properties I (with TT)

Time: Wednesday 9:30–11:15 Location: POT 251

HL 60.1 Wed 9:30 POT 251

Single line emission of InGaN quantum dots grown on AlGaN templates — •Elahe Zakizadeh, Carsten Laurus, Stephan Figge, Timo Aschenbrenner, Kathrin Sebald, Jürgen Gutowski, and Detlef Hommel — Institute of Solid State Physics, University of Bremen, Germany

InGaN quantum dots (QDs) are a good candidates for realizing single-photon emission in the blue to green spectral region at elevated temperatures, because of the large bandgap and high exciton binding energies of the nitrides. Up to now, temperature dependent measurements demonstrate thermal stability up to 150 K of the emission of a single InGaN quantum dot grown on GaN template.

In order to achieve single-line emission at even higher temperatures, an enhancement of the carrier confinement in the quantum dots is needed. This can be realized by growing InGaN quantum dots on AlGaN templates by metal organic vaper phase epitaxy.

In this contribution we present the optical properties of single InGaN quantum dots achieved by the micro-photoluminescence measurements. The thermal stability of the emission lines and their dependance on the excitation density will be discussed.

HL 60.2 Wed 9:45 POT 251

Electronic coupling and luminescence dynamics of hybrid inorganic core/organic shell nanostructures — •Stephanie Bley, Michael Diez, Angelina Vogt, Jürgen Gutowski, and Tobias Voss — Institute of Solid State Physics, Semiconductor Optics, University of Bremen, 28359 Bremen, Germany

Hybrid core/shell nanostructures allow for spectral tuning of light emission and absorption processes what is of substantial interest for light-sensing and energy harvesting applications. Here, we study the luminescence decay dynamics of colloidal CdSe quantum dots (QDs) in different solvents and on different semiconducting and insulating surfaces. The QDs are optically excited with light from an optical parametric amplifier pumped by a Ti:Sapphire laser system. The time resolved luminescence signal is detected using a streak camera. The radiative recombination processes in the quantum dots attached to different three-dimensional nanostructure surfaces can be strongly influenced by different electron tunneling processes from excited states of the quantum dots into the conduction band of the nanostructures. In this context the experimental results show that different solvents and materials significantly change the decay process of the QDs. Possible reasons for decay time variations, including different polarities of solvents and dielectric constants of the solids, will be discussed.

HL 60.3 Wed 10:00 POT 251

Cubic GaN/AlN quantum dots - Characterization of individual emission lines — •Dmitrij Bostanjoglo[1], Gordon Callsen[1], Stefan Kalinowski[1], Gerald Hönig[1], Matthias Bürger[2], Donat As[2], Toni Markurt[3], Martin Albrecht[3], Andrei Schliwa[1], Stephan Reitzenstein[1], and Axel Hoffmann[1] — [1]TU Berlin, Germany — [2]Universität Paderborn, Germany — [3]Leibniz Institut für Kristallzüchtung, Germany

Group III-nitride quantum dots (QDs) with a wurtzite crystal structure (WZ) are plagued by a large spatial electron-hole separation, due to built-in pyro- and piezoelectric fields. As a consequence, one observes large excitonic lifetimes from the ns- up to the us-range in such QDs accompanied by a strong reduction of the overall light output. As most natural alternative to the WZ QDs one can examine their zincblende (ZB) counterparts. By growing nitride QDs onto ZB substrates such as 3C-SiC, the metastable ZB structure can be stabilized leading to the absence of spontaneous and a reduced piezoelectric polarization. Hence, a drastic reduction of the excitonic life-

time down to the 100 ps regime is observed. However, prior studies lack an interpretation of the physical origin of the observed emission lines. We examined the ZB GaN/AlN QDs in a time-resolved micro-photoluminescence setup. The measured decay times of all occurring excitonic complexes yield values from 100 ps up to 5 ns. This observation clearly demonstrates an enhanced charge carrier overlap. Our conclusive identification of the emission lines is supported by an analysis of the power- and polarization-dependence of all occurring emission lines.

HL 60.4 Wed 10:15 POT 251

Observation of carrier relaxation dynamics in Quantum Dot Excited State Laser — Holger Schmeckebier[1], Dejan Arsenijevic[1], Dieter Bimberg[1], •Bastian Herzog[2], Yücel Kaptan[2], Nina Owschimikow[2], Ulrike Woggon[2], Vissarion Mikhelashvili[3], and Gadi Eisenstein[3] — [1]Institute of Solid-State Physics, Technical University Berlin, Germany — [2]Institute of Optics and Atomic Physics, Technical University Berlin, Germany — [3]Electrical Engineering Dept. Technion - Israel Institute of Technology, Haifa, Israel

Single- and two-color Heterodyne pump-probe measurements were used to investigate the carrier dynamics of an InAs/InGaAs quantum dot based excited state laser at room temperature. Our main attention has been attracted by the excitonic ground state relaxation dynamics before and after the onset of excited state lasing, giving information about possible carrier relaxation paths. We found an ultrafast recovery with higher device currents, showing no change at and above the excited state lasing threshold. This could be an indication for a decoupling of the ground state gain recovery from the excited state gain dynamics. Two-color pump-probe experiments were performed to identify the excited state and ground state sub-ensemble belonging to the equal dot sub-ensemble.

HL 60.5 Wed 10:30 POT 251

Deterministic fabrication of quantum-dot microlenses for enhanced photon extraction efficiencies — •Manuel Gschrey, Marc Seifried, Luzy Krüger, Jan-Hindrik Schulze, Tobias Heindel, Sven Rodt, André Strittmatter, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, D-10623, Germany

The realization of building blocks for long-distance quantum communication is a major driving force for the development of advanced nanophotonic devices, like efficient quantum-dot-based single-photon sources. One major challenge of a deterministic device fabrication using self-assembled quantum dots (QDs) results from their random growth, which reduces the yield of usable nanophotonic devices. Another issue is the low extraction efficiency (EE), due to the high refractive index of the surrounding semiconductor material, where total internal reflection at the surface occurs already for very small angles. To overcome these obstacles we apply a recently developed cathodoluminescence (CL) lithography technique [1] to fabricate and position microlenses on top of preselected single InGaAs QDs. This in-situ lithography technique is based on low-temperature CL spectroscopy, to identify the spectral features and spatial positions of the statistically grown QDs, prior to the lithography step. To obtain optimum EE, the position and shape of the lens is directly taylored in the CL-system by means of 3D electron-beam lithography. By using this technique we fabricated microlenses that allow for a sixfold increase in EE as compared to plain surfaces - [1] M. Gschrey et al., APL 102, 251113 (2013).

HL 60.6 Wed 10:45 POT 251

Non-resonant and resonant optical spectroscopy of single self-assembled quantum dots, weakly coupled to a two dimensional electron gas — •Annika Kurzmann[1], Benjamin Merkel[1], Arne Ludwig[2], Andreas 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-Universitaet Bochum, Universitaetsstr. 150, 44780 Bochum, Germany

Self-assembled quantum dots (QDs) are promising candidates for single-photon sources and as hosts for spin qubits. For such applications, the QDs are often embedded in a diode structure which allows controlled charging by tunneling of electrons from a 3D, n-doped reservoir, with fast tunneling times in the order of nanoseconds. Here we show results from photoluminescence, differential reflection, resonant fluorescence, and correlation measurements on a single InAs QD, coupled weakly (tunneling times in the order of milliseconds) to a two-dimensional electron gas (2DEG).

By tuning the electrical field, we are able to occupy the QDs with single charge resolution and observe different excitonic emission lines simultaneously over a large voltage range under non-resonant excitation. This unusual behavior can be explained by auto- and cross-correlation measurements of the exciton and trion recombination line and resonant optical measurements, which give in sight into the capture rates of electrons and holes into the dot states.

HL 60.7 Wed 11:00 POT 251

Charge noise and spin noise in a semiconductor quantum device — •Andreas Kuhlmann[1], Jonathan Prechtel[1], Julien Houel[1], Arne Ludwig[1,2], Dirk Reuter[2], Andreas Wieck[2], Martino Poggio[1], and Richard Warburton[1] — [1]University of Basel, Switzerland — [2]Ruhr-Universität Bochum, Germany

Self-assembled QDs are potentially excellent single-photon sources. The linewidths are in the best case a factor of two larger than the transform-limit. Optimizing performance demands an understanding of noise and a strategy to circumvent its deleterious effects.

There are two sources of noise inherent to the semiconductor: charge noise and spin noise[1]. We present an investigation of noise in an ultra-clean semiconductor quantum device, using a minimally-invasive, ultra-sensitive, local probe: resonance fluorescence from a single QD. We present noise spectra with 6 decades of resolution in the noise power over 6 decades of frequency, from 0.1 Hz to 100 kHz. Significantly, we have discovered a spectroscopic way to distinguish charge noise from spin noise. We present a dynamic feedback technique to remove charge noise from the device[2]. We show that nuclear spin noise is the dominant dephasing mechanism that limits performance as a single-photon source. For the charged exciton, we demonstrate a significant decrease in the spin noise with resonant laser excitation. This noise reduction for the charged exciton is exploited to demonstrate transform-limited optical linewidths even when the measurement is performed very slowly.

[1] A. V. Kuhlmann et al., Nature Phys. 9, 570 (2013). [2] J. H. Prechtel et al., Phys. Rev. X 3, 041006 (2013).

HL 61: Organic electronics and photovoltaics III (organized by CPP)

Polymers, Solar Cells, OFETs, OLEDs, Spectroscopy

Time: Wednesday 9:30–12:45 Location: ZEU 260

HL 61.1 Wed 9:30 ZEU 260

Structural Degradation of Polymer Solar Cells — •Christoph J. Schaffer[1], Claudia M. Palumbiny[1], Martin A. Niedermeier[1], Christian Jendrzejewski[1], Gonzalo Santoro[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department - LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]DESY, Notkestr. 85, 22607 Hamburg

A major challenge in organic photovoltaics (OPV) is to elongate their lifetimes. Several mechanisms of organic solar cell degradation have been proposed in literature within the last years. However, insufficient research has been done on determining the role of transitions in the nanomorphology of the active layer of bulk-heterojunction (BHJ) polymer solar cells as an aspect of degradation. These transitions would strongly affect the properties of solar cells since the active layer morphology plays a crucial role in the energy conversion process.

We present a direct evidence of morphological degradation on a nanometer scale in polymeric solar cells by simultaneous in-situ GISAXS and current-voltage tracking on a running P3HT:PCBM solar cell. The loss of short-circuit current with time is fully modeled by the observed morphological transitions [1].

[1] C. J. Schaffer et al., *Adv. Mater.* **2013**, DOI: 10.1002/adma.201302854

HL 61.2 Wed 9:45 ZEU 260

Controlling nanomorphology in bulk heterojunction solar cells via addition of third component — •Eva M. Herzig[1], Ammara R. Akhtar[2], Anna Naumann[2], Shuai Guo[2], Gregory Tainter[2], Jianqi Zhan[2], Jan Perlich[3], Stephan V. Roth[3], Christine M. Papadakis[2], and Peter Müller-Buschbaum[2] — [1]TU München, MSE, Lichtenbergstr. 4, 85748 Garching — [2]TU München, Physik-Department,, James-Franck-Str. 1, 85748 Garching — [3]DESY, Notkestr. 85, 22603 Hamburg

Nanomorphology and effciency of organic solar cells are closely linked. It is therefore desirable to have control over the self-assembly process responsible for the morpholgy formation of the active material. Employing grazing incidence small and wide angle x-ray scattering(GISAXS & GIWAXS) as well as spectroscopy and microscopy methods allows us to characterize organic thin films on the nanoscale with high statistical relevance. Using these methods we thoroughly investigate the morphological changes upon the addition of a third polymeric component showing that the self-assembly process is altered. We find that the amount of the third component controls the phase separation in the bulk heterojunction active layer. Adjusting the preparation route to support crystallization of the active material leads to an increased solar cell performance for a tuned ternary solar cell system.

HL 61.3 Wed 10:00 ZEU 260

Layer by layer solution processing of nanostructured all-polymer solar cells — •Thomas Pfadler, Mihael Coric, Jonas Weickert, Karl-Philipp Strunk, and Lukas Schmidt-Mende — University of Konstanz

Organic solar cells have the potential to become an important low-cost alternative to conventional solar cells. However, before this can happen, the energy harvesting potential of organic solar cells must become more comparable with that of the pervading technology. This research is focusing on nanoimprint lithography (NIL), a low-cost lithographic method for high-throughput patterning applicable to organic semiconductors. This technique can be used to tailor an organic solar cells active material on a nanometer scale. A promising application of NIL aims to control the nanostructure of a donor-acceptor interface in an organic all-polymer device. The electron accepting polymer is structured. A stiff polymer network featuring a nanostructured topography is developed by the usage of a photoactivable crosslinker molecule (sFPA). The crosslinked polymer matrix is not dissolved during spincoating the donor polymer allowing fully solution processed device fabrication with controlled nanostructured donor-acceptor interfaces. Target of this approach is to investigate nanostructured bi-layer devices with controlled interfaces to finally enhance the overall efficiency by maximizing the interfacial area, increasing the exciton separation yield and ensuring direct pathways to the electrodes.

HL 61.4 Wed 10:15 ZEU 260

The role of processing additives in Organic Solar Cells after the preparation process — •Stefan Väth[1], Andreas Baumann[1], Andreas Sperlich[1], Carsten Deibel[1], Milutin Ivanovic[2], Heiko Peisert[2], Thomas Chassé[2], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Eberhard Karls University Tübingen, 72076 Tübingen — [3]ZAE Bayern, 97074 Würzburg

Processing additives are widely used in the preparation of new high performance bulk heterojunction organic solar cells to improve the power conversion efficiency (PCE) significantly. They act as selective solvent for fullerenes and are therefore improving the morphology of the active area. Nevertheless the question wether or not these co-solvents remain in the organic solar cells after the preparation process occurs. This question could be solved by investigating blends consisting of the material system PTB7:$PC_{60}BM$ processed with the additives diiodooctane (DIO), octanedithiol (ODT) and without additives as reference. We used the spin sensitive measurement technique light induced Electron Paramagnetic Resonance (LESR) to distinguish between positive polarons on the polymer and negative charges on the fullerene by their different g-factors. Together with Photoelectron Spectroscopy (PES) measurements we could show that the additive DIO remains partly inside the active layer of organic solar cells even after a high vacuum preparation step. We propose that they do not only lead to an improved morphology, but also to a doping effect.

HL 61.5 Wed 10:30 ZEU 260

Radiative and non-radiative recombination in organic solar cells — •Kristofer Tvingstedt, Philip Pelchmann, Vladimir Dyakonov, and Carsten Deibel — Experimental Physics VI Julius Maximilian University of Würzburg 97074 Würzburg

Although several organic solar cells has reached close to unity internal quantum efficiency at short circuit conditions, the open circuit voltage is still very far from its potential upper limit due to substantial charge recombination of various types, which remains to be accurately determined. In this work we evaluate the limiting mechanisms in OPVs by employing complementary steady state measurements of recombination as a function of charge carrier density by thoroughly evaluating the diode ideality factor. The diode ideality is directly related to the order of recombination and we first assess it via light intensity dependent open circuit voltage characterization under the influence of a varying temperature. We focus our study on the ratio between radiative and non-radiative recombination via the interfacial charge transfer state as determined by absolute CT electroluminescence efficiency measurements, also as a function of temperature. The charge transfer state governs the radiative recombination in OPV bulk heterojunctions and is therefore crucial to evaluate in this context. Improving the radiative efficiency of OPVs will substantially increase the open circuit voltage and eventually put these promising photovoltaic converters in efficiency parity with their inorganic counterparts.

HL 61.6 Wed 10:45 ZEU 260

Electronic Structure of Fullerene Heterodimer in Bulk-Heterojunction Blends — •Andreas Sperlich[1], Oleg G. Poluektov[2], Jens Niklas[2], Kristy L. Mardis[3], and Vladimir Dyakonov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg and ZAE Bayern, 97074 Würzburg — [2]Chemical Sciences and Engineering Division, ANL, Argonne, Illinois 60439, USA — [3]Department of Chemistry and Physics, Chicago State University, Chicago, Illinois 60628, USA

To increase performance of organic solar cells, the optimization of the electron-accepting fullerenes has received less attention. Here, we report an electronic structure study of a novel covalently linked C_{60}-C_{70}-heterodimer in blend with the polymer PCDTBT. Upon optical excitation of polymer:heterodimer solid films, the electron is shared between both C_{60} and C_{70} cages. In contrast, in the solution the electron is localized on one half of the dimer. Electronic structure calculations reveal that for the heterodimer two nearly iso-energetic minima exist, essentially the cis and trans conformers. These conformers have different edge-to-edge distance between the two cages and therefor the

electron is either shared between two dimer halves (cis) or localized on one half of the heterodimer (trans). By comparison with the experimental data, we conclude that the cis conformation is preferable in films, and the trans conformation in solution. These findings demonstrate how electronic coupling of the fullerene acceptor molecules is influenced by their packing in blends, which may have an impact on the charge carrier generation efficiency in solar cells.

15 min. break

HL 61.7 Wed 11:15 ZEU 260

Cyclic potential growth mechanism for electropolymerized polythiophenes as anode buffer layers in P3HT-PCBM solar cells — •Sidhant Bom, Marlis Ortel, and Veit Wagner — Research Center for Functional Materials and Nanomolecular Science, Jacobs University, Bremen, Germany

A new method for electro-polymerization of polythiophenes as anode buffer layer (ABL) is presented. The ABL is used in a bulk-heterojunction solar cell with P3HT-PCBM as active material. Electro-polymerized thiophenes (ePT) are grown electrochemically with a standard three electrodes system on conductive contacts. We find a distinct impact of the time variation of the growth potential on the obtained layer properties. A new time dependent cyclic potential electro-polymerization method is systematically compared to a standard constant potential method. AFM topography reveals that a uniform homogeneous film of ePT is obtained by the time dependent cyclic potential growth method. The devices were fabricated with a 10 nm ePT between the active layer and PEDOT:PSS with aluminum as cathode. With a cyclic potential method, about 20% enhancement in short circuit current was observed in contrast to 10% enhancement with constant potential method. Improvements by the ePT layer are attributed to better band alignment of the HOMO levels and a LUMO offset of 0.2eV which gives its electron blocking characteristics. In summary, the cyclic potential method results in a better quality of ePT layers with good homogeneity and area coverage leading to further improvements in device performance.

HL 61.8 Wed 11:30 ZEU 260

Intrinsic charge carrier mobility in PCDTBT:$PC_{71}BM$ blend thin films investigated by simultaneous transient absorption and transient microwave conductivity measurements — •Andreas Fritze[1], Jeremias Weinrich[1], Vladimir Dyakonov[1,2], and Carsten Deibel[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

PCDTBT is a promising low-bandgap polymer for photovoltaic applications that has demonstrated unique recombination dynamics compared to the model P3HT system. Usually, the recombination dynamics in organics blends is expected to be proportional to the macroscopic charge carrier mobility, which is influenced by trapping and therefore potentially depends on the charge carrier concentration. For PCDTBT blends, we want to determine if the recombination dynamics are indeed governed exclusively by the low macroscopic mobility or if it is dominated by the, high local mobility. Therefor, we performed simultaneous measurements of transient absorption (TAS) and transient microwave conductivity on PCDTBT:$PC_{71}BM$ thin films on a 10 ns to 1 ms time scale. TAS probes the charge carrier density, whereas the microwave experiment is sensitive to the intrinsic, high frequency conductivity. By investigating the charge carrier dynamics and conductivity at different laser pump intensities and temperatures, we can separate the effects of mobility relaxation from carrier concentration dependent mobility in order to understand the dominant loss mechanism in organic solar cells.

HL 61.9 Wed 11:45 ZEU 260

On the role of the effectiv mass, ground state complexes and interfacial dipoles on exciton dissocitation in organic donor-acceptor systems — •Anna Köhler — University of Bayreuth, Bayreuth, Germany

Efficient exciton dissociation at a donor-acceptor interface is a necessary condition for obtaining high efficiency polymeric solar cells. Despite its importance, this step is still not fully understood. A central question is how and why, after photoexcitation of the donor and transfer of an electron onto the acceptor, the the e-h pair can overcome their considerable mutual Coulomb potential. Possibilities that are currently discussed include the degree of delocalization of both an exciton and a charge in a conjugated polymer, ground state charge transfer complexes as well as interfacial dipoles that may exist at the donor-acceptor interface in the ground state, and the degree of energetic and structural order/disorder. In this talk I will show how we combine insight gained from ultrafast pump-probe spectroscopy, field dependent photocurrent measurements, photoemission measurements and modeling to assess which factors control the dissociation process.

HL 61.10 Wed 12:00 ZEU 260

Non-photochemical self-quenching mechanism in conjugated polymers revealed by control of chain length and morphology — •Florian Steiner, Jan Vogelsang, and John M. Lupton — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D- 93040 Regensburg

Unraveling the complex photophysics of multichromophoric systems like conjugated polymers (CPs) is an ongoing interdisciplinary task. Some of the pressing questions in CP photophysics are: (i) what unit absorbs and emits the light in a CP? (ii) What processes take place between the absorption and emission event? And (iii) what is the interplay between excitation energy transfer between chromophores and non-radiative fluorescence decay? Answering these questions will lead to a fundamental understanding of the photophysics of CPs, which in turn can highlight important loss mechanisms regarding the efficiency in CP-based devices, such as self-quenching.

We illustrate that control of size and morphology in combination with several single-molecule techniques leads to a universal picture of the self-quenching mechanism in CPs by addressing these questions. As a model system we chose the device-relevant prototypical CP poly(3-hexylthiophene). Morphological control, combined with well-defined sub-populations of different sizes, enabled us to correlate a diverse set of photophysical observables (brightness, emission polarization, emission spectra, photon antibunching) with each other and the size. Finally, the increasing fluorescence self-quenching with size and morphological order is rationalized with a comprehensive photophysical model.

HL 61.11 Wed 12:15 ZEU 260

Conformations and electronic structure of Oligo-PPEs Investigated by Pulsed Electron Paramagnetic Resonance Spectroscopy — Patrick Korf, Friederike Schütze, Christian Hintze, Stefan Mecking, and •Malte Drescher — Department of Chemistry, University of Konstanz, Germany

Poly(para-phenyleneethynylene)s (PPE) are versatile polymers that are synthetically easily accessible.

Owing to their application in organic electronics and cell microscopy their microscopic and electronic properties are of high interest.

Herein we report the investigation of the electronic structure including the photo-excited triplet state of rod-like Oligo-PPEs. The lifetime, relaxation rates and populations of the triplet sublevels are quantitatively analyzed at cryogenic temperatures in a glassy toluene matrix via time-resolved EPR with synchronized UV laser flash excitation. The photo-physical properties are studied depending on the size of the delocalized π-electron system by varying the number of repeat units in the Oligo-PPEs.

In addition, their microscopic material properties are studied in particles with confined size constituted by block coplymers of PEGylated Oligo-PPEs. The molecular conformation is investigated by EPR distance measurements in solution, in bulk material as well as in particles. The data suggest that the rod-like Oligo-PPEs are present in a collapsed state in the particles.

HL 61.12 Wed 12:30 ZEU 260

Structural and electrical characterization of Hex-5T-Hex oligothiophene thin films during film formation — •Eduard Mikayelyan[1], Linda Grodd[1], Ullrich Pietsch[1], Artem. V. Bakirov[2], Maxim. A. Shcherbina[2], Sergei N. Chvalun[2], and Souren Grigorian[1] — [1]University of Siegen — [2]Enikolopov Institute of Synthetic Polymeric Materials of Russian Academy of Sciences

Organic semiconductors are attractive for electronics due to the low cost processing methods and their high electrical conductivity. Thiophene based polymers and oligomers are demonstrating relatively high mobility, excellent luminescence properties which used for application in solar cells, radio-frequency identification, etc. [1, 2]. We have investigated the thiophene based oligomer Hex-5T-Hex. Structural characterization has been performed by grazing incidence x-ray diffraction (GIXD)method, in particular we probed the crystallite orientations in prefabricated thin films. The 3D structure of Hex-5T-Hex

oligomer evaluated from the in-plane (010), (020) and (021) reflections is consistent with 2D structure suggested from 5T based oligomer self-assembled monolayer (SAM) [3]. Additionally, we found the (100) and (100)' reflections in out-of-plane direction characterizing two different stacking along thiophene backbone axis. In order to correlate the structural properties of oligothiophene thin films with the electrical characteristics both properties were probed simultaneous during film formation. This work was supported by BMBF, project number 05K10PSC.

HL 62: Spintronics I (with MA/O/TT)

Time: Wednesday 10:15–12:00 Location: POT 006

HL 62.1 Wed 10:15 POT 006

Spin dynamics on the metallic side of the metal to insulator transition — •Jan G. Lonnemann, Kim Niewerth, Jens Hübner, and Michael Oestreich — Leibniz Universität Hannover - Abteilung Nanostrukturen, Hannover, Germany

Several theoretical works treat the spin dynamics in zinc-blende semiconductors, like GaAs, around the metal-to-insulator transition. Most of them fail to explain the extremely long lifetimes experimentally observed [1]. Recently, it was argued that the Dyakonov-Perel mechanism (DP), usually only applicable in the conduction band, can be extended towards hopping transport (HT) present in the impurity band [2]. The theoretical calculations predict a dependence on the carrier density differing strongly from the DP spin relaxation expected for the conduction band electrons. We present extremely low excitation Hanle depolarization measurements on precisely n-doped MBE grown samples in the range of carrier concentrations from 2 to $10 * 10^{16}\,\mathrm{cm}^{-3}$. The density dependence of the spin lifetimes extracted from our measurements indicates that the dephasing due to HT is not the dominant mechanism. Remarkably, there is no significant difference in the spin lifetimes obtained from measurements on MBE material, with extremely low compensation ratios, as compared with samples from commercial wafers. This further indicates that dephasing due to HT is not the dominant mechanism, since HT depends strongly on the compensation ratio.

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

HL 62.2 Wed 10:30 POT 006

Nanomechanical read-out and manipulation of a single spin — •Heng Wang and Guido Burkard — University of Konstanz, Department of Physics

The single electron spin in quantum dot is a promising candidate as a qubit for quantum computation and quantum information. We investigate detection as well as manipulation of the single spin in a suspended carbon nanotube quantum dot. The detection and the manipulation are based on the spin-mechanical coupling induced from the intrinsic spin-orbit coupling. We use a Jaynes-Cummings model with a quantized flexural mode of the resonator to describe the system. An external electric field is used to drive the resonator and to induce an the interaction between the single electron in the quantum dot and the external driving field. The spin states can be identified by measuring the mechanical motion of the nanotube, which is detected by observing the current through a nearby charge sensor. Arbitrary-angle rotations about arbitrary axes of the single electron spin can be achieved by varying the frequency and the strength of the external electric driving field.

HL 62.3 Wed 10:45 POT 006

Time-resolved electrical detection of the inverse spin Hall Effect after ps optical excitation — •Manfred Ersfeld[1], Ivan Stepanov[1], Sammy Pissinger[1], Christopher Franzen[1], Sebastian Kuhlen[1], Mihail Lepsa[2], and Bernd Beschoten[1] — [1]2nd Institute of Physics, RWTH Aachen University, Germany — [2]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich GmbH, Germany

Electrical detection of spin currents give an insight into the microscopic mechanisms of spin transport and play an important role in spin electronics. In previous experiments spin currents due to spin Hall effect have been imaged in optical measurements as spin accumulation.[1]

Here we report on the first time-resolved electrical detection of spin precession in n-InGaAs in time-resolved measurements of the inverse spin Hall effect. Net spin currents are achieved by applying electric fields and by polarization of the electrons with circularly polarized picosecond laser pulses. Electron spin precession in an external magnetic field can be monitored using a phase-triggered sampling oscilloscope as an oscillating voltage perpendicular to the applied electric field. Temperature dependent measurements of the spin Hall effect are presented. Time-resolved Faraday rotation measurements on the same sample under identical experimental conditions show good agreement between the measured spin dephasing times and the g-factor in the spin Hall measurements.

This Work has been supported by DFG through FOR 912

[1] Y. K. Kato et al., Science 306, 1910 (2004)

HL 62.4 Wed 11:00 POT 006

Terahertz out-of-plane resonances due to spin-orbit coupling — •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

A microscopic kinetic theory is developed which allows to investigate non-Abelian SU(2) systems interacting with mean fields and spin-orbit coupling under magnetic fields in one, two, and three dimensions. The coupled kinetic equations for the scalar and spin components are presented and linearized with respect to an external electric field. The dynamical classical and quantum Hall effect are described in this way as well as the anomalous Hall effect for which a new symmetric dynamical contribution to the conductivity is presented. The coupled density and spin response functions to an electric field are derived including arbitrary magnetic fields. The magnetic field induces a staircase structure at frequencies of the Landau levels. It is found that for linear Dresselhaus and Rashba spin-orbit coupling a dynamical out-of-plane spin response appears at these Landau level frequencies establishing terahertz resonances. (EPL, 104 (2013) 2700)

HL 62.5 Wed 11:15 POT 006

Resonant spin amplification in intrinsic bulk germanium — •Jan Lohrenz, Timo Paschen, and Markus Betz — Experimentelle Physik 2, TU Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund

Recent experiments have revealed the possibility to optically orient electron spins in bulk germanium via indirect optical transitions. However, the temporal limitations to both the spin lifetime and the coherence of photogenerated electrons have remained unexplored so far. Here we demonstrate resonant spin amplification in intrinsic bulk germanium using a 90 MHz femtosecond pulse train at 0.8 eV central photon energy. Most importantly, we find remarkably long spin lifetimes exceeding 50 ns at temperatures of up to 60 K, limited by Elliott Yafet type processes. Consistent with model simulations we also find pronounced signatures of the g-factor anisotropy in germanium in the resonant spin amplification data.

HL 62.6 Wed 11:30 POT 006

Ultrahigh Bandwidth Spin Noise Spectroscopy — •Fabian Berski, Hendrik Kuhn, Jan G. Lonnemann, Jens Hübner, and Michael Oestreich — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany

We advance all optical spin noise spectroscopy (SNS) in semiconductors to detection bandwidths of several hundred gigahertz by employing a sophisticated scheme of pulse trains from ultrafast laser oscillators as an optical probe [1]. The ultrafast SNS technique avoids the need for optical pumping and enables nearly perturbation free measurements of extremely short spin dephasing times. We apply the technique to highly-n-doped bulk GaAs where magnetic field dependent measurements show unexpected large g-factor fluctuations. Calculations suggest that such large g-factor fluctuations do not necessarily result from extrinsic sample variations but are intrinsically present in every doped semiconductor due to the stochastic nature of the dopant distribution.

[1] Berski, F., et al., Phys. Rev. Lett. **111**, 186602 (2013).

HL 62.7 Wed 11:45 POT 006

Effect of Nuclear Quadrupole Moments on Electron Spin Coherence in Semiconductor Quantum Dots — •Erik Welander[1], Evgeny Chekhovich[2], Alexander Tartakovskii[2], and Guido Burkard[1] — [1]Department of Physics, University of Konstanz, Germany — [2]Department of Physics and Astronomy, University of Sheffield, United Kingdom

We theoretically investigate the influence of the fluctuating Overhauser field on the spin of an electron confined to a quantum dot. The fluctuations arise from nuclear spin being exchanged between different nuclei via the nuclear magnetic dipole coupling. We focus on the role of the nuclear interaction from electric quadrupole moments (QPM), which generally cause a reduction in internuclear spin transfer efficiency. By dividing the nuclear problem into subcells we are able to describe $10^4 - 10^5$ nuclei, which are realistic numbers for a quantum dot. The effects on the electron spin coherence time are studied by modeling an electron spin echo experiment. We find that the QPM cause an increase in the electron spin coherence time and that an inhomogeneous distribution, where different nuclei have different QPM, causes an even larger increase than a homogeneous distribution.

HL 63: Invited Talk Axel Hoffmann

Time: Wednesday 12:00–12:30 Location: POT 006

Invited Talk HL 63.1 Wed 12:00 POT 006

Exciton-phonon coupling in nitride-based nanostructures — G. Callsen[1], G. Hönig[1], S. Kalinowski[1], J. Settke[1], C. Kindel[1], J. Brunnmeier[1], T. Markurt[2], M. Albrecht[2], S. Kako[3], A. Schliwa[1], Y. Arakawa[3], and •A. Hoffmann[1] — [1]Technical University of Berlin, 10623 Berlin, Germany — [2]Leibniz Institute for Crystal Growth (IKZ), 12489 Berlin, Germany — [3]University of Tokyo, Tokyo 153-8505, Japan

We review the exciton-phonon coupling in nitride-based nanostructures such as e.g. GaN/AlN quantum dots (QDs). Generally, nanostructures based on strongly polar group III-nitrides represent ideal candidates for analyzing the exciton-phonon interaction in contrast to only weakly polar materials as e.g. the group III-arsenides. Occurring large excitonic dipole moments inherent to nitride QDs facilitate an efficient coupling to acoustical and optical phonons, clearly observable in μPhotoluminescence spectra. We reveal a strong QD size and geometry dependence of the Huang-Rhys factor, as a measure of the exciton-LO-phonon coupling strength, and the LO-phonon energy, based on a unique conjunction of experimental and theoretical results. The given observation can be regarded as general phenomena in strongly polar nanostructured materials and highlight current limitations in regard to applications at non-cryogenic temperatures.

HL 64: Frontiers of electronic structure theory - Non-equilibrium phenomena at the nano-scale IV (organized by O)

Time: Wednesday 10:30–13:15 Location: TRE Ma

Topical Talk HL 64.1 Wed 10:30 TRE Ma

From Rydberg Crystals to Bound Magnons - Probing the Non-Equilibrium Dynamics of Ultracold Atoms in Optical Lattices — •Immanuel Bloch — Max-Planck Institut für Quantenoptik, Garching, Germany — Ludwig-Maximilians-Universität, Munich, Germany

Ultracold atoms in optical lattice form an ideal testbed to probe the non-equilibrium dynamics of quantum many-body systems. In particular recent high-resolution imaging and control techniques allow to probe dynamically evolving non-local correlations in an unprecedented way. As an example, I will focus in my talk on the dynamical excitation of spatially ordered Rydberg structures that are formed through laser exctiation from ground state Mott insulating atoms. In addition, I will show how single-spin and spin-pair impuritites can be used to directly reveal polaron dynamics in a strongy interacting superfluid or the bound state of two magnons in a Heisenberg ferromagnet - a problem discussed first theoretically more than 80 years ago by H.A. Bethe. New atom interferometric schemes to directly probe the Green's function of a many-body system through the impurity dynamics will be discussed.

HL 64.2 Wed 11:00 TRE Ma

Correlated Light-Matter Interactions in Cavity QED — •Johannes Flick[1], Heiko Appel[1], and Angel Rubio[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

In the electronic structure community, the quantized nature of the electrons is usually (approximately) incorporated, whereas the electromagnetic field is mostly treated classically. In contrast, in quantum optics, matter is typically simplified to models with a few levels, while the quantized nature of light is fully explored. In this work, we aim at treating both, matter and light, on an equal quantized footing.
We present exact solutions for fully quantized prototype systems consisting of atoms or molecules placed in optical one- or two-dimensional high-Q cavities and coupled to the quantized electromagnetic modes in the dipole or quadrupole coupling regime. We focus on spontaneous emission, strong-coupling phenomena, dipole-dipole couplings including van-der-Waals interactions, and Förster resonance energy transfer (FRET), all beyond the rotating-wave approximation. This work has implications for a future development of a time-dependent density functional theory formulation of QED [1,2] for correlated multi-photon configurations.

[1] M. Ruggenthaler, F. Mackenroth, and D. Bauer, Phys. Rev. A **84**, 042107 (2011).
[2] I. Tolkatly, Phys. Rev. Lett. **110**, 233001 (2013).

HL 64.3 Wed 11:15 TRE Ma

Optimized effective potential approach to time-dependent density functional theory for many-electron systems interacting with cavity photons — •Camilla Pellegrini[1], Johannes Flick[2], Heiko Appel[2], Ilya V. Tokatly[1,3], and Angel Rubio[1,2] — [1]Nano-bio Spectroscopy Group and ETSF Scientific Development Centre, Departamento de Física de Materiales, Universidad del País Vasco UPV/EHU, E-20018 San Sebastían, Spain — [2]Fritz-Haber Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany — [3]IKERBASQUE, Bilbao, Spain

In a recent paper [1] time dependent density functional theory has been generalized to many-electron systems strongly coupled to quantum electromagnetic modes of a microcavity. Here we construct an approximation for the corresponding exchange-correlation (xc) potential by extending the optimized effective potential (OEP) method to the electron-photon system. The derivation of the OEP equation employing the non-equilibrium Green's function formalism, and the first order approximation for the electronic self-energy is presented. Beyond the mean field level, the electron-photon coupling generates a time non-local photon-mediated interaction between the electrons, whose propagator enters the exchange-like diagram. We further show the approximated xc-potential for a model two-level diatomic molecule with one electron coupled to photon modes. The comparison between the obtained results and the exact numerical ones in the different coupling regimes (from weak up to ultra-strong) is discussed. [1] I.V. Tokatly, Phys. Rev. Lett. 110, 233001(2013)

HL 64.4 Wed 11:30 TRE Ma

Correlated photon-electron wavefunctions in cavity Quantum Electrodynamics — •Heiko Appel[1], Johannes Flick[1], Rene Jestaedt[1], and Angel Rubio[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

Experimental progress in recent years has enabled the fabrication of Fabry-Perot resonators with high optical quality factors (high-Q). Such cavities allow to study the interaction of matter with a quantized light field at the single-photon level (Nobel prize 2012). In this talk we present the real-time evolution of correlated photon-electron wavefunctions in optical one- and two-dimensional high-Q cavities. We discuss implications for a multi-component density functional theory for Quantum Electrodynamics [1,2] based on the time-dependent electron density and the photon energy density.

[1] M. Ruggenthaler, F. Mackenroth, and D. Bauer, Phys. Rev. A **84**, 042107 (2011).
[2] I. Tolkatly, Phys. Rev. Lett. **110**, 233001 (2013).

HL 64.5 Wed 11:45 TRE Ma

Photoelectron driven plasmaron excitations in (2x2)K/Graphite — •Bo Hellsing — Department of Physics, Gothenburg University, Sweden

A new type of plasmarons formed by the compound of photoelec- trons and acoustic surface plasmon (ASP) excitations is investigated in the system p(2 * 2)-K/Graphite. The physics behind these types of plasmarons, e-plasmarons, is different from the ones re- cently found in graphene and quantum well systems, where the loss features results from the photohole-plasmon interaction in the material, h-plasmarons. Based on the first principles scheme, Time dependent density functional (TDDFT), we calculated the linear response due to the presence of the escaping photo-electron and determine the ASP dispersion. The coupling between the photoelectron and the ASP gives rise to excitation of the e- plasmarons manifested by a broad dispersive feature shifted about 0.5 eV below parabolic K induced quantum well band (QWB) in agreement with the ARPES experiment by Agdal et al. The e-plasmarons should be considered as a source of the loss satellite structure in ARPES for 2D systems. In addition they are important to take into account in theoretical studies of different compounds as they reflect an additional channel for excitations of plasmons. This could then increase the photon-plasmon conversion yield which obviously is of interest in the field of plasmonics.

HL 64.6 Wed 12:00 TRE Ma

Charge-transfer excitations in organic systems from many-body perturbation theory — •Xavier Blase[1], Carina Faber[1,2], Paul Boulanger[1], Claudio Attaccalite[1], and Ivan Duchemin[2] — [1]Institut Néel, CNRS and UJF, Grenoble, France — [2]L_SIM/INAC, CEA, Grenoble, France

Charge-transfer excitations in organic systems lies at the heart of a large variety of physical phenomena, from photosynthesis to photovoltaics, photocatalysis or DNA denaturation. From a theoretical point of view, such nonlocal excitations are well known to lead to difficulties within the TDDFT framework, leading to the development of range-separated hybrids. We present here the merits of the Bethe-Salpeter formalism and demonstrate its ability to reproduce *cold* and *hot* Frenkel or charge-transfer excitations with remarkable accuracy [1-3]. Our calculations are based on a recent Gaussian basis implementation of the GW and Bethe-Salpeter formalism, the Fiesta initiative [1-4], allowing all-electron or pseudopotential excited states calculations for systems comprising several hundred atoms. Recent developments towards discrete and continuous embedding techniques within the many-body perturbation framework will be presented.

References: [1] C. Faber, I. Duchemin, T. Deutsch, X. Blase, Phys. Rev. B, 86, 155315 (2012). [2] I. Duchemin, T. Deutsch, X. Blase, Phys. Rev. Lett. 109, 167801 (2012). [3] I. Duchemin and X. Blase, Phys. Rev. B 87, 245412 (2013). [4] X. Blase, C. Attaccalite, V. Olevano, Phys. Rev. B 83, 115103 (2011).

HL 64.7 Wed 12:15 TRE Ma

Charge transfer from first principles: self-consistent *GW* applied to donor-acceptor systems — •Fabio Caruso[1,2], Viktor Atalla[1], Angel Rubio[1,3], Matthias Scheffler[1], and Patrick Rinke[1] — [1]Fritz Haber Institute, Berlin, Germany — [2]University of Oxford, UK — [3]Universidad del País Vasco, San Sebastián, Spain

Charge transfer in donor-acceptor systems (DAS) is determined by the relative alignment between the frontier orbitals of the donor and the acceptor. Semi-local approximations to density functional theory (DFT) may give a qualitatively wrong level alignment in DAS, if the ionisation potential of one molecule erroneously ends up above the electron affinity of the other. An unphysical fractional electron transfer will then result in weakly interacting DAS [1]. *GW* calculations based on first-order perturbation theory (G_0W_0) correct the level alignment. However, the ground state is unaffected by the G_0W_0 approach, and the charge-transfer properties remain on the level of the initial DFT calculation [1]. We demonstrate that self-consistent *GW* (sc*GW*) – based on the iterative solution of the Dyson's equation – provides an ideal framework for the description of charge transfer in DAS. The sc*GW* level alignment is in agreement with experimental reference data. In addition ground- and excited-state properties are described at the same level of theory. As a result, the electron density in DAS is consistent with the level alignment between donor and acceptor, leading to a qualitatively correct description of charge-transfer properties.

[1] V. Atalla, M. Yoon, F. Caruso, P. Rinke, and M. Scheffler, Phys. Rev. B **88**, 165122 (2013).

HL 64.8 Wed 12:30 TRE Ma

What Koopmans' compliant orbital-density dependent functionals can do for you: a comprehensive benchmark of the G2-set — •Giovanni Borghi[1], Ngoc Linh Nguyen[1], Andrea Ferretti[2], Ismaila Dabo[3], and Nicola Marzari[1] — [1]École Polytechnique Fédérale de Lausanne, Lausanne (VD), CH — [2]Centro S3, CNR–NANO, Modena, IT — [3]Department of Materials Science and Engineering, Penn State University, University Park (PA), USA

In this talk we present the results of benchmark calculations of the structure and electronic-structure of all molecules in the g2 set, using different flavours for Koopmans' compliant (KC) functionals. Results are compared not only to LDA and PBE, but also to orbital-density dependent calculations with the Perdew-Zunger self-interaction correction.

Our results assess the accuracy of Koopmans' compliant functionals in improving semilocal functionals to predict electronic eigenvalues and in particular ionization energies, with an accuracy that for molecules seems to be comparable or superior to that of many-body (GW) approaches. We also highlight how the Koopmans' condition tends to preserve the potential energy surface of the underlying functional, with higher reliability than e.g. PBE in structural predictions, while also providing good estimates of atomization energies.

The talk will also provide a general introduction to the theory of Koopmans' compliant functionals and their implementation in existing electronic structure codes.

Ref. Dabo *et al.*, PRB 82, 115121 (2010), and Psik highlight (2012).

HL 64.9 Wed 12:45 TRE Ma

The electronic structure of quinacridone: Optimally tuned range-separated hybrid functional versus GW results — Daniel Lüftner[1], Sivan Refaely-Abramson[2], Michael Pachler[1], Michael G. Ramsey[1], Leeor Kronik[2], and •Peter Puschnig[1] — [1]Institut für Physik, Karl-Franzens-Universität Graz, Austria — [2]Department of Materials and Interfaces, Weizmann Institute of Science, Israel

Quinacridone is an organic molecule (C20H12N2O2) utilized in the formation of organic pigments. It has also been discussed for usage in organic electronics particularly due to its stability under ambient conditions and its tendency to form self-assembled supramolecular networks. Here, we report on its electronic structure, both, for the isolated molecule as well as for the alpha- and beta- bulk molecular crystal polymorphs. We employ an optimally tuned range-separated hybrid functional (OT-RSH) within density functional theory as well as GW corrections within a many-body perturbation theory framework. A comparison of the theoretical results obtained with the different levels of theory and a subsequent comparison with experimental data from angle-resolved photoemission spectroscopy emphasize the need for going beyond simple semi-local DFT-functionals in order to obtain the correct orbital ordering. Furthermore the comparison indicates that the results obtained with OT-RSH greatly improve those of standard DFT functionals and achieve an agreement with experiment at the level of GW calculations, thus making the OT-RSH an alternative to the computationally more expensive GW approach.

HL 64.10 Wed 13:00 TRE Ma

GW many-body perturbation theory for electron-phonon coupling calculations — •Carina Faber[1,2], Paul Boulanger[1], Ivan Duchemin[1,2], and Xavier Blase[1] — [1]Institut Néel, CNRS, Grenoble, France — [2]INAC, CEA, Grenoble, France

We study within many-body perturbation theory the electron-phonon coupling in organic systems, taking as paradigmatic examples the fullerene molecule and the pentacene crystal [1,2]. We show that the

strength of the electron-phonon coupling potential is dramatically underestimated at the LDA level, while GW calculations offer an excellent agreement with experiments [1]. Further, combining GW calculations of the electronic band structure and of the electron-phonon coupling in crystalline pentacene, we show that the hole bands dispersion can be reconciled with photoemission experiments, by solving non-perturbatively (DMFT) the effect of electron-phonon coupling on the electronic self-energy [2]. We finally explore various approximations that may allow to combine the GW formalism with convenient linear response formalisms beyond the frozen-phonon techniques. Our calculations are performed with the Fiesta package, a Gaussian based GW and Bethe-Salpeter code allowing all-electron or pseudopotential calculations with various resolution of the identity techniques and without any plasmon pole approximation [3,4].

[1] C. Faber et al., Phys. Rev. B 84, 155104 (2011) [2] S. Ciuchi et al., Phys. Rev. Lett. 108, 256401 (2012) [3] C. Faber, I. Duchemin, T. Deutsch, X. Blase, Phys. Rev. B, 86, 155315 (2012). [4] I. Duchemin, T. Deutsch, X. Blase, Phys. Rev. Lett. 109, 167801 (2012).

HL 65: Devices

Time: Wednesday 11:30–13:15 Location: POT 151

HL 65.1 Wed 11:30 POT 151

Influence of Charge Trapping on Memory Characteristics of Si:HfO2-Based Ferroelectric Field Effect Transistors — •Milan Pešić[1], Stefan Mueller[1], Stefan Slesazeck[1], Alban Zaka[2], Tom Herrmann[2], Ekaterina Yurchuk[1], Uwe Schröder[1], and Thomas Mikolajick[1] — [1]NaMLab gGmbH / * IHM TU Dresden, Dresden, Germany — [2]GLOBALFOUNDRIES Dresden Module One LLC & Co. KG, Dresden, Germany

The Ferroelectric field effect transistors (FeFET) devices have never reached maturity due to limited scalability, low retention and CMOS incompatibility. Only recently, these obstacles seem to have been resolved by the discovery of ferroelectric properties in silicon doped hafnium dioxide (Si:HfO2). This concept proven that possess the potential of realizing highly-scaled ultra low-power memory cells.

One of the main challenges in Si:HfO2 FeFET implementation is the memory window degradation caused by charge trapping effects. In order to analyze the interplay between ferroelectric switching and parasitic charge trapping, a FeFET model including nonlocal tunneling, charge trapping and ferroelectric switching effects was implemented in TCAD Sentaurus Device.

The charge trapping model was qualitatively calibrated based on electrical characterization of Si:HfO2-FeFETs fabricated on a 28 nm bulk technology. From the characterization results, simulation parameters were extracted. In our study we present how bulk traps inside the ferroelectric (Si:HfO2) as well as interface traps at the SiO2 / silicon bulk substrate interfere with the ferroelectric memory characteristics.

HL 65.2 Wed 11:45 POT 151

Non-volatile capacitance change in BiFeO3-coated photocapacitive MIS diodes — •l p Selvaraj[1], t You[1], v John[1], h Zeng[2], d Bürger[1], i Skorupa[1], a Lawerenz[3], o g Schmidt[1,4], and h Schmidt[1] — [1]Faculty of Electrical Engineering and Information Technology, Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]State Key Laboratory of Electronic Thin Films and Integrated Devices, University of Electronic Science and Technology of China, 610054 Chengdu, China — [3]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik GmbH, 99099 Erfurt, Germany — [4]Institute for Integrative Nanosciences, IFW Dresden, 01069 Dresden, Germany

Metal-BiFeO3-metal thin film structures can be switched between a high resistance state (HRS) and a low resistance state (LRS), when a positive and negative writing bias is applied, respectively. The current investigation deals with the effect of light-irradiation on the capacitance of BiFeO3-coated metal-insulator-semiconductor (MIS) diodes. N-type conducting BiFeO3 thin films of nominal thickness 70, 140, 210, 280, 350 and 490 nm have been grown by pulsed laser deposition on p-type silicon wafers substrates having an 163 nm thick SiN layer. The DC bias for the capacitance measurements was swept from +10 V to -15 V and back under different light-irradiation at a sweep rate of ca. 59 mV/s. It has been found that under dark conditions two nonvolatile capacitance minima can be found at -3.8 V and at -6.8 V possibly when the BiFeO3 is in the HRS and LRS state, respectively. The retention measurement result shows non-volatile memory in capacitance which can be used for photocapacitive detectors.

HL 65.3 Wed 12:00 POT 151

RF- and DC Characterization of the High-k to InGaAs Interface in Gate Last nMOSFETs — •Guntrade Roll, Mikael Egard, Sofia Johansson, Erik Lind, and Lars-Erik Wernersson — EIT, Lund University, Lund, Sweden

InGaAs MOSFETs are a promising candidate for low power and high-frequency application. Due to high-injection velocity and mobility it is possible to reach high on-currents at low source/drain voltages. An improved high-k to channel interface quality and low source/drain resistance are challenges currently under research. We have developed a gate last nMOSFET process flow, which gives an excellent extrinsic transconductance of 1.9mS/μm (L_G=55nm) and a source/drain resistance of 199Ω/μm. The presentation will focus on the evaluation of $InGaAs/Al_2O_3/HfO_2$ interface quality, using RF and DC characteristics. A hopping gate leakage via defects to the transistor raised source/drain is observed. Prestress border defects are filled by trapping when the transistor is turned on. This leads to a transconductance frequency dispersion and current-voltage hysteresis. Reliability is a key issue for all future technologies. The degradation after constant gate stress and hot carrier stress is analyzed. The border trap density is increased by constant gate stress. The threshold bias shift due to trapping is the main reliability problem, which has to be overcome by further improving the high-k processing.

HL 65.4 Wed 12:15 POT 151

Subnanosecond relaxation of free carriers in compensated n- and p-type germanium — •Nils Dessmann[1], Sergey Pavlov[2], Valery Shastin[3], Roman Zhukavin[3], Veniamin Tsyplenkov[3], Stephan Winnerl[4], Martin Mittendorff[5], Nikolai Abrosimov[6], Helge Riemann[6], and Heinz-Wilhelm Hübers[1,2] — [1]Technische Universität Berlin, Berlin, Deutschland — [2]Deutsches Zentrum für Luft- und Raumfahrt, Berlin, Deutschland — [3]Institute for Physics of Microstructures, Nizhny Novgorod, Russland — [4]Helmholtz-Zentrum Dresden-Rossendorf, Dresden-Rossendorf, Deutschland — [5]Technische Universität Dresden, Dresden, Deutschland — [6]Leibniz-Institut für Kristallzüchtung, Berlin, Deutschland

The relaxation of free holes and electrons in highly compensated germanium doped with gallium (p-Ge:Ga:Sb) and antimony (n-Ge:Sb:Ga) has been studied by a pump-probe experiment with the free-electron laser FELBE at the Helmholtz-Zentrum Dresden-Rossendorf. The relaxation times vary between 20 ps and 300 ps and depend on the incident THz intensity and compensation level. The relaxation times are about five times shorter than previously obtained for uncompensated n-Ge:Sb and p-Ge:Ga. The results support the development of fast photoconductive detectors in the THz frequency range.

HL 65.5 Wed 12:30 POT 151

Nickel-related defects and their interaction with H in n- and p-type Si. — •Leopold Scheffler[1], Vladimir Kolkovsky[1], Philipp Saring[2], and Jörg Weber[1] — [1]Technische Universität Dresden, 01069 Dresden, Germany — [2]Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

In the present study we focus our attention on Ni-related defects in n- and p-type Si and investigate their interaction with H. Previously, three dominant deep level transient spectroscopy (DLTS) peaks with the activation energies of EC-0.08 eV (E45), EC-0.4 eV (E230) and EV+0.17 eV (H80) were assigned to the double acceptor, single acceptor and single donor states of substitutional Ni. [1,2] However, in our study the concentration profiles of E45 and E230 were found to be different both in samples with a nickel concentration of NNi ˜ 1x1013cm-3 and NNi ˜ 6x1013cm-3 as determined from E230. This observation suggests a different origin of the dominant DLTS peaks in Ni-doped Si. After wet chemical etching or a dc H plasma treatment a number of additional minor peaks appear in the DLTS spectra. We will show that these peaks are correlated with H and some of them could be assigned to NiH-related complexes. The origin of these defects will be discussed.

[1] M. Shiraishi, J.-U. Sachse, H. Lemke, and J. Weber, Mater. Sci. Eng. B 58, 130 (1999)
[2] H. Kitagawa and H. Nakashima, Jpn. J. Appl. Phys. 28, 305 (1989)

HL 65.6 Wed 12:45 POT 151

Brittle to Ductile transition in silicon nanopillars — •Anton Davydok[1], Thomas W. Cornelius[1], Zhe Ren[1], Francesca Mastropietro[1], Michael Texier[1], Christophe Tromas[2], Ludovic Thilly[2], Marie-Ingrid Richard[1,3], and Olivier Thomas[1] — [1]IM2NP, Marseille, France — [2]PPrime institute, Poitiers, France — [3]ID01 beamline, ESRF, Grenoble, France

In recent years, nanostructures attracted enormous attention due to novel properties which, are not observed for bulk materials. When the object size becomes comparable to intrinsic length scales, finite-size and quantum size effects occur influencing the physical properties. For instance, while bulk silicon is brittle at ambient conditions and ductile at elevated temperatures, Si nanopillars of sufficiently small diameter are ductile at room temperature. In this work, we report on studies of the brittle-to-ductile transition of Si nanopillars as a function of their diameter. Pillars of various sizes were fabricated by electron beam lithography on a Silicon-on-insulator wafer and mechanically deformed employing a nano-indenter. Their structure and defects induced by the deformation were investigated by electron microscopy as well as by micro- and nanofocused X-ray diffraction. In addition, preliminary finite-element method calculations will be presented.

HL 65.7 Wed 13:00 POT 151

The consecutive photoresponse performance of porous silicon carbide ultraviolet photodetectors — •Nima Naderi[1,2] and Md Roslan Hashim[2] — [1]Division of Semiconductors, Materials and Energy Research Center, Karaj, Iran — [2]Nano-Optoelectronics Research Laboratory, School of Physics, Universiti Sains Malaysia, Penang, Malaysia

This work reports on improvement in the optical and electrical properties of ultraviolet (UV) photodetectors based on porous silicon carbide (PSC). Porous samples were prepared through the optimization of the current density in the UV-assisted electrochemical etching of n-type silicon carbide (SiC) substrates. The current density can be considered an important parameter in controlling the etching rate and morphology of the porous samples. Thus, it can be used to enhance the optical properties of electrochemically etched PSC layers. Therefore, the electrical properties of PSC-based photodetectors such as response time and recovery time can be controlled by optimization of current density in the photoelectrochemical etching of SiC substrate.

HL 66: Quantum dots: Optical properties II (with TT)

Time: Wednesday 11:30–13:00 Location: POT 251

HL 66.1 Wed 11:30 POT 251

Revealing the local environment noise of a quantum dot through resonance fluorescence intensity statistics — •Megan Stanley, Clemens Matthiesen, and Mete Atatüre — Cavendish Laboratory, University of Cambridge, JJ Thomson Avenue, Cambridge CB3 0HE, UK

The electronic level structure and optical transitions of quantum dots are subject to fluctuating electric fields from nearby charge traps and a noisy Overhauser field from local nuclear spins [1]. The resultant inhomogeneous electron spin dephasing and reduced photon spectral purity are detrimental to the use of dots in quantum information processing [2]. We combine the intensity autocorrelation of resonance fluorescence (RF) and full photon counting statistics to capture the amplitudes and timescales of environment-induced fluctuations. Full counting statistics offer a robust and technically undemanding method to quantify steady-state spectral diffusion. In particular, it allows us to distinguish blinking or switching from continuous spectral shifts when this is not obvious from RF timetraces. Charge and nuclear spin contributions to noise are distinguished in autocorrelations via a detailed exploration of detuning and excitation power dependent sensitivities in comparison to a theoretical model. We find electric field noise to dominate down to timescales of 100us. Finally, we expose nuclear spin noise exclusively by decoupling the fluorescence from the electric field fluctuations using a two-colour noise compensation technique. [1] A. V. Kuhlmann et al., Nature Phys. 9, 570-575 (2013) [2] C. Santori et al., Nature 419, 594-597 (2002)

HL 66.2 Wed 11:45 POT 251

cQED-controlled anticorrelation between axial and lateral emission of quantum dot - micropillar cavities — •Caspar Hopfmann[1], Micha Strauss[2], Christian Schneider[2], Sven Höfling[2,3], Martin Kamp[2], Alfred Forchel[2], and Stephan Reitzenstein[1] — [1]Institute of Solid State Physics, Technische Universität Berlin, D-10623 Berlin, Germany — [2]Technische Physik, Universität Würzburg, D-97074 Würzburg, Germany — [3]University of St Andrews, North Haugh, KY16 9SS United Kingdom

Cavity quantum electrodynamics (cQED) in high quality quantum dot (QD) microcavities has been subject of extensive research interest in recent years. This includes the study of fundamental cavity effects in the weak and strong coupling regime as well as their application in non-classical light sources. Here, we present an advanced optical characterization method to obtain comprehensive insight into the relevant cQED effects in QD-micropillar cavities. In contrast to conventional approaches in which the micropillar is addressed only in axial direction via its top facet, we implement additionally an in-plane excitation and detection scheme. In this unique configuration, excitation and detection capabilities are available synchronously in the axial and in-plane direction which opens up appealing opportunities for a broad study of cQED effects. For instance, it allows one to investigate the interplay between coupling emission from the QDs into resonator modes and leaky modes, respectively. Indeed, we demonstrate a cQED-controlled anti-correlation between single-QD emission through the top facet via resonator modes and emission through the side-walls via leaky modes.

HL 66.3 Wed 12:00 POT 251

Stark shifts in single and vertically stacked GaAs QDs — •Arne Ungeheuer, Achim Küster, Andreas Graf, David Sonnenberg, Christian Heyn, and Wolfgang Hansen — Institut für Angewandte Physik, Universität Hamburg, 20355 Hamburg, Germany

We study the optical properties of single GaAs quantum dots (QDs) and quantum dot molecules (QDMs) in vertical electrical fields. The QDs and QDMs are fabricated using molecular beam epitaxy in combination with the local droplet etching (LDE) technique [1]. Using Al-droplets on AlGaAs substrates, nanoholes of some ten nanometers depth are drilled and subsequently filled with GaAs to form QDs or with a GaAs/AlGaAs/GaAs sequence to form QDMs. Here, we report on the electric field-dependent energy-shift of the excitonic states due to the quantum-confined Stark-effect. Using a Schottky-diode structure and a micro-photoluminescence setup we observe a red-shift up to 25 meV.
[1] D. Sonnenberg et al., Appl. Phys. Let. **101**, 183113 (2012)

HL 66.4 Wed 12:15 POT 251

Robust population inversion using an excitonic V-type three level system in a single InGaAs quantum dot — •Dirk Mantei[1], Jens Förstner[1], Simon Gordon[1], Yves Alexander Leier[1], Ashish Kumar Rai[2], 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. For instance they are used to realize quantum gates or single photon sources. 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. We experimentally demonstrate and theoretically describe this concept, which is based on the polarization-selective excitation of a fine structure split exciton ground state in a single InGaAs quantum.

HL 66.5 Wed 12:30 POT 251

Photocurrent spectroscopy of single InAs quantum dots at 1500 nm — •Simon Gordon[1], Matusala Yacob[2], Yves Alexander Leier[1], Dirk Mantei[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 high resolution 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 resonantly excited by a tunable single-frequency diode laser. By changing the applied reverse voltage the resonance energy of the quantum dot is tuned by the quantum confined Stark effect with respect to the laser line. We observe clear ground state absorption of single dots over a large tuning range in the photocurrent response. The highly resolved absorption lines show for the investigated samples no fine-structure splitting. This behavior could be caused by single electron charging, which leads to the decay of trions.

HL 66.6 Wed 12:45 POT 251

Excitons in InAs-quantum dots measured by capacitance-voltage spectroscopy — Patrick Labud, •Arne Ludwig, Andreas D. Wieck, and Dirk Reuter — Ruhr-Universität Bochum, Lehrstuhl für Angewandte Festkörperphysik

Electron-electron and hole-hole interaction has been studied intensively on self-assembled quantum dot (QD) samples using capacitance-voltage spectroscopy (C-V) since two decades. The energetic positions of the charging peaks are considerably affected by the Coulomb interaction energies and in standard C-V spectra only the Coulomb repulsion is seen.

In this contribution, we present C-V data obtained under nonresonant illumination from a light emitting diode. Under these conditions, additional charging peaks appear due to attractive Coulomb interaction between illumination induced holes and electrons, tunnelling into the QD.

We are able to resolve up to five additional charging peaks belonging to an X^0, X^{1+}, X^{2+}, X^{3+}, X^{4+}-complex, formed upon electron charging. The individual Coulomb energies are calculated from the charging gate voltage and the charging dynamics is discussed.

HL 67: Quantum information systems I (with MA/TT)

Time: Wednesday 15:00–16:30 Location: POT 006

HL 67.1 Wed 15:00 POT 006

Improving the efficiency of passive Hall effect circulator — •Giovanni Viola[1] and David DiVincenzo[1,2] — [1]Institute for Quantum Information , RWTH Aachen — [2]Department of Theoretical Nanoelectronics, Peter Gruenberg Institute, Forschungszentrum Juelich

Low temperature microwave technology and the implementation of quantum computation require circulators as building blocks. Three-port circulators are examples of non-reciprocal devices; they should be passive, low noise and must operate at and below microwave frequencies. It is known that the Hall effect in the quantum regime shows non reciprocal behavior, and it can be utilized in a straightforward way in the realization of highly lossy circulators as well as gyrators. We have analyzed the physical origin of this lossy behaviour and, based on this understanding, developed a novel device that improves efficiency by dealing with the galvanic loss of the earlier designs. These novel circulators and gyrators are particularly suitable for current experiments: they are characterized by low loss and should be suitable for low temperature operation.

HL 67.2 Wed 15:15 POT 006

Large-scale density functional theory study of localization of donor electrons in phosphorus-doped silicon — •Pengxiang Xu[1], Elias Rabel[2], Wei Zhang[1], Riccardo Mazzarello[1], Rudolf Zeller[2], and Stefan Blügel[2] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen, 52074 Aachen, Germany — [2]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The spin of an electron bound to a Phosphorus impurity in lightly Phosphorus-doped Silicon is a promising system for the realization of a spin quantum bit. By using two highly scalable density functional theory codes, KKRnano and QUICKSTEP, we investigate the structural and electronic properties of large models of P-doped Si containing up to 10^4 atoms, focusing in particular on those properties which are relevant to their application as spin qubits.

Computation of the electronic structure of a P impurity as a function of the isotropic doping fraction enable us to determine the doping potential, the doping density and the exchange interaction between donor electrons up to inter-impurity distances of approximately six nanometers.

Our density functional calculations reveal details in the density and potential distribution of the dopants, which are not evident in calculations that do not include explicit treatment of the P donor atom and the relaxation of the crystal lattice.

HL 67.3 Wed 15:30 POT 006

Deterministic Entanglement of Distant Nitrogen Vacancy Centers on an Integrated Photonic Platform — •Janik Wolters[1], Julia Kabuss[2], Andreas Knorr[2], and Oliver Benson[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, AG Nano-Optik, Newtonstraße 15, 12489 Berlin — [2]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin

The nitrogen vacancy (NV) defect center in diamond has emerged as one of the most promising candidates for future solid state quantum technology. In particular recent progress on the integration of NV centers into photonic hybrid platforms attracted attention [1]. We explore the prospects of such an integrated quantum hybrid platform. The applicability of a robust, fast and deterministic entanglement scheme [2] is evaluated. Using realistic conditions and parameters (cavity quality factors, radiative dephasing and spectral diffusion) we find that significant entanglement can be generated between medium distant NV centers via a shared cavity mode. These studies outline a route towards deterministic quantum information processing on a realistic solid state platform.

[1] Wolters, J. et al. Enhancement of the zero phonon line emission from a single nitrogen vacancy center in a nanodiamond via coupling to a photonic crystal cavity. Appl. Phys. Lett. 97, 141108 (2010).

[2] Imamoglu, A. et al. Quantum Information Processing Using Quantum Dot Spins and Cavity QED. Phys. Rev. Lett. 83, 4204 (1999).

HL 67.4 Wed 15:45 POT 006

Interaction between differently charged states of the nitrogen vacancy in diamond — •Dion Braukmann[1], J. Debus[1], D. Dunker[1], V. Yu. Ivanov[2], D. R. Yakovlev[1], and M. Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44227 Dortmund, Germany — [2]Institute of Physics, Polish Academy of Sciences, 02668 Warsaw, Poland

The nitrogen vacancy (NV) in diamond is studied on account of its possible applications in spin-electronics. Temperature-stable properties are ranked among the main advantages of the NV center: Even at room temperature spin coherence times exceed one second.[1] The NV center appears in differently charged states. About 70% are negatively charged (NV^-), the rest are neutral (NV^0) centers. In contrast to the NV^-, the NV^0 is poorly investigated. For single NV centers it was shown that both charge states can transform into each other. In that context, an ensemble of NV centers has not been studied yet. We report on polarization-dependent optical characterization of ensembles of NV^- and NV^0 centers in diamond subjected to high magnetic fields, thus providing insight into their level structures. The talk will be focused on interactions between both charged states. We observe a strong increase in NV^- ZPL intensity and a characteristic resonance of

the NV^- ZPL energy when the NV^0 center is excited resonantly. This behavior can either be explained by a change in the charge state or by a Förster resonant energy transfer. Both possibilities will be discussed in detail.
[1] P. C. Maurer et al., Science, 336, 1283 (2012).

HL 67.5 Wed 16:00 POT 006

Few spin NMR of external spins using a strongly coupled sensor in diamond — •Christoph Müller[1], Xi Kong[2], Jiangming Cai[3], Kristina Melentijević[1], Alastair Stacey[4], Matthew Markham[4], Daniel Twitchen[4], Junichi Isoya[5], Sébastien Pezzagna[6], Jan Meijer[6], Jiangfeng Du[2], Martin Plenio[3], Boris Naydenov[1], Liam McGuinness[1], and Fedor Jelezko[1] — [1]Institute for Quantum Optics, University Ulm, Germany — [2]Hefei National Laboratory for Physics Sciences at Microscale and Depatment of Modern Physics, University of Science and Technology of China, Hefei, China — [3]Institute for Theoretical Physics, University Ulm, Germany — [4]Element Six, Ltd, Ascot, Berkshire, United Kingdom — [5]Research Center for Knowledge Communities, University of Tsukuba, Ibakiri, Japan — [6]Experimental Physics II, University Leipzig, Germany

Negatively charged nitrogen-vacancy (NV^-) centres in diamond, located around 2 nm below the diamond surface were used as a NMR sensor at room-temperature. Strong coupling between the electron spin of the NV^- centre and external nuclear ^{29}Si spins on the diamond surface made it possible to measure the NMR signal aroused by four nuclear spins. With the achieved signal to noise ratio, single spin sensitivity within seconds is possible. In addition, the field gradient created by the NV^- centre itself combined with compressed sensing enables to locate the detected individual nuclei with Angstrom resolution.

HL 67.6 Wed 16:15 POT 006

Increasing the creation yield of shallow nitrogen-vacancy centers by surface plasma termination — •Christian Osterkamp[1], Jochen Scharpf[1], Sebastien Pezzagna[2], Jan Meijer[2], Thomas Diemant[3], Rolf Jürgen Behm[3], Boris Naydenov[1], and Fedor Jelezko[1] — [1]Institut für Quantenoptik, Ulm University, Albert Einstein Allee 11, 89081 Ulm, Germany. — [2]Institut für Experimentelle Physik II, Abteilung Nukleare Festkörperphysik, Universität Leipzig, Linnestraße 5, 04103 Leipzig, Germany. — [3]Institut für Oberflächenchemie und Katalyse, Ulm University, Albert-Einstein-Allee 47, 89081 Ulm, Germany.

Single nitrogen-vacancy (NV) centers in diamond close to the crystal surface are very promising magnetic field sensors with very high sensitivity and nanometer spacial resolution. The fluorescence of single NVs can be detected and its electron spin can be polarized, read-out and manipulated at ambient conditions. Here we report the enhanced creation of very shallow (less than 3 nm below the diamond surface) NVs by using fluorine and oxygen plasma treatment. We observe a four fold increase - from 0.11 % to about 0.45 % in the production yield when the sample surface is terminated with fluorine or oxygen atoms [1]. This effect is explained by the stabilization of the NV's negative charge state which is influenced by the various impurities present on the diamond surface.
[1]: Osterkamp et al., Appl. Phys. Lett. 103 (19), S.193118. (2013)

HL 68: Heterostructures and interfaces

Time: Wednesday 15:00–17:00 Location: POT 051

HL 68.1 Wed 15:00 POT 051

Electronic properties of the ideal Fe/GaAs(110) interface — •Tim Ifflländer, Steffen Rolf-Pissarczyk, Lars Winking, Rainer G. Ulbrich, and Martin Wenderoth — IV. Physikalisches Institut, Georg-August-Universität Göttingen, Germany

In this study we present the investigation of the ideal Fe/GaAs(110) interface by scanning tunneling microscopy (STM) and spectroscopy (STS) in cross-sectional geometry. The Fe/GaAs(110) interface was grown at low temperature and subsequently annealed to room temperature yielding an epitaxial and atomically flat interface without any sign of compound formation [1]. Atomically resolved STS measurements across the Schottky contact reveal a continuum of states in the band gap of the semiconductor in the first few atomic layers at the interface. Furthermore, we report STS measurements of the electronic landscape of the space charge region (SCR) of the Schottky contact. The bending of the valence and conduction band along the SCR for differently n- and p-type doped Fe/GaAs(110) interfaces is demonstrated. To properly interpret the STS data the tip induced band bending has to be taken into consideration. This is addressed by means of a 3-dimensional finite element method calculation. A comparison of the measured and calculated data yields the Schottky barrier (SB) height of the interface and enables us to discuss our findings in the context of theoretical works on SB formation. This work was supported by the DFG SPP 1285.
[1] Winking et al. Appl. Phys. Lett. 92, 193102 (2008)

HL 68.2 Wed 15:15 POT 051

Early stages of nucleation in Cu/a-Si system — •Mohammed Ibrahim[1], Zoltán Balogh[1], Dietmar Baither[1], Patrick Stender[1], and Guido Schmitz[2] — [1]Institut für Materialphysik, University of Münster — [2]Institut für Materialwissenschaft, Universität Stuttgart

Laser-assisted atom probe shows a unique potential in the analysis of embedded Si/metal interfaces, owing to its ability to deliver 3D chemical mapping with near atomic resolution. It is therefore a complementary part to the 2D electron microscopic methods [1]. Recently, we observed that the reaction between Cu and a-Si to form silicide phases is strongly influenced by the deposition sequence. From that, if Cu deposited on a-Si, an instantaneous reaction happens at low temperature and a reacted layer increases linearly with increasing annealing time [2]. For the reverse case, high temperatures or long annealing time are required for the appearance of silicide at the interface [3]. In this work, we focus on the phase nucleation with higher nucleation barrier in case of a-Si deposited upon Cu. We observed an increase of roughness at the interface, the appearance of Cu rich particles in the a-Si bulk as well as spikes of high Cu contents protruding from the metallic Cu. As opposed to previous reports [4], these findings indicate that a significant nucleation barrier exists for nucleating the silicide at the interface. Nucleation happens at the a-Si side probably even inside the Si bulk.
[1] R. Schlesiger et al., Rev. Sci. Instrum., 81 (2010) 043703. [2] B. Parditka et al., Acta Mater., 61 (2013) 7173. [3] M. Ibrahim, et. al, Phys. Stat. Sol. C, DOI: 10.1002/pssc.201300370. [4] F. Hodaj , and. A. Gusak, Acta Mater., 52 (2004) 4305.

HL 68.3 Wed 15:30 POT 051

An XPS study on $Al_xGa_{1-x}N$/metal oxide hetero interfaces with ZnO and CuO_x, respectively — •Benedikt Kramm, André Portz, Philipp Hering, Achim Kronenberger, Angelika Polity, and Bruno K. Meyer — 1. Physikalisches Institut, Justus Liebig Universität, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

For semi-conductor devices the energy band alignment of hetero junctions is one of the crucial factors which deliver a judgment for a successful operating electronic device. For our research on the nitride-oxide hetero interface we fabricated various hetero junctions based on n-type aluminum gallium nitride alloys (with 7%, 11% and 15% aluminum content) plus pure n-type and p-type gallium nitride. Copper oxide and zinc oxide were on top, respectively. The nitrides were epitaxial grown on sapphire substrates whereas the oxide top layers were deposited by RF-magnetron sputtering as 50 nm thick poly crystalline thin films. To get knowledge of the energetic behavior, like the band offsets of the valence and conduction band, charging effects as well as diffusion and the shape of the oxy-nitrogen mixed interface we performed X-ray photoelectron spectroscopy. A special focus was on the naturally build oxygen overlayer on gallium nitride which is typically a few angstroms thick and how it affects the hetero interface. Furthermore we evaluated the shifting of the photoelectron signals due to the preferential sputtering effect during depth-profiling with argon-ion bombardment.

HL 68.4 Wed 15:45 POT 051

Heteroepitaxial growth of GaP on Si(111) — •Agnieszka Paszuk[1,2], Weihong Zhao[1,2], Matthias Steidl[1,2], Sebas-

tian Brückner[1,2], Anja Dobrich[1], Oliver Supplie[1], Peter Kleinschmidt[1,3], and Thomas Hannappel[1,2,3] — [1]Technische Universität Ilmenau, Institute for Physics, Ilmenau, Germany — [2]Helmholtz-Zentrum Berlin, Institute for Solar Fuels, Berlin, Germany — [3]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, Erfurt, Germany

III-V nanowires exhibit properties for new concepts of high efficiency solar cells. The use of Si instead of III-Vs as substrate benefits from large cost reduction. We prepare thin GaP films on Si as transition buffer layer for subsequent NW growth, since GaP is almost lattice matched to Si. GaP(111) exhibits two polarities, GaP(111)A and B type, which differ by an inversion of the crystal lattice. However, vertical growth of NWs requires GaP(111) layers with B-type polarity. Further, rotational domains might occur in GaP layers during heteroepitaxy, decreasing the crystal quality. Here, we show that surface preparation of Si(111) substrates strongly influences the subsequently grown GaP film polarity during heteroepitaxy by metalorganic vapor phase epitaxy (MOVPE). Low energy electron diffraction (LEED) can be applied to distinguish between the two GaP polarities, which exhibit two different surface reconstructions. X-ray diffraction (XRD) enabled analysis of rotational domains in the GaP buffer layer. Our MOVPE prepared GaP(111)B/Si(111) quasisubstrates enabled vertical growth of III-V NWs.

HL 68.5 Wed 16:00 POT 051

***In situ* RAS and *ab initio* DFT study of GaP/Si(100) interface structures** — •Oliver Supplie[1,2], Sebastian Brückner[1,2], Oleksandr Romanyuk[3], Peter Kleinschmidt[1,2], Henning Döscher[1,2,5], Frank Grosse[4], and Thomas Hannappel[1,2] — [1]Helmholtz-Zentrum Berlin, Institute Solar Fuels — [2]TU Ilmenau, Institut für Physik, FG Photovoltaik — [3]Institute of Physics, Academy of Sciences of the Czech Republic, Prague — [4]NREL, Golden, CO, USA — [5]Paul-Drude Institut für Festkörperelektronik, Berlin

GaP/Si(100) is considered as quasi-substrate for lattice-matched GaPN/Si photoelectrochemical tandem diodes [1]. The formation of the crucial polar-on-nonpolar heterointerface in vapor phase epitaxy ambient is studied here by *in situ* reflection anisotropy spectroscopy (RAS) in combination with *ab initio* density functional theory (DFT). We can choose between energetically and kinetically [2] driven Si(100) step formation, which results in either A-type or B-type majority domains of Si dimers. The sublattice orientation of the subsequently grown GaP film depends on the type of Si surface. In an abrupt interface model [3], Si–P bonds are found to be favored. *Ab initio* DFT calculations [4] show that Si–P bonds are energetically favored over Si–Ga bonds at abrupt interfaces. Charge can be compensated in an in-plane (2x1) interface unit cell with a Si to P (Ga) atomic mixing ratio of 0.5:0.5 which is favorable in thermodynamic equilibrium.
[1] Döscher et al., *ChemPhysChem* **13** (2012) 2899. [2] Brückner et al., *PRB* **86** (2012) 195310. [3] Beyer et al., *JAP* **111** (2012) 083534. [4] Romanyuk et al., *PRB* **88** (2013) 115312.

HL 68.6 Wed 16:15 POT 051

Effect of growth conditions on electrical properties of epitaxial GaP/Si (100) — •Emad H. Hussein[1,2], Fariba Hatami[1], and W. Ted Masselink[1] — [1]Institut für Physik, Mathematisch-Naturwissenschaftliche Fakultät I, Humboldt Universität zu Berlin, Newtonstrasse D-15, 12489 Berlin, Germany — [2]On leave from department of Physics, college of Science, Al-Mustansiriyah University, Baghdad, Iraq

Gallium phosphide layers were grown using gas-source molecular beam epitaxy on p-type silicon substrates of orientation (100). The growth temperature was varied between 250 and 550 °C. Samples grown at 250 and 400 °C were thermally annealed at 500 and 480 °C for 10 and 90 min, respectively. (Subsequent contact alloying was carried out at much lower temperature.) Current-voltage (I-V) and capacitance-voltage (C-V) measurements were carried out in the dark at room temperature. The structures were also characterized using x-ray diffraction. From I-V measurements, it was found that the GaP/Si heterostructures grown at 400 °C and annealed at 480 °C for 90 minutes exhibited rectifying characteristics. The C-V data show the increased dopant diffusion during the annealing process. Furthermore, the C-V allows us to characterize the location of the junction and the electrically active defects. We conclude that the electrical properties of the GaP/Si can be improved after long-time annealing due to reduction of the defects in the structure which is in agreement with the x-ray analysis.

HL 68.7 Wed 16:30 POT 051

THz Transmission Spectroscopy of Charge Carriers in Semiconductor Heterostructures with epitaxial, complementary doped gate — •Shovon Pal[1,2], Hanond Nong[2], Sascha Valentin[1], Arne Ludwig[1], Nathan Jukam[2], and Andreas D. Wieck[1] — [1]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum — [2]Arbeitsgruppe Terahertz-Spektroskopie und Technologie, Ruhr-Universität Bochum

Intersubband transitions take place between quasi-two-dimensional (2D) electronic states called subbands, which are formed due to confinement of electrons in the growth direction. Confined electrons in the ground subband absorb incident infrared radiation and are excited to higher subbands, resulting in transmission minima at intersubband resonance (ISR) frequencies. These frequencies lie in the THz domain and hence THz-transmission spectroscopy of these 2D charge carriers serves as an effective tool to investigate ISR. In the present work, an epitaxial, complementarly doped gate is used to control the 2D electron density in a modulation doped GaAs-AlxGa(1-x)As heterojunction to observe the ISR. Hall measurements of the sample show that the 2D electron density is n=1.76e11 cm-2. Density chopping measurements between the threshold voltage (n=0) and a certain gate voltage (n) were performed with the sample tilted at 30°, normalizing the transmission spectra T(n) via division by T(0). With a magnetic field in beam direction and the sample tilted at the same angle as before, half-field coupling of the cyclotron resonance with the ISR was observed. All measurements were performed at 4.2 K.

HL 68.8 Wed 16:45 POT 051

Investigation of interband dynamics in single InAs/GaAs quantum dots — •Daniel Stephan[1,2], Jayeeta Bhattacharyya[1], Manfred Helm[1,2], Yongheng Huo[3], Oliver Schmidt[3], Armando Rastelli[4], and Harald Schneider[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Technische Universität Dresden, Germany — [3]Leibniz Institute for Solid State Materials Research Dresden, Germany — [4]Johannes Kepler Universität, Austria

We investigate the dynamics of inter-sublevel transitions in single InAs/GaAs self-assembled quantum dots (QDs). By using a microphotoluminescence (PL) setup and low-density QD samples, we measure the PL emission from single QDs. The QDs is manipulated by a free-electron laser pulse tuned to the inter-sublevel transition energy, which excites carriers to a higher energy level, from which they decay non-radiatively back to the ground state. The PL is measured spectrally resolved, as well as time-resolved, employing time-correlated single photon counting. In time resolved measurements, the inter-sublevel dynamics causes quenching in the exponential PL decay. In contrast to previous studies on QD ensembles[1,2], the use of single dots eliminates effects such as inhomogeneous broadening and inter-dot transfer, providing a better understanding of inter-sublevel carrier dynamics.

[1] J. Bhattacharyya, et al., Applied Physics Letters 97, 031101 (2010).

[2] J. Bhattacharyya, et al., Applied Physics Letters 100, 152101 (2012).

HL 69: Emerging oxide semiconductors II (Focus session with DS)

Continuation of the morning session 'Emerging oxide semiconductors I'

Organizers: Oliver Bierwagen, Paul-Drude-Institut für Festkörperelektronik, Berlin, Norber Esser, Leibniz-Institut für Analytische Wissenschaften ISAS, Berlin, Rüdiger Goldhahn, Otto von-Guericke-Universität Magdeburg, and Marius Grundmann, Universität Leipzig.

Time: Wednesday 15:00–18:45 Location: POT 081

Topical Talk HL 69.1 Wed 15:00 POT 081

Electronic properties of the transparent semiconducting oxides Ga2O3 and In2O3 — •Recardo Manzke — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

The exploration of oxides from the perspective of semiconductor science and technology offers great opportunities for uncovering new physics as well as developing novel devices with unprecedented performance and functionality. In this talk the transparent semiconducting oxides (TSO) Ga2O3 and In2O3 will be presented. Regarding the electronic structure respectively band structure, crucial progress has been reached in the last years. Here Ga2O3 and, in particular, the (100) surface behaves like expected for a large-gap semiconductor. Against this, for In2O3 the occurrence of a charge accumulation layer is heavily debated. This possibly will restrict their potential for applications.

HL 69.2 Wed 15:30 POT 081

Dielectric function of In_2O_3 from the mid-infrared into the vacuum ultraviolet — •Rüdiger Goldhahn[1], Jakob Nixdorf[1], Christian Lidig[1], Klaus Irmscher[2], Zbigniew Gałazka[2], Oliver Bierwagen[3,4], James S. Speck[4], Christoph Cobet[5], and Martin Feneberg[1] — [1]Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg — [2]Leibniz-Institut für Kristallzüchtung, Berlin — [3]Paul Drude Institut für Festkörperelektronik — [4]University of California, Santa Barbara — [5]Johannes Kepler Universität, Linz

The optical properties of cubic bixbyite In_2O_3 are under intense discussion. There is not even a consensus about the direct or indirect nature of the fundamental band gap and the corresponding energies. Here, we present spectroscopic ellipsometry from the phonon region in the mid-infrared up to 10 eV using several different instruments including synchrotron radiation. The studies comprise bulk (111) crystals and epitaxial (001) thin films on (001) yttria-stabilized zirconia covering a wide range of electron concentrations (N_s). The dielectric function of In_2O_3 at high energies exhibits pronounced features related to critical points. By analyzing certain peculiarities of ellipsometric data, the fundamental band gap energy to be 2.77 ± 0.02 eV for low N_s. A continuous Burstein-Moss shift is found for increasing N_s. The analysis of the plasma frequency yields an electron effective mass of about $0.23m_0$.

HL 69.3 Wed 15:45 POT 081

Barrier height of Ag on In_2O_3 (111) single crystals — •maryam nazarzadehmoafi[1], stephan machulik[1], florian Neske[1], christoph janowitz[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, Berlin, Germany

The barrier height of a metal-semiconductor contact was studied by means of angle-resolved photoemission spectroscopy, which was implemented through stepwise Ag deposition on the (111) surface of In_2O_3 single crystals. Work function of Ag and electron affinity of In_2O_3 were measured in situ, being 4.21 ± 0.05 eV and 4.24 ± 0.05 eV, respectively. A slight barrier height of 0.15 ± 0.07 eV was determined by following the band bending of valence band and core level spectra with Ag coverage. Good agreement was observed when comparing the results to a calculation of the height by applying the Schottky-Mott rule, yielding the negligible value of 0.03 ± 0.05 eV. Therefore, the character of the contact is ohmic like. Additionally, the results revealed the existence of diffuse band-gap states for In_2O_3(111) and a Fermi level shift by 0.09 ± 0.02 eV due to the photovoltage effect with Ag deposition.

HL 69.4 Wed 16:00 POT 081

Metal contacts on the beta-Ga2O3 single crystal (001) surface — •Stephan Machulik[1], Maryam Nazarzadehmoafi[1], Mansour Mohamed[2], Andreas Siebert[1], Christoph Janowitz[1], Zbigniew Galazka[3], and Recardo Manzke[1] — [1]Humboldt Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin — [2]Assiut University, Physics Department, Faculty of Science, Assiut 71516, Egypt — [3]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, Berlin, Germany

Results of band structure measurements on beta-Ga2O3 single crystals were in good agreement with theoretical calculations [1], indicating a good theoretical understanding of this material. For application purposes in semiconductor technologies both Schottky and Ohmic metal-semiconductor contacts are required. ARPES and I/U measurements performed on n-doped Au-beta-Ga2O3(001) contacts confirmed Schottky-like behavior with a barrier height of 1.01 eV [2]. Motivated by the lower work function of silver we performed an ARPES study of Ag-beta-Ga2O3(001). The results point to a distinctly lower Schottky barrier, but the contact was not yet Ohmic. Additionally the work function depending on the layer thickness of Ag was studied.

[1] M. Mohamed, C. Janowitz, I. Unger, R. Manzke, Z. Galazka, R. Uecker, R. Fornari, J.R. Weber, J.B. Varley, C.G. van de Walle, Appl. Phys. Lett. 97, 211903 (2010)

[2] M. Mohamed, K. Irmscher, C. Janowitz, Z. Galazka, R. Manzke, R. Fornari, Appl. Phys. Lett. 101, 132106 (2012)

HL 69.5 Wed 16:15 POT 081

Sputtered SnO_2 degenerately doped with Ta or Sb - A comparative study for applications in transparent electronics — •Mirko Weidner and Andreas Klein — Technische Universität Darmstadt

In the emerging field of transparent electronics, indium oxide doped with tin (ITO) is still the predominately used electrode material, due to its high conductivity at low deposition temperatures. Due to the relative scarcity and high cost of Indium, alternatives are highly sought after. Tin oxide (SnO_2) is one of the few other materials that combine the properties of optical transparency and electrical conductivity. The material may serve as a transparent electrode in optoelectronic devices such as displays, touch screens, LEDs and thin film solar cells. In recent years, SnO_2 doped with Tantalum (TTO) has been shown to be a valid alternative to the established SnO_2 systems doped with Fluorine (FTO) or Antimony (ATO). However, little work has been published on the material, and thus far the question as to why Tantalum doping can yield better electrical conductivity than Antimony doping has not been raised or answered.
In this study, TTO and ATO thin films where sputter-deposited and characterized under similar conditions to maximize comparability between the two materials. Characterization of electrical conductivity and optical transmissivity was complimented by probing the materials' electronic structure by in-situ Photoelectron Spectroscopy (XPS/UPS) of the sample surfaces and by structural characterization by AFM and XRD.

HL 69.6 Wed 16:30 POT 081

Structural and electrical properties of Nb doped TiO_2 anatase films (2 - 17 at.%) sputtered with plasma emission control — •Sebastian Schipporeit[1], Sanat Kumar Mukherjee[1], Hans-Werner Becker[2], Andrew Paolo Cádiz Bedini[1], Christian Notthoff[1], Abdelkader Nebatti[1], Detlef Rogalla[1], Azadeh Soleimani-Estafani[1], and Dieter Mergel[1] — [1]Thin Film Technology Group, Faculty of Physics, University Duisburg-Essen — [2]University Bochum

Nb doped TiO_2 films were deposited using radio frequency magnetron sputtering with a metallic Ti target and introducing O_2 and Ar gas into the chamber. Nb wires were put onto the sputter track of the Ti target and the oxidation state of the target was controlled using a Ti line of the plasma emission. The films were analysed with XRD, RBS, SEM, EDX and XPS. After annealing at 400 °C, all films are polycrystalline and inhibit anatase structure. The Nb/(Nb+Ti) content varies from 2 to 17 at.%. The lattice parameter a and the unit cell volume

increase in a similar manner compared to TiO_2:Nb single crystals.

The films with the lowest resistivity of $7{\cdot}10^{-4}$ Ωcm (Nb content: 10 at.%) were coated with an oxidation state of the target in the transition region between metallic and oxidic modes. The Nb is incorporated as Nb^{5+} into the anatase lattice. In films with higher resistivity, the donor effect of Nb might be compensated by Ti vacancies (acceptors). The oxygen content is higher than in stoichiometric TiO_2. Ogyxen interstitials might increase the mass density in the films.

Coffee break (15 min.)

Topical Talk HL 69.7 Wed 17:00 POT 081

Surface properties of In_2O_3 and other semiconducting metal oxides — •Ulrike Diebold — Institute of Applied Physics, TU Vienna, Austria

The atomic-scale surface properties of semiconducting oxides influence, and often even dominate, their performance in a variety of applications. Often, local effects such as defects can severely affect the local electronic structure and surface chemistry. Our group uses STM in combination with DFT and area-averaging spectroscopies to investigate such phenomena at the atomic scale. Recent results on single crystalline In_2O_3 and other metal oxides will be discussed.

HL 69.8 Wed 17:30 POT 081

STM and STS at the InO(111) cleavage surface — Robert Zielinski, Andrea Lenz, Josephine Schuppang, Mario Dähne, and •Holger Eisele — Technische Universität Berlin, Institut für Festkörperphysik, 10623 Berlin, Germany

The freshly cleaved In2O3(111) surface is investigated by UHV cross-sectional scanning tunneling microscopy and spectroscopy in order to achieve knowledge about its intrinsic electronic surface states. Atomically resolved STM images show a topographic contrast, which can be related with recent density functional theory calculations, and indicate a local charge enhancement within the surface unit cell. Scanning tunneling spectra reveil intrinsic states within the fundamental bulk band gap. Furthermore, the Fermi level is energetically located within the bulk band gap. This finding leads to the assumption that electron accumulation at this surface is not an intrinsic property, but related to extrinsic effects, such as e.g., non-stoichiometric material re-organization.

HL 69.9 Wed 17:45 POT 081

Electrical properties of In2O3 single crystals: distinction between surface and bulk conductivity — •Klaus Irmscher, Mike Pietsch, Wolfram Troeder, and Zbigniew Galazka — Leibniz-Institut für Kristallzüchtung, Berlin

Transparent semiconducting oxides such as In2O3, SnO2 or ZnO have the tendency to form surface electron accumulation layers. The highly conductive surface layers may have strong implications in the emerging field of transparent oxide electronics. For instance, the implementation of active elements like Schottky diodes depends on whether the accumulation of electrons at the surface can be suppressed in a controlled manner. Investigations on the origin of the surface electron accumulation in In2O3 were hitherto performed on thin crystalline films. Here, we present temperature dependent Hall effect measurements of melt-grown In2O3 bulk single crystals. The samples had electron concentrations between 10^16 and 10^19 cm-3 at room temperature depending on post-growth annealing conditions. The temperature dependent electron concentrations measured from 15 to 750 K show clear contributions due to surface electron accumulation. To differentiate between bulk and surface proportions the data evaluation is based on a two-layer model. This enables a clear attribution of donor concentration changes due to sample annealing under oxidizing or reducing conditions to surface-near and bulk regions, respectively. We discuss the possible influence of oxygen vacancies, hydrogen donors and surface adsorbates.

HL 69.10 Wed 18:00 POT 081

Electronic surface properties of stoichiometric and defect-rich indium oxide films prepared by MOCVD — •Marcel Himmerlich[1], Chunyu Wang[2], Volker Cimalla[2], Oliver Ambacher[2], and Stefan Krischok[1] — [1]Institut für Physik and Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, PF 100565, 98684 Ilmenau, Germany — [2]Fraunhofer-Institut für Angewandte Festkörperphysik, Tullastraße 72, 79108 Freiburg, Germany

The influence of metalorganic chemical vapor deposition conditions on the indium oxide surface properties is investigated using photoelectron spectroscopy (PES). It is shown that the growth conditions have a strong influence on the physical properties and that films prepared at 200°C or below are highly oxygen-deficient and rich in defects, influencing the surface chemical and electronic properties and resulting in the existence of excess electrons, which are partially localized at the remaining indium atoms. This configuration results in the existence of reactive defect sites, which cause high ozone sensitivity. The PES results are compared to the electronic properties of crystalline In_2O_3 films in cubic bixbyite and rhombohedral structure. The influences of the surface stoichiometry and high defect density, ozone oxidation and UV photoreduction on variations in surface band bending, electron accumulation, work function and formed surface dipoles as well electron transport and sensor characteristics are analyzed.

HL 69.11 Wed 18:15 POT 081

Stability of low-index bcc-In_2O_3 surfaces under O-Rich-, In-Rich-, and Sn-doping molecular beam epitaxy conditions: An Experimental Study — •Oliver Bierwagen[1,2], Patrick Vogt[1], and James S. Speck[2] — [1]Paul-Drude-Institut, Berlin,Germany. — [2]University of California, Santa Barbara, USA.

Molecular beam epitaxy of bixbiyte In_2O_3 on (001) oriented ZrO_2:Y (YSZ) substrates typically results in {111} faceted surfaces whereas on (111) smooth films are obtained [1]. This behavior has been explained by theory calculations that found the surface free energies of low index bixbiyte surfaces to increase from (111) to (011) to (001) surfaces [2]. On the other hand, it was found that In-rich growth conditions [1] or high Sn-doping [6] lead to the formation of smooth, unfaceted (001) In_2O_3 films on YSZ(001). These results are in-line calculations of stoichiometry-dependent surface free energy [5]. Our experimental study of In_2O_3 on YSZ(001), (011), (111) grown by MBE under O-rich, In-rich and high Sn-doping conditions suggest the following relative surface free energies: (111) lowest under all conditions, (001) significantly lowered by In-rich conditions and Sn-doping. A flat (011) surface was not observed suggesting a higher surface free energy than predicted by theory. Our experimental results compare well to theory of [5]. [1] Bierwagen, Appl. Phys. Lett. 95, 262105 (2009). [2] Walsh and Catlow, J. Mater. Chem. 20, 10438 (2010). [4] Bierwagen and Speck, J. Appl. Phys. 107, 113519 (2010). [5] Agoston and Albe, Phys. Rev. B 84, 045311 (2011). [6] Taga, Jpn. J. Appl. Phys. 37, 6585 (1998).

HL 69.12 Wed 18:30 POT 081

Surface structure of metal oxides via classical and quantum mechanical rainbow scattering — •Marco Busch[1], Eric Meyer[1], Jan Seifert[1], Helmut Winter[1], Klaus Irmscher[2], and Zbigniew Galazka[2] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstrasse 15, D-12489 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Strasse 2, D-12489 Berlin, Germany

Fast light atoms and molecules with energies from 200 eV up to several tens of keV are grazingly scattered from clean and flat metal oxide surfaces. The angular distributions of projectiles scattered in the regime of axial surface channeling show intensity maxima, which can be described with the concept of the classical rainbow scattering and offer the determination of the interaction surface potential. However, for decreasing projectile energy one can observe Bragg peaks in the angular distributions, which can be interpreted within the framework of quantum mechanics only. As examples, we present investigations of the quantum scattering from the cleaved (100) surface of β-Ga_2O_3 single crystals, grown by the Czochralski method. The splittings of Bragg peaks and their intensity modulations were so far exploited to deduce information on the arrangement of atoms in the topmost surface layer. Furthermore, diffraction effects were present in the regime of surface channeling, where quantum scattering is considered for the motion parallel to the surface. For the thermal induced reconstruction of the $(11\bar{2}0)$ and (0001) surface of Al_2O_3 we found also a preservation of the longitudinal coherence and observed Laue circles of higher orders.

HL 70: Semiconductor laser I: VECSEL and cascade lasers

Time: Wednesday 15:00–17:15 Location: POT 112

HL 70.1 Wed 15:00 POT 112

Interband-Cascade-Lasers — •Matthias Dallner, Robert Weih, Florian Hau, Sven Höfling, and Martin Kamp — Technische Physik and Wilhelm-Conrad-Röntgen-Research Center for Complex Material Systems, Universität Würzburg, Am Hubland, 97074 Würzburg

Interband cascade lasers (ICLs) are promising candidates to meet the demand for efficient and relieable laser sources in the mid-infrared wavelength region coming from a variety of applications such as high sensitivity tunable laser absorption spectroscopy (TLAS) or medical diagnostics. Grown on GaSb-substrates ICLs are able to cover a wide spectral range from 3 μm to 5.7 μm in cw operation above room temperature. Long wavelength devices based on InAs substrates, utilizing highly doped InAs-layers instead of superlattice claddings in view of a higher thermal conductivity, have shown laser emission up to 10.4 μm. In this talk recent results on both, GaSb-based and InAs-based long wavelength ICLs are presented.

For ICLs grown on both substrates, GaSb and InAs, several design optimizations concerning the active region and the waveguide were examined. As a result GaSb based dry etched ridge waveguide lasers with more than 100 mW of cw output power at room temperature in the 3.5 μm wavelength range could be fabricated. For the plasmon waveguide InAs-ICLs a maximum lasing temperature of -13 $°C$ in cw operation for a narrow ridge waveguide laser was achieved at 6 μm. In pulsed operation threshold current densities below 1 kA/cm^2 were measured.

HL 70.2 Wed 15:15 POT 112

Monomode Interband Cascade Lasers in the MIR wavelength range — •Julian Scheuermann[1], Michael von Edlinger[1], Robert Weih[2], Lars Nähle[1], Christian Zimmermann[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 University of Würzburg and Wilhelm-Conrad-Röntgen-Research Center for Complex Material Systems, Am Hubland, 97074 Würzburg, Germany

Interband cascade lasers (ICLs) have evolved into important laser sources in the mid infrared (MIR) spectral range. Compared to quantum cascade lasers, they offer significant advantages with respect to threshold power density as well as overall power consumption. In contrast to conventional diode lasers, they are able to cover the entire wavelength region from 3 to 6 microns. This is extremely interesting for high accuracy gas sensing, since many gas species have their strongest absorption features in this range, including e.g. CH4, formaldehyde or NO. Novel monomode ICLs in the MIR wavelength range suited for applications in tunable laser absorption spectroscopy are presented in this talk. The focus is on the design and processing of distributed feedback ICLs and their temperature dependent characteristics. Vertical sidewall gratings defined by electron beam lithography and an optimized dry etch process are the key components to achieve application-grade device performance and monomode emission with high side mode suppression ratio. Continuous wave operation at temperatures up to 80°C with threshold currents below 80 mA was observed.

HL 70.3 Wed 15:30 POT 112

In-phase supermode emission based on an evanescently coupled semiconductor laser array — •Alexander Reinhold[1], Christian Zimmermann[1], Julian Scheuermann[1], Wolfgang Zeller[1], Johannes Koeth[1], and Martin Kamp[2] — [1]nanoplus Nanosystems and Technologies GmbH, Oberer Kirschberg 4, D-97218 Gerbrunn, Germany — [2]Technische Physik and Wilhelm-Conrad-Röntgen-Research Center for Complex Material Systems, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Various fields of application demand compact, low cost, coherent light sources with high brilliance and emission of a single spectral mode. Suitable monolithic device concepts like semiconductor ridge waveguide arrays are extremely promising to achieve a narrow beam divergence with a high optical output power. Such arrays exhibit lateral mode coupling of adjacent ridge waveguides, leading to a distinct number of index guided supermodes with a large mode extension at the facet. For an array with a predefined number of ridge waveguides, coupled mode analysis postulates a distinct number of allowed supermodes with only the first order in-phase supermode exhibiting lateral single lobe emission. We have designed and fabricated arrays based on an AlGaAs/GaAs laser structure with an InGaAs double quantum well active region. In order to obtain devices with spectral single mode emission we have also realised arrays with wavelength selective elements. We achieved in-phase supermode emission with a lateral beam divergence of 5,6 ° at full width half maximum (FWHM) and optical output powers beyond 100 mW.

HL 70.4 Wed 15:45 POT 112

Organic microlasers in vertical and lateral geometry — •Tim Wagner, Markas Sudzius, Andreas Mischok, Robert Brückner, Hartmut Fröb, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr Str. 1, 01069 Dresden

Optical microcavities can trap light in a very compact volume by different mechanisms, for example, by total internal reflection or distributed Bragg reflection. As a result, properties such as confinement, positive optical feedback, wavelength selectivity and outcoupling mechanisms are realized in entirely different ways.

In this work, we compare lasing characteristics of two conceptually different structures — vertical-cavity surface-emitting lasers and distributed feedback lasers — which are based on the same set of materials and technology. The active material in all structures is a blend of the red laser dye DCM doped by 2 wt% into the host material Alq_3.

Although based on conceptually different microresonator structures, both devices show similar lasing thresholds I_{th} and comparable optical confinement factors β. A systematic analysis of these characteristics allows us to identify dominating mechanisms, which are responsible for the lasing thresholds, and let us justify the balance between the positive optical feedback, which is defined by the optical resonator, against the different kinds of optical losses. Based on the results obtained, devices combining concepts of VCSEL and DFB will be discussed further.

HL 70.5 Wed 16:00 POT 112

Single-frequency vertical-external-cavity surface-emitting laser with output power exceeding 10 W and sub-MHz linewidth — •Fan Zhang[1], Bernd Heinen[1], Matthias Wichmann[1], Christoph Möller[1], Bernardette Kunert[2], Wolfgang Stolz[1], Arash Rahimi-Iman[1], and Martin Koch[1] — [1]Department of Physics, Philipps-Universität Marburg, Marburg D-35032, Germany — [2]NAsP III/V GmbH, Marburg D-35041, Germany

Vertical-external-cavity surface-emitting lasers (VECSELs) provide high power, highly coherent continuous-wave emission and a broad wavelength coverage (from UV to mid-IR) depending on the chip design. Moreover, the laser cavity can be extended by optical components, which allows for single-frequency operation. In recent years, single-frequency VECSELs have been intensively investigated. They have the potential to combine a high output power, a narrow linewidth and a large frequency tunability in one device. Such lasers are desirable tools for numerous applications, ranging from spectroscopy, metrology to optical free-space telecommunication. Here, we demonstrate a single-frequency VECSEL working at 1030 nm, and exceeding 10 W output power with sub-MHz linewidth at the same time. A maximum output power of 11 W is achieved at a net incident pump power of 42 W. Furthermore, an external Fabry-Perot cavity was used as frequency discriminator to measure the stability of the free-running laser. At a sampling time of 1 ms, we yield a considerably narrow linewidth, which is mainly limited by the mechanical vibrations and acoustical noise, of 750 kHz.

HL 70.6 Wed 16:15 POT 112

SESAM mode-locked AlGaInP-VECSEL emitting femtosecond pulses — •Roman Bek, Grizelda Kersteen, 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

Since 2000, semiconductor saturable absorber mirrors (SESAMs) have been used for passive mode locking of vertical external-cavity surface-emitting lasers (VECSELs) emitting in the infrared spectral range. These laser systems are able to produce femtosecond pulses with an

average power of several watts. In contrast, the first passively mode-locked VECSEL emitting picosecond pulses in the visible spectrum could only be realized in 2013.

We present the first SESAM mode-locked VECSEL producing femtosecond pulses at a wavelength of 664 nm and a repetition rate of 836 MHz. We use an absorber containing two quantum wells close to the surface and an additional fused silica coating. Due to a plane diamond heatspreader bonded onto the gain chip, we observe side pulses with a time delay of 8.95 ps. The laser spectrum shows the superposition of a soliton-like part and a "continuum" which has already been observed for soliton-like mode-locked semiconductor disk lasers in the infrared spectral range.

HL 70.7 Wed 16:30 POT 112

Frequency doubled AlGaInP-VECSELs for interference lithography — •Hermann Kahle, Clarissa Wink, Jonas Weber, Ulrich Rengstl, Hendrik Niederbracht, Thomas Schwarzbäck, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen and Research Center SCoPE, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

The wide range of applications in biophotonics, television technologies, spectroscopy and lithography made the vertical external-cavity surface-emitting laser (VECSEL) an important category of power scalable lasers. We present an optically pumped, frequency doubled AlGaInP-VECSEL with a total of 20 compressively strained quantum wells (QWs). The QW packages are placed in a separate confinement heterostructure in a resonant periodic gain (RPG) design within strain-compensating quaternary AlGaInP barriers and cladding layers, respectively. The VECSEL operates in continuous-wave operation at fundamental wavelengths around 660 nm. Wavelength tuning measurements of the fundamental and frequency doubled output, realized by rotation of an intra-cavity birefringent filter will be shown. High power ultraviolet output can be used as light source for interference lithography. Details of the fabrication, characterization, laser setup as well as test structures of the application aiming on pre-structuring of semiconductor samples will be shown. A new power-scaling concept for semiconductor disk lasers towards high UV laser power for large area lithography is under investigation.

HL 70.8 Wed 16:45 POT 112

Continuously tunable, self-seeded GaSb-based semiconductor disk laser emitting around 2.05μm — •Peter Holl, Sebastian Kaspar, Steffen Adler, Marcel Rattunde, Andreas Bächle, Rolf Aidam, and Joachim Wagner — Fraunhofer-Institut für Angewandte Festkörperphysik, Tullastrasse 72, D-79108 Freiburg, Germany

Semiconductor disk lasers, also known as vertical-external-cavity surface-emitting laser (VECSEL), combine the wavelength versatility of semiconductor laser with the capability of a nearly diffraction-limited high-power output. Due to the broad gain spectrum of the semiconductor gain material, VECSELs are an attractive option to build a wavelength tunable laser source, which are needed for applications like high resolution spectroscopy.

In this presentation we will report on a tunable, self-seeded VECSEL emitting around 2.05 μm. An intra-cavity SiC heatspreader dissipates the heat of the active region to ensure high output power. At the same time we were able to overcome etalon effects that limit the selectable wavelengths to discrete values by using a wedged heatspreader, thus avoiding plane-parallel surfaces. The heatspreader inserts a tilted surface in the cavity acting as beam splitter, whose reflection is used to self-seed the laser. For this purpose the outcoupled beam is led onto a diffraction grating providing wavelength selective feedback into the cavity.

The achieved continuous tuning range around 2.05μm spans over 30nm, while the output power exceeds 400mW at room temperature.

HL 70.9 Wed 17:00 POT 112

Emission intensity modulation of a VCSEL by ultrafast acoustics — •Jan Tepper[1], Thomas Czerniuk[1], Christian Brüggemann[1], Sebastian Brodbeck[2], Christian Schneider[2], Martin Kamp[2], Sven Höfling[2], Boris Glavin[3], Dimitri Yakovlev[1,4], Andrey Akimov[4,5], and Manfred Bayer[1] — [1]Experimentelle Physik 2a, TU Dortmund, Dortmund, Germany — [2]Technische Physik, Universität Würzburg, Würzburg, Germany — [3]V. E. Lashkaryov Institute of Semiconductor Physics, Kiev, Ukraine — [4]A. F. Ioffe Physical-Technical Institute, Russian Academy of Sciences, St. Petersburg, Russia — [5]School of Physics and Astronomy, University of Nottingham, Nottingham, United Kingdom

We report an ultrafast intensity modulation of a VCSEL's laser emission of up to 50% peak-to-peak by shifting the active medium's spectral profile using an acoustic strain pulse.

The sample under investigation is an AlAs/GaAs based microcavity, which inhabits quantum wells as the active medium. Its emission intensity strongly depends on how well the active medium's wavelength matches the cavity mode. By using high energy femtosecond laser pulses, we generate a strain pulse travelling through the sample. This strain pulse subsequently reaches the QWs and alters their band gap, which leads to an emission intensity modulation with an amplitude of 50% from peak to peak. Due to the small spatial separation of the QWs, the corresponding modulation frequencies lie in the THz regime. Qualitatively, the results can be described by rate equations in which the strain is treated as a perturbation of the laser's gain.

HL 71: Energy materials: Silicon-based photovoltaics

Time: Wednesday 15:00–17:15 Location: POT 151

HL 71.1 Wed 15:00 POT 151

Strained Lonsdaleite Silicon as a Potential Absorber for Photovoltaics — •Claudia Rödl[1,2,3], Tobias Sander[2,3], and Friedhelm Bechstedt[2,3] — [1]Laboratoire des Solides Irradiés, Ecole Polytechnique, CNRS, CEA-DSM, 91128 Palaiseau cedex, France — [2]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany — [3]European Theoretical Spectroscopy Facility (ETSF)

Si in the diamond structure is one of the the key materials in photovoltaics, since it is abundant in nature and can be grown in extremely good quality. However, its fundamental band gap of 1.2 eV is indirect and only phonon-assisted absorption occurs in the visible spectral range. The direct absorption edge at 3.2 eV lies in the ultraviolet spectral region. Today a large variety of Si polymorphs is known, whereof some are semiconductors with direct gaps smaller than 3.2 eV.

Here, we calculate the optical absorption spectrum of Si in the lonsdaleite structure, also known as wurtzite Si, one of the most promising candidates for strong absorption in the visible spectral range. It features a direct band gap of 1.6 eV matching ideally with the solar spectrum. The quasiparticle band gap and the dielectric function including excitonic effects are calculated from first principles by many-body theory (*GW* method, Bethe-Salpeter equation). The optical absorption at the onset is compared to the absorption of diamond Si and discussed in terms of dipole-allowed and forbidden transitions. We study in detail the influence of hydrostatic pressure, uniaxial, and biaxial strain on the band gap and the optical absorption.

HL 71.2 Wed 15:15 POT 151

Passivation of Silicon surfaces by Aluminum oxide layers: a DFT simulation study — •Francesco Colonna[1,2] and Christian Elsässer[1,2] — [1]Albert-Ludwigs University, Freiburg Materials Research Center (FMF), Freiburg, Germany — [2]Fraunhofer IWM, Freiburg, Germany

By the Atomic Layer Deposition of Aluminum oxide on a Silicon (100) surface, followed by a heat-treatment, it is possible to obtain an excellent surface passivation [1], which is expected to play a significant role in future photovoltaic application.

In the present study we investigate the interplay between the electronic structure at the interface and the local atomic environments of Aluminum oxide by means of density functional theory (DFT) simulation methods. Observations show that passivation is associated with a change in the proportion of local tetrahedral and octahedral cation coordination in the passivation layer. We model a number of stoichiometric or oxygen-rich interfaces between Silicon and k-Alumina, which entails both tetrahedra and octahedra. We also study the role played by additional Hydrogen at the interface. We relate the local features of the interface to the presence of electronic defect levels in the band gap,

as computed by means of a self-interaction corrected [2] local-density approximation of DFT.

[1] G. Agostinelli et al., Solar Energy Materials and Solar Cells 90 (18-19), 3438-3443 (2006). [2] W. Körner and C. Elsässer, Physical Review B 81, 085324 (2010).

HL 71.3 Wed 15:30 POT 151

Electronic properties of nano-textured 'black' silicon — •Manuel Salzberger, Michael Algasinger, Svetoslav Koynov, and Martin Stutzmann — Walter Schottky Institut, Technische Universität München, 85748 Garching, Germany

Nano-textured silicon, also referred to as black silicon (b-Si), shows a reflectivity below 5% in the whole range of Si absorption [1]. Furthermore, the nano-texture exhibits efficient light trapping effects, making it interesting for application in thin film solar cells. However, all black Si solar cells reported up to now show a poor external quantum efficiency in the short wavelength range due to elevated surface recombination. Besides the enlarged surface area, also the potential distribution within the nano-texture can affect the recombination rate.

Electrical measurements of nano-textured thin Si films were performed in order to investigate the influence of the structure depth on the electronic properties. The b-Si nano-textures were prepared with an Au-catalyzed wet-chemical etch process. Cross-sectional scanning electron microscopy images show a nano-texture consisting of c-Si hillocks, reaching deep into the substrate. From the comparison with a planar reference sample, the influence of the nano-texture on the electrical conductivity will be investigated. From these findings, a better knowledge of the potential distribution within the nano-texture and, thus, a possible reduction of the surface recombination can be realized.

[1] S. Koynov, M. S. Brandt, and M. Stutzmann, Appl. Phys. Lett. 88, 203107 (2006).

HL 71.4 Wed 15:45 POT 151

Subnanometer thin silicon oxide films for the application as passivating interlayer in silicon heterojunction solar cells — •Wenjia Lu, Caspar Leendertz, Heike Angermann, Lars Korte, and Bernd Rech — Helmholtz-Zentrum Berlin, Institute for Silicon Photovoltaics, Kekuléstr. 5, 12489 Berlin, Germany

Subnanometer thin silicon oxide (SiO_x) has previously been applied as interlayer between crystalline silicon (c-Si) wafers and hydrogenated amorphous silicon ((p)a-Si:H). To optimize such thin SiO_x passivation layers, oxidations on silicon wafers with different crystal orientations were performed by different oxidation methods. Native oxide and wet-chemical oxides of different thickness and after different chemical wafer pre-treatment processes are compared. The layer thickness (d_{ox}) was measured with spectral ellipsometry, while field-dependent photovoltage measurements and minority charge carrier lifetimes have been applied in order to assess the interface passivation quality and to determine the interface defect density (D_{it}) and charge (Q_{it}). For the native oxides a correlation between the defect density and the charge indicates that the overall charge is dominated by electrons trapped in defects. This relationship cannot be found for the wet-chemical oxides which show superior passivation quality. The highest passivation quality is obtained for the (111) surfaces after NH4F pre-treatment for SiO_x layers of only 0.5 nm thickness. With a low D_{it}, a negative Q_{it} that supports emitter band bending and a low thickness, this wet-chemical oxide seems most suitable to be used as a buffer layer between the n-type c-Si absorber and the (p)a-Si:H emitter.

HL 71.5 Wed 16:00 POT 151

Comparison of Room Temperature Electroluminescence and Photoluminescence from Silicon Solar Cells — •Beatrice Pötschick, Karsten Kurasch, and Jörg Weber — Institut für Halbleiterphysik, Dresden, Germany

A set up for the detection of spatially- and spectrally-resolved luminescence from Si solar-cells was constructed. A thermoelectrically-cooled InGaAs-camera was connected to a spectrometer for investigations in the spectral range from 900 to 1700nm. After validating the performance of our system, we discuss the results of electroluminescence experiments on Si solar cells. The results are compared to spectrally resolved photoluminescence measurements from the same solar cells. Clear spectral differences of the two techniques are detected and related to different areas on the solar cell. The origin of these differences will be discussed.

HL 71.6 Wed 16:15 POT 151

Iron-related traps in near-junction volume of crystalline silicon solar cells — •Teimuraz Mchedlidze and Jörg Weber — Technische Universität Dresden, 01062 Dresden, Germany

Deep traps of majority carriers were detected recently in the near-to-junction volume (NJV) of fully processed crystalline solar cells [1]. The traps were detected using mesa-structured n+p-junctions prepared on the processed Si solar cells by deep level transient spectroscopy (DLTS). In this report we present an investigation of the trap formation at various stages of the standard solar cell fabrication process. The samples fabricated from the Czochralski-grown crystals with various initial iron contents were investigated. Total iron content in the samples was determined by DLTS in the as-grown samples subjected to high-temperature annealing followed by fast quenching. The NJV trap density at various steps of the solar cell fabrication process correlated with the iron content in the starting material and dropped strongly with the distance from the junctions. The traps were detected already after phosphorus diffusion and further fabrication processes varied their density depending on the initial iron content in the wafers. The results suggest that the iron-related NJV traps are formed during/after the phosphorus diffusion process. Our results could help in tailoring the solar cell fabrication process parameters to the content of contaminants in the feedstock.

[1] T. Mchedlidze, L. Scheffler, J. Weber, M. Herms, J. Neusel, V. Osinniy, C. Möller, and K. Lauer, Appl. Phys. Lett., 103, 013901 (2013).

HL 71.7 Wed 16:30 POT 151

Formation of near junction and bulk traps in crystalline silicon solar cells — •Teimuraz Mchedlidze[1], Christian Möller[2], Kevin Lauer[2], and Jörg Weber[1] — [1]Technische Universität Dresden, 01062 Dresden, Germany — [2]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik GmbH, Konrad-Zuse-Str. 14, 99099 Erfurt, Germany

Utilization of low quality feedstock for Si crystal growth was acknowledged as a valuable strategy for further price reduction of solar cell production. However, this strategy requires correct determination of the acceptable limits for the feedstock cleanness and relevant tailoring of the solar cell fabrication process. Recently we reported on influence of the fabrication steps on the bulk lifetime in the wafers produced from the various feedstock materials [1]. Deep traps of majority carriers were detected in the similar samples in near to the junction volume (NJV) using mesa-structured n+p-junctions prepared from the processed Si solar cells by deep level transient spectroscopy (DLTS) [2]. In this report we compare results from lifetime measurement and from DLTS for various quality crystals at various stages of solar cell fabrication process. Apparently, the NJV traps differ from those formed in the wafer bulk. However, in the both cases the trap densities correlate with the total content of iron in the crystals. The analyses of our results allow suggesting changes to the solar cell fabrication processes minimizing the influence of iron contamination.

[1] K. Layer, et al., Energy Proc., 38, 589 (2013) [2] T. Mchedlidze, et al., Appl. Phys. Lett., 103, 013901 (2013)

HL 71.8 Wed 16:45 POT 151

Nanostructuring of silicon and surface passivation of silicon nanostructures for organic-inorganic hybrid solar cell absorbers — •Stefanie Greil[1], Xin Zhang[1], Matthias Zellmeier[1], Silvia Janietz[2], Norbert Nickel[1], and Jörg Rappich[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium-Photovoltaik, Kekuléstr. 5, 12489 Berlin (Germany) — [2]Fraunhofer-Institut für Angewandte Polymerforschung IAP, Abteilung Polymere und Elektronik, Geiselbergstr. 69, 14476 Potsdam (Germany)

Metal assisted chemical etching (MACE) using Ag nanoparticles as catalysts is an outstanding method for nanostructuring Si wafers to modify its optical properties for photovoltaic applications. To obtain regular nanostructure arrays, MACE processes are combined with shadow nanosphere lithography. Self assembled polystyrene nanosphere masks were realized by Langmuir-Blodgett techniques. For further variations in diameter and spacing of the Si nanotrucures, reactive ion etching of the polystyrene nanosphere masks is applied. As MACE processes always lead to etching induced surface defects in the resulting Si nanostuctures, suitable post-etching surface treatments are necessary. As a direct surface passivation process, the application of electrochemical functionalization by methyl groups is examined. Another approach is to remove the damaged surface of the Si nanostuctures by subsequent electrochemical oxidation and Si oxide dissolution. Finally, the influences of the nanostructured substrate and its different surface pas-

sivation are studied on hybrid solar cells with a thiophene/Si interface.

HL 71.9 Wed 17:00 POT 151

Surface characterization of arsenic terminated Si(111) substrates with MOVPE for III-V nanowire solar cells — •Weihong Zhao[1], Agnieszka Paszuk[1], Matthias Steidl[1], Sebastian Brückner[1], Anja Dobrich[2], Johannes Luczak[2], Peter Kleinschmidt[1,3], Henning Döscher[1] und Thomas Hannappel[1,2,3] — [1]Technische Universität Ilmenau, Institut für Physik, Fachgebiet Photovoltaik, D-98684 Ilmenau — [2]Helmholtz-Zentru Berlin, Institut für Solare Brennstoffe und Energiespeichermaterialien, D-14109 Berlin — [3]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, D-99099 Erfurt

III-V nanowires grown on Si(111) substrates by metal-organic vapor phase epitaxy (MOVPE) enable a promising new solar cell concept meeting the demands of high-quality-low-cost photovoltaics. GaP buffer layers grown on Si(111) substrates represent suitable quasi-substrates since GaP is almost lattice-matched to Si. Apparently, preparation of atomically flat Si (111) surfaces is an essential step as a precondition for adjacent GaP heteroepitaxy. However, little is known about preparation and surface properties of Si(111) surfaces in MOVPE with H2 ambient. A contamination-free transfer system enabled us to study the MOVPE prepared surfaces with numerous UHV based surface science tools. We found that a dedicated wet-chemical pretreatment is crucial to obtain atomically flat Si(111) surfaces. Moreover, the GaP heteroepitaxy leads to an unfavorable A-type surface for growing vertical nanowires. We successfully applied a controlled arsenic termination procedure during the epitaxy for changing the surface polarity.

HL 72: Quantum dots: Transport properties

Time: Wednesday 15:00–16:15 Location: POT 251

HL 72.1 Wed 15:00 POT 251

Decoherence of an entangled states of a strongly-correlated double quantum dot structure through tunneling processes — •Carlos Alberto Büsser and Fabian Heidrich-Meisner — Department of Physics and Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-University Munich, Germany

The entanglement of the spin state of two quantum dots is investigated out of equilibrium. First, we prepare a two-dot system in a perfect singlet state at time $t = 0$. For $t > 0$, one of the dots is tunnel-coupled to leads, including a finite voltage. Using the time-dependent density matrix renormalization group method, we study the time evolution of the spin correlations and the concurrence as a function of time since electrons hopping on and off the tunnel-coupled dot lead to decoherence. We observe that the spin correlation between the dots decays exponentially determining a decoherence rate. A similar rate can be defined for the concurrence. We study the dependence of these rates on voltage, tunnel coupling, and Coulomb repulsion and compare our numerical results to a master-equation approach derived for the weak-coupling limit.

This work was supported by the Deutsche Forschungsgemeinschaft (DFG) through FOR 912 under grant-no. HE5242/2-2.

HL 72.2 Wed 15:15 POT 251

Resonant tunnelling structures for reducing the erase time in a quantum dot-based memory — •Ismail Firat Arikan[1,2], Nathanael Cottet[3], Tobias Nowozin[1], Dieter Bimberg[1], and Nurten Öncan[2] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany — [2]Department of Physics, Faculty of Science, Istanbul University, 34314 Vezneciler, Istanbul, Turkey — [3]ICFP, Departement de Physique, Ecole Normale Superieure, Paris, France

A memory based on self-organized quantum dots (QDs) is a promising candidate to combine the individual advantages of both DRAM and Flash, such as a long storage time (years), a fast write time (ns) and a good endurance. While the results are promising for the write performance, a trade-off exists for the erase performance: If the localization energy of the QDs is increased to further increase the storage time, the erase time also increases due to the increased tunnelling barrier. The solution to eliminate this trade-off between storage and erase time is to use a superlattice structure which implements resonant tunnelling as erasing mechanism. The transparency of such a structure is designed in such a way that it can be switched between very high and very low values by applying a bias voltage. In this work, a scheme for designing such a superlattice structure is presented. The structures are then simulated by using a one-dimensional Poisson-Schrödinger Solver and the Non-Equilibrium Green Function's formalism. For simple structures, first measurements are presented.

HL 72.3 Wed 15:30 POT 251

Spin-Spectroscopy of InAs Quantum Dots Defined in Gated Nanowires — •Sebastian Heedt[1], Thomas Gerster[1], Paul Wenk[2], Stefan Kettemann[3], Werner Prost[4], Jürgen Schubert[1], Detlev Grützmacher[1], and Thomas Schäpers[1] — [1]Peter Grünberg Institute (PGI-9) and JARA-Fundamentals of Future Information Technology, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [3]School of Engineering and Science, Jacobs University Bremen, 28759 Bremen, Germany — [4]Solid State Electronics Department, University Duisburg-Essen, 47057 Duisburg, Germany

The aim of this study is to investigate spin coherence properties of quantum dots defined in InAs nanowires by multiple top-gates and high-k dielectrics. This way, accurate control over the local potential landscape inside the nanowire is achieved and the quantum dots are tuned to the few-electron regime. An external magnetic field applied perpendicular to the nanowire axis strongly affects the quantum dot energy levels. Hence, the electron g factor can be determined and two-electron states exhibit an avoided-crossing in dependence of the magnetic field. The resulting energy gap gives a measure for the spin relaxation length inside the InAs quantum dot, which is compared with results from weak antilocalization in phase-coherent transport measurements. Spin relaxation exhibits a strong dependence on external electric fields yielding a cross-over from weak antilocalization to weak localization. Also, it is substantially affected by the confinement.

HL 72.4 Wed 15:45 POT 251

Two-path Transport Measurements with Bias Dependence on a Triple Quantum Dot — •Monika Kotzian, Maximilian C. Rogge, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, 30167 Hannover, Germany

We present transport measurements on a lateral triple quantum dot with a star-like geometry and one lead attached to each dot. [1] The research on triple quantum dots is motivated by fundamental physics and by the fact that it can work as a single qubit. [2] 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. Two of the leads are used as source contacts and one lead as a drain contact. Thus the setup provides the possibility of applying two different bias voltages to the system to study the interaction between the paths. By controlling the potentials via the four gates of the device resonances of two and all three dots can be generated. [3,4] Signatures of three dots can be detected in both transport paths. In the region of the triple dot resonance we observe a sharp suppression of the dc current depending on bias voltage, which we attribute to current blocking due to the presence of an interference phenomenon - a dark state.

[1] M. C. Rogge, R. J. Haug, Phys. Rev. B 77, 193306 (2008). [2] P. Hawrylak, M. Korkusinski, Solid State Comm. 136 (2005), pp. 508-512. [3] L. Gaudreau, et al., PRL 97, 036807 (2006). [4] M. C. Rogge, R. J. Haug, New Journal of Physics 11, 113037 (2009).

HL 72.5 Wed 16:00 POT 251

Temperature Driven Current Modulation in a Capacitively Coupled Double Quantum Dot — •Holger Thierschmann[1], Marcel Mittermüller[1], Luis Maier[1], Wolfgang Hansen[2], Hartmut Buhmann[1], and Laurens W. Molenkamp[1] — [1]Physikalisches Institut (EP3), Universität Würzburg, Germany — [2]Insitut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Universität Hamburg, Germany

In recent years multi-terminal devices with interacting quantum dots

(QD) have received an increasing attention. Especially subjected to a temperature difference such systems are expected to exhibit interesting effects, e.g. efficiently converting heat into a directed current [1]. Here we present measurements on a QD system consisting of two capacitively coupled dots. One of the QDs (QD1) can exchange energy and particles with a heat reservoir at a temperature T1 while the other (QD2) couples to two electron reservoirs at a lower temperature T2. In the vicinity of the triple points of the charge stability diagram we observe a strong dependence of the current through QD2 on the temperature of the heat reservoir T1. The sign of the current change is determined by the relative position of the dots' chemical potentials with respect to the reservoirs. I(QD2) can be related to the heat induced charge fluctuations.

[1] R. Sánchez and M. Büttiker, Phys. Rev. B 83, 085428 (2011)

HL 73: Organic electronics and photovoltaics IV (organized by CPP)

Spectroscopy, OFETs, OLEDs, Photo switches

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

HL 73.1 Wed 15:00 ZEU 260

Comprehensive efficiency analysis of organic light-emitting diodes featuring horizontal emitter orientation and triplet-to-singlet up-conversion — •Tobias Schmidt[1], Bert Scholz[1], Christian Mayr[1], Andreas Rausch[2], Thomas Wehlus[2], Dirk Michaelis[3], Norbert Danz[3], Thilo Reusch[2], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]OSRAM Opto Semiconductors GmbH, Leibnizstrasse 4, 93055 Regensburg, Germany — [3]Fraunhofer Institute for Applied Optics and Precision Engineering, 07745 Jena, Germany

The external quantum efficiency (EQE) of an organic light-emitting diode can strongly be affected by orientation of the emissive dipole moments, and for fluorescent dyes, by triplet-to-singlet up-conversion leading to an enhanced radiative exciton fraction (η_r), exceeding the spin-statistical limit of 25 %. By a combination of EQE investigations with time resolved photo- and electroluminescence measurements we are able to quantify the lower limit of the additionally created singlet excitons, e.g. by thermally activated delayed fluorescence, as well as the factors being responsible for light-outcoupling. For the investigated fluorescent system the EQE is boosted by two effects. First, due to horizontal alignment of the transition dipole moments, the outcoupling factor is enhanced by a factor of 1.3. Second, the enhanced η_r value of 36 %, results in an additional efficiency increase by a factor of 1.44. As a consequence of the combination of both effects the EQE almost doubles and values up to 5 % are achieved for direct emission in spite of a comparatively low emitter efficiency of 40 % only.

HL 73.2 Wed 15:15 ZEU 260

Multi-analytical investigation of SAM formation in printing relevant timescales III: OFET devices — •Milan Alt[1,2,6], Janusz Schinke[2,3], Sabina Hillebrandt[2,5], Marc Hänsel[2,4], Kaja Deing[2,6], Uli Lemmer[1,2], and Norman Mechau[1,2] — [1]Karlsruher Institute of Technology — [2]InnovationLab, Heidelberg — [3]TU Braunschweig — [4]TU Darmstadt — [5]Uni Heidelberg — [6]Merck KGaA

Self-assembled monolayers (SAMs) can be used to effectively reduce contact resistances originating from energetic misalignments at metal-semiconductor interfaces. Solution processing of SAMs has been intensively studied and is in principle compatible with high throughput printing techniques. However, most studies on SAMs feature immersion in very dilute solutions for many hours, in some cases up to several days. The objective of this work is to understand SAM accumulation with a focus on short time scales in order to estimate weather the deposition of well performing SAMs can be speeded up sufficiently to be compatible with typical film drying times in printing. We combined analytical characterization of SAM treated metal surfaces via photoelectron- and IR-spectroscopy, as well as Kelvin Probe with measurements of the actual injection barriers in OFET devices. We chose the widely used 1H,1H,2H,2H-Perfluorodecanethiol SAM and investigated its quality and charge injection performance in dependency of the process parameters immersion time and molecular concentration. Additionally, we studied the impact of ambient condition on SAM deposition and the resulting SAM performance, in order to account for a realistic fabrication environment.

HL 73.3 Wed 15:30 ZEU 260

Multi-analytical investigation of SAM formation on printing-relevant time scales I: Kelvin probe and photoelectron spectroscopy — •Janusz Schinke[1,5], Marc Hänsel[2,5], Milan Alt[3,4,5], Sabina Hillebrandt[2,5], Eric Mankel[6,5], Wolfram Jaegermann[6,5], Wolfgang Kowalsky[1,5], and Robert Lovrincic[1,5] — [1]TUBS, Inst. f. Hochfrequenztechnik — [2]Uni HD, Kirchhoff-Inst. für Physik — [3]Karlsruher Inst. f. Technologie — [4]Merck KGaA — [5]InnovationLab GmbH, Heidelberg — [6]TUD, Materials Science Inst.

In organic electronic devices, charge injection at the contacts is crucial for electrical performance. The devices require electrodes with a sufficiently low contact resistance at the metal-semiconductor interface to inject into or collect charge carriers from the transporting layer. A smart way to align the energetics at the interface is the use of self-assembled monolayers (SAMs). We have studied the properties of 1H,1H,2H,2H-Perfluorodecanethiol using photoelectron spectroscopy (XPS/UPS), infrared spectroscopy (IR), ambient Kelvin probe (KP), and contact angle (CA) measurements and the injection barriers were also measured in actual devices - organic field effect transistors. Using these methods we were able to obtain a very deep understanding of the whole SAM adsorption process, as well as the impact of immersion time, concentration and the influence of ambient conditions on the resulting monolayer and its performance. With this knowledge we estimate optimized parameters to speed up the treatment process, in contrast to most studies where long immersion times are used, to be compatible with typical times used in standard printing methods.

HL 73.4 Wed 15:45 ZEU 260

Multi-analytical investigation of SAM formation on printing-relevant time scales II: infrared-reflection-absorption-spectroscopy — •Sabina Hillebrandt[1,5], Janusz Schinke[2,5], Milan Alt[3,4,5], Robert Lovrincic[2,5], Tobias Glaser[1,5], and Annemarie Pucci[1,5] — [1]Universität Heidelberg, Kirchhoff-Institut für Physik — [2]Technische Universität Braunschweig, Institut für Hochfrequenztechnik — [3]Karlsruher Institut für Technologie — [4]Merck KGaA, Darmstadt — [5]Innovationlab GmbH, Heidelberg

In organic semiconductor devices the improvement of charge carrier injection between metal contact and organic semiconductor is a major concern. Self-assembled monolayers (SAMs) built up interface dipoles on metal surfaces that can increase or lower the work function of the material. Therefore SAMs can be used as injection layers. The properties of solution-processed SAMs such as orientation and interface dipole are influenced by various factors like concentration of the molecule in solution, immersion time and purity of the solution or substrate.

Infrared-reflection-absorption-spectroscopy (IRRAS) is very sensitive to changes in the orientation of SAMs on metal surfaces, thus we performed IRRAS measurements on SAMs consisting of 1H,1H,2H,2H-perfluorinated decanethiol on evaporated gold substrates. Orientation, ordering and quality of the SAM were investigated under systematic variation of immersion time and concentration of the molecule in solution. Taking into account realistic printing conditions we also investigated very short immersion times and high concentrations as well as the impact of oxygen in solvent and substrate on the layer formation.

HL 73.5 Wed 16:00 ZEU 260

Towards fully printed organic light-emitting diodes: investigation of solution processed electron injection layers — •Sebastian Stolz[1,4], Gerardo Hernandez-Sosa[1,4], Michael Scherer[2,4], Eric Mankel[3,4], Robert Lovrinčić[2,4], Janusz Schinke[2,4], Uli Lemmer[1,4], and Norman Mechau[1,4] — [1]Karlsruhe Institute of Technology, Light Technology Institute — [2]Technische Universität Braunschweig, Institut für Hochfrequenztechnik — [3]Technische Universität Darmstadt, Materials Science Institute, Surface Science Division — [4]InnovationLab GmbH, Heidelberg

The fabrication of organic light-emitting diodes (OLEDs) by high throughput printing techniques requires the development of solution processable electron injection layers. Today, either alkali salts or low work-function alkaline earth metals are used as cathode layers in

OLEDs. As these materials are highly reactive, they cannot be easily solution processed. In this work, we present blue fluorescent light-emitting diodes which use silver in combination with Polyethylenimine (PEI) and Polyethylenimine-ethoxylated (PEIE) as cathode layer. We demonstrate that both materials can be effectively used as electron injection layers in OLEDs and correlate the performance of the devices to the characteristics of the PEI(E) layers. Photoelectron spectroscopy is used to estimate the polymer thickness and the corresponding change in cathode work-function while the homogeneity of the layers is evaluated by AFM measurements. We show that OLEDs using PEI/PEIE and silver as cathode layer yield an improved performance and shelf lifetime compared to reference devices that use calcium, instead.

15 min. break

HL 73.6 Wed 16:30 ZEU 260

Micro-structured organic field effect transistor on commercial poly(urethane) resin as substrate and gate dielectric — Jan Hartel, Derck Schlettwein, and •Christopher Keil — Institute of Applied Physics, Laboratory of Materials Research, Justus-Liebig-University Giessen, Germany.

Dielectric layers of a commercial cross-linked poly (urethane) (PU) were prepared on a conductively coated film and served as gate dielectric and as substrate for the growth of an organic semiconductor film in an alternative approach to all-organic field effect transistors (OFET). A method was developed to process micro-structured electrodes on top of the PU dielectric layer which proved superior to the traditional lift-off-procedure. The influence of the aspect ratio of the electrodes within the organic transistor on a given dielectric layer will be discussed with respect to the calculation of the relative permittivity and the gate capacitance. A method is proposed to compensate short electrode effects which would otherwise lead to an underestimation of the gate capacitance and hence to a miscalculation of the OFET properties.

HL 73.7 Wed 16:45 ZEU 260

Time-resolved potentiometry of organic thin film transistors — •Jan Murawski, Tobias Mönch, Moritz Philipp Hein, Peter Milde, and Lukas M. Eng — Technische Universität Dresden, Institut für Angewandte Photophysik

High speed application still poses a challenge for organic thin film transistors (OTFTs) due to their low charge carrier mobilities, high driving voltages, and low on/off-current ratios. Few investigations have been reported on the switching dynamics of OTFTs on the nanoscale, even fewer in the relevant temporal operation regime as required for high speed applications. Yet, such investigations are crucial for understanding the bottle-necks in OTFTs dynamic performance.

Here, we introduce time-resolved Kelvin probe force microscopy (tr-KPFM) to track the time evolution of surface potential wave fronts inside the channel of a pentacene-based bottom-gate coplanar OTFT. The relevant dynamical evolution proceeds in the microsecond regime and is easily resolved by our quantitative tr-KPFM method. Comparing our experiment with simulations reveals the presence of Schottky barriers in the real device to be responsible not only for a reduced effective electric field across the transistor channel (and thus a reduced field mobility) but also for inducing a delayed re-injection of charge carriers at the electrode-semiconductor interface. Although the charge-carrier mobility would allow for faster switching, charging the Schottky barrier constitutes the bottle-neck to be overcome for higher working frequencies in OTFTs.

HL 73.8 Wed 17:00 ZEU 260

High-Mobility, Low-Voltage Organic TFTs based on Air-Stable DNTT Derivatives: Time-Dependent Improvement in Contact Resistance and Dynamic Performance — •Ulrike Kraft[1,3], Ute Zschieschang[1], Kazuo Takimiya[2], Edwin Weber[3], and Hagen Klauk[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]RIKEN Advanced Science Institute, Wako, Japan — [3]Technical University Bergakademie Freiberg, Germany

The organic semiconductor dinaphtothienothiophene and its derivatives C10-DNTT and diphenyl-DNTT provide larger carrier mobilities and better air stability than, e.g., pentacene. We present a detailed comparison of the thin-film morphology, static and dynamic performance and stability of low-voltage (3 V) thin film transistors based on vacuum-deposited films. Freshly fabricated TFTs (channel length: 100 um) have hole mobilities ranging from 3 cm2/Vs (DNTT) to 5 cm2/Vs (diphenyl-DNTT), with on/off ratios of 10ˆ7.

During the first few hours after fabrication, the effective mobility of short-channel TFTs (L=1 um) increases by about 20-30%, due to an improvement in the contact resistance (measured with TLM). The dependence of this effect on the exposure to different gas atmospheres, humidity and to light was investigated. To study the impact on the dynamic performance of the TFTs, we fabricated unipolar ring oscillators on flexible PEN substrates. The stage delay of DNTT TFTs (L=1 um) measured at 3 V drops from 920 to 410 ns during the first 4 days of exposure to ambient air, which is the shortest delay reported for flexible organic TFTs at supply voltages <10 V.

HL 73.9 Wed 17:15 ZEU 260

Continuously tunable organic semiconductor distributed Feedback (DFB) lasers as an example for optical components built from shape-memory polymers — •Senta Schauer[1], Xin Liu[2], Tobias Meier[1], Marc Schneider[1], Matthias Worgull[1], Uli Lemmer[1,2], and Hendrik Hölscher[1] — [1]Karlsruhe Institute of Technology, Institute of Microstructure Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [2]Karlsruhe Institute of Technology, Light Technology Institute, Engesserstraße 13, 76131 Karlsruhe, Germany

Phase gratings are important tools for many applications in optics and photonics, e.g., they serve as resonators in DFB-lasers. We manufactured Bragg gratings from a shape-memory polymer (SMP) to tune their period over a wide range without any mechanical components. SMPs can remember a predefined shape and recover to it even after strong deformations, if they are triggered by a stimulus. We used the polyurethane Tecoflex(R), which is a thermally triggered SMP, to fabricate nanostructured gratings via hot embossing. After stretching, these gratings feature an increased period which shrinks back to its original length after the activation of the recovery process. In order to demonstrate the practical applicability of these gratings as useful components for photonics, we successfully fabricated continuously tunable DFB-lasers based on SMP grating substrates with Alq3:DCM serving as active material. By changing the grating period via the shape-memory effect, the emitted wavelength of the laser changes likewise. So far we demonstrated shifts of the emission spectrum by 30nm.

HL 73.10 Wed 17:30 ZEU 260

Optical studies of excitonic precursor spin species under magnetic resonance in organic light emitting diodes. — •Hermann Kraus, Sebastian Bange, and John M. Lupton — Universität Regensburg, 93040 Regensburg, Deutschland

Large magnetoresistance effects e.g. due to spin-dependent recombination rates are well-known for OLEDs [C. Boehme et al., Nat. Nano 8, 612 (2013)], although models are still under debate given that they remain hard to verify from a measurement of integrated current and luminance values[J. M. Lupton et al., Nature Mat. 7, 598 (2008)]. Spin resonance of paramagnetic species enables direct manipulation of carrier and excitonic precursor spins, providing a wealth of new insight into dynamic spin properties. Previous work on electrical or optical detection of spin manipulation [W. J. Baker et al., Nature Comm. 3, 898 (2012); W. J. Baker et al., Phys. Rev. B 84, 165205 (2011)] misses out on the opportunity to directly observe the presence of triplet exciton species that are at the heart of spin-dependent recombination models. A few polymeric and small-molecular compounds are now known to exhibit reasonable triplet emission without modification of the polaron pair and exciton dynamics by strong spin-orbit interaction [D. Chaudhuri et al., Angew. Chem. Int. Ed. DOI 10.1002/anie.201307601(2013); J. M. Lupton et al., Phys. Rev. Lett. 89 167401(2002)]. Those materials are ideal candidates to directly track spin singlet and triplet excitonic species in organic light-emitting diodes under conditions of magnetic resonance, by comparing the fluorescence (singlet) to phosphorescence (triplet) intensity.

HL 73.11 Wed 17:45 ZEU 260

***Ab-initio* quantum dynamics simulation of photo-induced molecular switching: Azobenzene on coinage metals** — •Reinhard J. Maurer and Karsten Reuter — Department Chemie, Technische Universität München, Germany

The constant pursuit towards further miniaturization of electronic devices slowly reaches the point where individual molecules may serve as the main functional units. Unfortunately, more often than not, an inherent molecular function is quenched by overly strong coupling to the environment; a permanent danger, specifically in the case of metal surface adsorption. Nevertheless, metal surface adsorption may also in-

troduce new functionality, such as in the case of photo-induced molecular switching of tetra-*tert*-butyl-functionalized Azobenzene (TBA) on Au(111). In this work we attempt a full *ab-initio* description of the explicit nuclear and electronic dynamics to analyze a novel substrate-mediated process that was suggested for this system [1]. The immense system size and a continuum of electronic states demand an effective modelling approach explicitly accounting only for the most important degrees of freedom. Employing an efficient density-functional theory based ΔSCF approach [2] we construct and analyze the involved excited-state potential energy surfaces (PESs), and establish a mixed-quantum classical dynamics simulation. A particular focus is the effect of the image-charge induced changes on the excited-state PESs and the excited-state lifetime- and temperature-dependence of the quantum yield. [1] Wolf, Tegeder, Surf. Sci. **603**, 1506–1517 (2009); [2] Maurer, Reuter, J. Chem. Phys. **139**, 014708 (2013)

HL 73.12 Wed 18:00 ZEU 260

Reversible switching and light-induced structural changes in spin-coated thin films of Azobenzene-polymers — •Christopher Weber[1], Tobias Liebig[1], David Bléger[2], Stefan Hecht[2], Jürgen Rabe[1], and Stefan Kowarik[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik — [2]Humboldt-Universität zu Berlin, Institut für Chemie

Functionalized surfaces with molecules whose conformation can be reversibly switched between two isomeric forms by light are relevant for future devices -e.g. for switching adaptive materials, storing two states in memory applications, and switching current in molecular electronics. Here we use grazing incidence x-ray diffraction (GIXD), atomic force microscopy (AFM) and differential reflectance spectroscopy (DRS) to study light-induced structural changes in spin-coated thin films of Azobenzene-polymers with Alkyl side-chains. In solution, the individual Azobenzene-polymer shrinks upon UV-irradiation. Submonolayers of Azobenzene-polymers on Silicon oxide are still switchable with high efficiency, but do not show the same shrinking behavior, as suggested by AFM measurements before and after UV-illumination. Increasing the thickness to multilayers drastically changes the switching behavior, because of strong sterical hindrance. Interestingly, GIXD shows that the in-plane Bragg peaks corresponding to the coherent ordering of the Alkyl side-chains disappear when the sample is illuminated with UV-light and partially reappear after a few minutes in the dark, showing that switching is still possible in the crystalline state albeit with slower kinetics.

HL 74: Invited Talk: Heidemarie Schmidt (organized by DF)

Time: Wednesday 15:00–15:45 Location: GER 37

Invited Talk HL 74.1 Wed 15:00 GER 37

Smart multiferroic thin films for cognitive computing — •Heidemarie Schmidt — Technische Universität Chemnitz, Department of Materials for Nanoelectronics, Reichenhainer Str. 39, 09126 Chemnitz

Cognitive systems promise to penetrate complexity and assist people and organizations in better decision making [1]. We have successfully prepared metal-multiferroic-metal (MMM) structures with the multiferroic material BiFeO3 and BiFeTiO3. All those MMM structures exhibit nonvolatile resistive (meristive) switching. Investigations of memristive switching is driven by promising applications of power-efficient memristive nanostructures including data storage, logic systems, cognitive computing and artificial neural networks. Prominence of work on memristive systems might be visualized by the near-future breakthrough in computing technology, where classical Von Neumann architecture is replaced by cognitive systems. In this talk I present three new functionalities of smart MMM structures including nonvolatile multilevel resistive switching [2], nonvolatile reconfigurable logics and nonvolatile second and higher harmonics generation [3] which are very promising for the development of cognitive computing. [1] J. E. Kelly III, S. Hamm, Smart Machines: IBM*s Watson and the Era of Cognitive Computing, Columbia University Press, 2013 [2] Y. Shuai et al., J. Appl. Phys. 109 (2011); Appl. Phys. Lett. 98 (2011); Appl. Phys. Exp. 4 (2011); 111 (2012); IEEE Electron Device Letters 34 (2013); Scientific Reports 3 (2013) [3] N. Du et al., Rev. Sci. Instr. 84 (2013)

HL 75: Transport: Majorana fermions (organized by TT)

Time: Wednesday 15:00–18:00 Location: HSZ 03

HL 75.1 Wed 15:00 HSZ 03

Majorana spin liquid and dimensional reduction in Cs_2CuCl_4 — •Tim Herfurth, Simon Streib, and Peter Kopietz — Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Strasse 1, 60438 Frankfurt, Germany

The low-temperature behavior of the magnetic insulator Cs_2CuCl_4 can be modeled by an anisotropic triangular lattice spin 1/2 Heisenberg antiferromagnet with two different exchange couplings J and $J' \approx J/3$. We show that in a wide range of magnetic fields the experimentally observed field dependence of the crossover temperature T_c for spin-liquid behavior can be explained within a mean-field theory based on the representation of spin operators in terms of Majorana fermions. We also show that for small magnetic fields the specific heat and the spin susceptibility both exhibit a maximum as a function of temperature at $T_c = J/2$. In the spin-liquid regime, the Majorana fermions can only propagate along the direction of the strongest bond, in agreement with the dimensional reduction scenario advanced by Balents[1].
[1] Nature **464**, 199 (2010)

HL 75.2 Wed 15:15 HSZ 03

Supersymmetry in the Majorana Cooper pair box — •Jascha Ulrich and Fabian Hassler — Institut für Quanteninformation, RWTH Aachen

Over the years, supersymmetric quantum mechanics (SUSY QM) has evolved from a toy model of high energy physics to a research direction of its own. Although many examples of SUSY QM systems have been found, systems that can be naturally realized are generally scarce. In this work, we argue that the interaction of fermionic subgap Majorana bound states with the underlying Cooper pair condensate provides a natural setting for SUSY QM. We show that the extension of the conventional Cooper pair box by an anomalous Majorana-Josephson coupling realizes SUSY QM for certain values of gate voltage and Josephon/Majorana-Josephson coupling ratio. We show that the resulting degeneracy of all subgap energy levels can be probed directly in a tunneling experiment and discuss the various transport signatures. An observation of the predicted level degeneracy would provide evidence for the presence of a Majorana-induced anomalous Josephson coupling.

HL 75.3 Wed 15:30 HSZ 03

Robustness of exchange protocols of Majorana fermions in quantum wire networks — •Rolf W. Reinthaler[1], Chao Lei[2], Allan H. MacDonald[2], and Ewelina M. Hankiewicz[1] — [1]Faculty of Physics and Astrophysics, University of Würzburg, Würzburg, Germany — [2]Department of Physics, University of Texas at Austin, USA

The ends of one-dimensional spinless p-wave superconductors support Majorana bound states [1], whose non-trivial exchange statistics makes them promising candidates for topological quantum computation [2]. The huge advantage of using networks of 1D nano wires is that the Majorana fermions can be manipulated and exchanged by purely electrical means [3]. By applying a tight binding approach we solve the time dependent Bogoliubov-de Gennes equations for the Kitaev chain model [1]. We analyze how the robustness of the exchange protocols is affected by non-adiabatic effects as well as by a finite overlap of the Majorana bound states.

We acknowledge financial support by the DFG grant HA 5893/3-1.

[1] A. Y. Kitaev, Physics-Uspekhi **44** (2001) 131
[2] D. A. Ivanov, PRL **86** (2001) 268
[3] J. Alicea et al., Nature Physics **7** (2011) 412

HL 75.4 Wed 15:45 HSZ 03

Absence of Aharonov-Bohm effect of chiral Majorana fermion edge states — •Sunghun Park[1,4], Joel Moore[2,3], and Heung-Sun Sim[1] — [1]Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 305-701, Korea — [2]Department of Physics, University of California, Berkeley, California 94720, USA — [3]Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA — [4]Institute for Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany

Majorana fermions in a superconductor hybrid system are charge neutral zero-energy states. For the detection of this unique feature, we propose an interferometry of a chiral Majorana edge channel, formed along the interface between a superconductor and a topological insulator under an external magnetic field perpendicular to the surface of the topological insulator. The superconductor is of a ring shape and has a Josephson junction that allows the Majorana state to enclose continuously tunable magnetic flux. Zero-bias differential electron conductance between the Majorana state and a normal lead is found to be independent of the flux at zero temperature, manifesting the Majorana feature of a charge neutral zero-energy state. To compare with a non-Majorana case, we consider the same setup on graphene. In this case, the setup has no Majorana states and shows Aharonov-Bohm effects.

HL 75.5 Wed 16:00 HSZ 03

Fractional Josephson effect in a quadruple quantum dot — •Björn Sothmann, Jian Li, and Markus Büttiker — Département de Physique Théorique, Université de Genève, CH-1211 Genève 4, Switzerland

A double quantum dot coupled to an s-wave superconductor and subject to an inhomogenous magnetic field can host a pair of zero-energy Majorana fermions when the dot properties are tuned appropriately [1]. Here, we demonstrate the possibility to generate a fractional 4π Josephson effect in two such double dots tunnel-coupled to each other. We discuss the robustness of this effect with respect to perturbations away from the special point in parameter space where the uncoupled doube dots host Majorana fermions. We point out the possibility to generate Josephson effects with a period of 8π and 12π in strongly-coupled double dots.

[1] M. Leijnse and K. Flensberg, Phys. Rev. B **86**, 134528 (2012)
[2] B. Sothmann, J. Li, M. Büttiker, New J. Phys. **15**, 085018 (2013)

15 min. break.

Invited Talk HL 75.6 Wed 16:30 HSZ 03

Majorana Fermions in Chains of Magnetic Atoms on the Surface of a Superconductor — •Ali Yazdani — Princeton University

In this talk, I will describe a proposal and related experiments for realization of Majorana fermions in chains of magnetic atoms on the surface of a conventional superconductors. I will describe model calculations that motivate the experimental studies, which show that a spiral spin textured chain of atoms give rise to a topological superconducting phase when place in contact with a s-wave superconductor. Remarkably, only chains of as long as few tens of atoms is required to realize this phase in the calculations. I will also describe experiments in which we use in situ assembly of magnetic atoms on the surface of an s-wave superconductor and spectroscopic mapping with a scanning tunneling microscope (STM) to search for signatures of Majorana fermions at the end of such chains. Spin-polarized STM experiments in which we probe the spin texture of such chains will also be described.

[1] S. Nadj-Perge, I.K. Drozdov, B.A. Bernevig, and A. Yazdani, Phys. Rev. B 88, 020407 (2013)
[2]J. Klinovaja, P. Stano, A. Yazdani, and D. Loss, Phys. Rev. Lett. 111, 186805 (2013)

HL 75.7 Wed 17:00 HSZ 03

Disordered one-dimensional topological superconductors — •Michael Wimmer[1,2], Inanc Adagideli[3], and Aykut Teker[3] — [1]Universiteit Leiden, The Netherlands — [2]TU Delft, The Netherlands — [3]Sabanci University, Istanbul, Turkey

It is well-established that disorder is harmful to a topological phase in p-wave superconductors [1]. Recently, it has been proposed to engineer ap-wave superconductor using conventional materials: a nanowire with strong spin-obrit coupling in proximity to a s-wave superconductor and in a magnetic field ("s-wave Rashba wires"), and first experimental results have been obtained [2].

We present a simple and intuitive method to link topological properties of superconducting wires to their normal state properties. This allows to describe ensemble-averaged topological properties as well as individual systems. In particular, we show that the effect of disorder is quite different in p-wave superconductors and s-wave Rahsba wires: While disorder is always harmful for the former, topology can be created by disorder in the latter [3].

[1] P. Brouwer *et al.* Phys. Rev. B **84**, 144526 (2011)
[2] V. Mourik *et al.* Science **336**, 1003 (2012)
[3] I. Adagideli, M. Wimmer, A. Teker. arXiv:1302.2612 (2013)

HL 75.8 Wed 17:15 HSZ 03

Majorana Fermions in Antiferromagnetically doped Superconductors — •Andreas Heimes, Panagiotis Kotetes, and Gerd Schön — Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany

Recently the field of Majorana fermions (MFs) in solid state physics has attracted great attention. Among the many existing proposals for their experimental realization and detection, one can distinguish a class of self-tuned MF systems, consisting of spiral spin chains on s-wave superconductors. We propose an alternative MF platform based on a chain of antiferromagnetically (AFM) ordered magnetic impurities on top of a conventional superconductor, which has the advantage that it allows for an external tunability by experimental parameters: The transition to the MF regime is achieved and controlled by the combination of a supercurrent flow and a Zeeman field. In fact, the latter can be considerably weak since the presence of the AFM order relaxes the requirement of a large Zeeman energy. Evenmore, the currently existing STM technology renders our proposal directly experimentally accessible.

HL 75.9 Wed 17:30 HSZ 03

Majorana fermions in quasi-1d Rashba semiconductor/superconductor heterostructures without the requirement of a Zeeman field — •Panagiotis Kotetes, Alexander Shnirman, and Gerd Schön — Karlsruhe Institute of Technology

Recent experiments have provided the first promising indications of Majorana fermions (MFs) in heterostructures consisting of Rashba semiconducting wires and superconductors in the presence of a Zeeman field. By performing a complete classification of engineered topological superconductors (TSCs) [1] we predict that MFs are accessible in quasi-1d Rashba semiconductors with proximity induced superconductivity, even in the absence of magnetism. The only requirement is the presence of a Josephson current, flowing transversely to the principal axis of the quasi-1d structure. Here, we demonstrate how MFs emerge within our proposal when multi-wire or multi-channnel semiconductors are involved. The crucial effect of the supercurrent flow is to convert the inter-wire/channel spin-orbit coupling into an effective Zeeman term. Our results can motivate a new set of experiments using the already developed devices but in different configurations, providing in this way an accessible and irrefutable method for confirming the emergence of MFs.

[1] P. Kotetes, New J. Phys. 15, 105027 (2013)

HL 75.10 Wed 17:45 HSZ 03

Quantum spin liquid with a Majorana Fermi surface on the three-dimensional hyperoctagon lattice — •Maria Hermanns and Simon Trebst — Institut für Theoretische Physik, Universität zu Köln

Motivated by the recent synthesis of β-Li_2IrO_3 – a spin-orbit entangled $j = 1/2$ Mott insulator with a three-dimensional lattice structure of the Ir^{4+} ions – we consider generalizations of the Kitaev model, believed to capture some of the microscopic interactions between the Iridium moments, on various trivalent lattice structures in three spatial dimensions. Of particular interest is the so-called hyperoctagon lattice – a cubic non-Bravais lattice, which is probably best described as the premedial lattice of the hyperkagome lattice – for which the ground state is a gapless quantum spin liquid where the gapless Majorana modes form an extended Majorana Fermi surface. We demonstrate that this Majorana Fermi surface is inherently protected by lattice symmetries and discuss possible instabilities when allowing for a reduction in lattice symmetries. We discuss these findings also in light of recent results obtained for the hyperhoneycomb lattice.

HL 76: Graphene: Electronic properties (organized by O)

Time: Wednesday 16:00–19:15 Location: WIL C107

HL 76.1 Wed 16:00 WIL C107

Monomer Doping of Self-Assembled Graphene Nanoribbons for Band Gap Alignment — •Christopher Bronner[1,3], Stephan Stremlau[1,3], Marie Gille[2], Felix Brausse[2], Anton Haase[1], Stefan Hecht[2], and Petra Tegeder[1,3] — [1]Freie Universität Berlin — [2]Humboldt-Universität zu Berlin — [3]Ruprecht-Karls-Universität Heidelberg

In order to exploit the technologically interesting electronic properties of graphene, several concepts have been discussed which would lead to the opening of a band gap. One approach is spatial confinement of the charge carriers in quasi-one-dimensional graphene nanoribbons (GNRs). The band gap of a GNR scales inversely with its width and particularly nanometer-scale widths are desirable for application e.g. in transistor devices. Since the electronic properties of GNRs depend critically on their structure, precise synthesis is necessary but challenging for conventional methods such as lithography. In contrast, self-assembly from molecular precursors is an intriguing approach which has been employed to fabricate defect-free GNRs with well-defined widths and edge structures. Only this high level of structural precision allows introduction of dopant atoms at specific doping sites and concentrations in the graphene lattice. Nitrogen doping has been known to shift the band structure of GNRs with respect to the Fermi level which is interesting for GNRs in contact with electrodes and other device materials. Using surface-sensitive electron spectroscopies we demonstrate a continuous down-shift of the band structure with increased nitrogen doping of the monomers.

HL 76.2 Wed 16:15 WIL C107

Transport in chemically gated graphene p-n junctions — •Jens Baringhaus[1], Alexander Stöhr[2], Ulrich Starke[2], and Christoph Tegenkamp[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, 30167 Hannover, Germany — [2]Max-Planck Institut für Festkörperforschung, 70569 Stuttgart, Germany

The chirality of charge carriers in graphene allows them to get through potential barriers without any reflection (known as Klein tunneling). To study this effect the fabrication of well-defined p-n junctions is necessary. We use the intercalation of Ge to convert the buffer layer on the SiC(0001) surface into graphene with local p-type or n-type doping depending on the local Ge coverage. The buffer layer is initially patterned using optical lithography, to fabricate isolated n-p, n-p-n and p-n-p structures. The n- and p-type doping (340 meV, -290 meV) is confirmed by STS which also reveals very narrow p-n junctions with a length below 5 nm. The corresponding electric fields are as high as 10^6 V/cm and therefore significantly higher than those induced by field effects, providing a perfect environment to study Klein tunneling. Transport experiments are carried out by means of a 4-tip STM system, on n-p-n as well as p-n-p structures. Their resistance was found to be strongly dependent on temperature and the inner barrier length. While short barriers (< 200 nm) appear almost transparent, the resistance increases rapidly for barrier widths exceeding the coherence length (> 600 nm). The resistance of a single p-n junction fits to the theoretically predicted value for a Klein tunneling junction.

HL 76.3 Wed 16:30 WIL C107

Exceptional ballistic transport in epitaxial graphene nanoribbons — Jens Baringhaus[1], Frederik Edler[1], Claire Berger[2], Walter A. de Heer[2], and •Christoph Tegenkamp[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, 30167 Hannover, Germany — [2]Georgia Institute of Technology, Atlanta, Georgia 30332-0430, USA

The patterning of graphene into graphene nanoribbons is an essential task for the development of graphene based devices. For such ribbons with a well-ordered edge geometry the presence of one-dimensional edge states has been predicted. We use a selective graphitization process on SiC-mesa structures to produce graphene nanoribbons with a width of 40 nm. The local electronic properties of the ribbons are investigated by means of a 4-tip STM. In combination with a SEM, the precise positioning of all four tips on the nanometer range is possible to perform local transport measurements. Additionally, local tunneling spectroscopy reveals characteristic features of ferromagnetic zig-zag graphene nanoribbons. Transport experiments carried out on the very same ribbon show a conductance close to e^2/h for a wide temperature range from 30 K up to room temperature and probe spacings between 1 μm and 10 μm. Description within the Landauer formalism is possible assuming ballistic transport dominated by a single channel. Transport in the second zeroth subband is only detectable for probe spacings smaller than 1 μm due to the short localization length of carriers in this subband manifesting in the increase of the conductance to 2 e^2/h at probe spacings below 200 nm.

HL 76.4 Wed 16:45 WIL C107

Electrical Transport in Freestanding Epitaxial Graphene: Evidence of an AB-Stacked Bilayer — •Johannes Jobst[1,2], Shriram Shivaraman[3], Michael G. Spencer[3], and Heiko B. Weber[2] — [1]Leiden University, Kamerlingh Onnes Laboratorium, P.O. Box 9504, NL-2300 RA Leiden, Netherlands — [2]Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — [3]School of Electrical and Computer Engineering, Cornell University, Ithaca, NY 14853, USA

We investigate the properties of freestanding epitaxial graphene devices, which are created using a photo-electrochemical etching technique. This technique allows to selectively remove the silicon carbide (SiC) substrate on which the graphene was grown by thermal decomposition of SiC. We focus on completely freestanding devices of various geometries and devoid of any graphene-substrate interactions. We prepare freestanding Hall bars in order to study the low-temperature transport and Shubnikov-de Haas oscillations. We find evidence that the buffer layer is transformed to an additional graphene layer upon the etching process, and that the formed bilayer is AB stacked. Inhomogeneities in the buffer layer or introduced during the etching process are discussed.

HL 76.5 Wed 17:00 WIL C107

Scattering mechanisms in Tl-doped epitaxial graphene — •Carola Strasser[1], Bart Ludbrook[2], Andrea Damascelli[2], Christian R. Ast[1], and Klaus Kern[1,3] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]Quantum Matter Institute, UBC, Vancouver, BC V6T 1Z4, Canada — [3]Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Since the charge carrier density in graphene can very easily be tuned by means of chemical doping this approach counts as a promising way to design graphene-based future electronic devices. It was shown [1] that the Fermi level can be shifted over a wide range in either direction. But one has to consider that the dopants do not just donate or take the electrons but they have an impact on the electronic structure: they act as scattering centres and change the charge carrier mobility.

We investigated small amounts of Thallium atoms on a monolayer of epitaxial graphene by angular resolved photoemission spectroscopy and did a careful analysis of the line width. Although Tl is very weakly bound and at first sight a paradigm long-range scatterer, we found that it introduces a sizeable short-range contribution. Only by using a model which combines both, long-range and short-range scattering we were able to describe our observations. This allowed us to put an upper limit on the dielectric constant for Tl-doped epitaxial graphene.

[1] H. Liu et al., *J. Mater. Chem.* **21**, 3335 (2011)

HL 76.6 Wed 17:15 WIL C107

Excited electron dynamics in spatially aligned 7a-graphene nanoribbons on Au(788) — •Nils Fabian Kleimeier[1], Alexander Timmer[1], Harry Mönig[1], Xinliang Feng[2], Klaus Müllen[2], Harald Fuchs[1], and Helmut Zacharias[1] — [1]Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Max-Planck-Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Photoelectron spectroscopy of spatially aligned straight 7-armchair graphene nanoribbons (7-aGNRs) on Au(788) was carried out under ultra high vacuum conditions utilizing a time-of-flight spectrometer and a multi-anode detector. We found two unoccupied states at energies of E_1=3.6 eV and E_2=3.9 eV above the Fermi energy by exciting the sample with different photon energies (3.94 eV to 4.35 eV) from a femtosecond OPA. When exciting the sample with ultrashort pules (20 fs) at λ=390 nm ($h\nu$=3.15 eV) by frequency- doubling the output of a femtosecond Ti:sapphire laser amplifier, these states can further be investigated by 3-photon photoemission using a third state at an energy of

E_3-E_F=0.6 eV as intermediate. All three states are in agreement with IPE measurements we performed previously on this system [1]. Thus the electronic dynamics of the state can be measured by time-resolved 3-photon photoemission spectroscopy with cross-polarized laser pulses. Preliminary evaluation of these measurements indicates electronic lifetimes of the unoccupied states of $\tau \sim$110 fs and 85 fs for the states at E-E_F 3.9 eV and 3.6 eV, respectively.

References: [1] S. Linden et al., Phys. Rev. Lett. 108 (2012) 216801

HL 76.7 Wed 17:30 WIL C107

Optical characterization of atomically precise graphene nanoribbons — •Richard Denk[1], Michael Hohage[1], Jinming Cai[2], Pascal Ruffieux[2], Roman Fasel[2], and Peter Zeppenfeld[1] — [1]Experimental Physics, JKU Linz, Altenbergerstrasse 69, 4040 Linz, Austria — [2]nanotech@surfaces, EMPA, Überlandstasse 129, 6800 Dübendorf, Switzerland

Graphene nanoribbons (GNRs) promise high potential for future nanoscale electronic devices. While 2-dimensional graphene is semimetallic, electron confinement and edge effects in narrow (<10nm) GNRs can result in the opening of a band gap. The electronic and optical properties, however, strongly depend on the structural details of the GNRs. Only recent advances in the bottom-up fabrication of atomically precise GNRs [1] have enabled reliable experimental investigations of well-defined GNRs.

We have studied the fabrication process and the optical properties of GNRs on Au(788) using reflectance difference spectroscopy (RDS), taking advantage of the optical anisotropy due to the uniaxial alignment of the GNRs parallel to the step edges of the vicinal Au(788) surface. We find that the optical properties of the GNRs are highly anisotropic and dominated by three excitonic transitions, in excellent agreement with theoretical calculations.

[1] J. Cai at el, Nature, 466 (2010) 470.

HL 76.8 Wed 17:45 WIL C107

Electronic and transport properties of BNC heterostructures, a first-principles investigation. — •Simon Dubois and Jean-Christophe Charlier — Institute of Condensed Matter and Nanosciences, UCL, Louvain-La-Neuve, Belgium

Two dimensional hexagonal BN (h-BN), an isomorph of graphene with a lattice mismatch of only 1 .7%, is a wide gap insulator as its bulk counterpart. Advances in the synthesis of hybrid BNC heterostructures offer new opportunities to engineer the electronic properties of low-dimensional systems. Recently, it has been shown that the introduction of h-BN nanodomains into graphene enables to induce a tunable band gap in the honeycomb lattice. Lateral junctions between electrically conductive graphene and insulating h-BN provide new ways to embed electrically isolated elements within single atomic layers. Not only the two-dimensional BNC heterostructures hold promises for new applications but also the corresponding quasi-1D nanoribbons as well as the few layers structures obtained by plane stacking.

We report on the properties of low energy carriers in various kind of BNC heterostructures investigated by means of first-principles calculations: quasi one dimensional junctions made of h-BN and graphene ribbons, two-dimensional atomic layers made of hybridized domains, as well as few-layers stacks.

HL 76.9 Wed 18:00 WIL C107

Time- and Angle-Resolved Photoemission Studies of Epitaxial Graphene — •Søren Ulstrup[1], Jens C. Johannsen[2], Federico Cilento[3], Alberto Crepaldi[3], Michele Zacchigna[3], Jill A. Miwa[1], Philip D. C. King[4], Cephise Cacho[5], Edmond Turcu[5], Emma Springate[5], Felix Fromm[6], Christian Raidel[6], Thomas Seyller[6], Fulvio Parmigiani[3], Marco Grioni[2], and Philip Hofmann[1] — [1]Aarhus University, Aarhus, Denmark — [2]EPFL, Lausanne, Switzerland — [3]Sincrotrone Trieste, Trieste, Italy — [4]University of St. Andrews, St. Andrews, United Kingdom — [5]STFC Rutherford Appleton Laboratory, Didcot, United Kingdom — [6]Technical University of Chemnitz, Chemnitz, Germany

Understanding of the ultrafast carrier dynamics in graphene is of central importance for many electronic and optoelectronic applications. With the advent of high harmonic laser-based time- and angle-resolved photoemission (TR-ARPES) it is possible to gain a direct view of the non-equilibrium electronic structure around the Dirac point in graphene with femtosecond time resolution. Here, we characterize the dynamic processes around the Dirac point in epitaxial graphene using TR-ARPES measurements. In particular, we study the time-scales and significance of hot electron thermalization processes and electron-phonon coupling, and address the possibility of carrier multiplication.

HL 76.10 Wed 18:15 WIL C107

Electronic and Transport Properties of Epitaxial Graphene on the Atomic Scale — •Philip Willke[1], Thomas Druga[1], Alexander Schneider[2], Rainer Ulbrich[1], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Georg-August Universität Göttingen, Germany — [2]Lehrstuhl für Festkörperphysik, FAU Erlangen, D-91058, Germany

The application of graphene in future devices requires a thorough understanding of its transport properties on the nanometer scale. We present a scanning tunneling potentiometry study at 6 K of electron scattering in mono- and bilayer graphene on n-doped SiC. Using STP we combine the imaging of local transport fields and sample topography. By probing simultaneously the thermovoltage signal [1] created due to slightly different temperatures of sample and tip, we can moreover obtain sensitive information on the electronic structure at the Fermi energy. We demonstrate how both transport and electronic information can be disentangled from STP measurements. We identify substrate steps and monolayer-bilayer junctions as local scattering centers which impede the electronic current and create local voltage drops that we compare to recent measurements at 72 K. [2] Moreover, wrinkles and substrate inhomogeinities have been identified as further sources of scattering. We acknowledge the financial support by the SPP 1459 "Graphene".

[1] K. J. Engel, M. Wenderoth, N. Quaas, T. Reusch, K. Sauthoff and R.Ulbrich, Phys. Rev. B 63, 165402 (2001)

[2] S. H. Ji et al., Nature Materials 11, 114-119 (2012)

HL 76.11 Wed 18:30 WIL C107

Exchange coupling between 3*d*-transition metal adatoms and Ni(111) mediated by graphene — •Simon Fichtner, Paolo Ferriani, and Stefan Heinze — Institut für Theoretische Physik und Astrophysik, Christian-Albrecht-Universität zu Kiel, D-24098 Kiel, Germany

Recently, 3*d*-transition metal (TM) adatoms on graphene have been intensively studied both experimentally (e.g. [1]) and theoretically (e.g. [2]). However, the possibility to stabilize their magnetic moment by exchange coupling to an underlying magnetic substrate has received little attention so far. Graphene on Ni(111) is a very good candidate in this respect as it has been experimentally shown to grow pseudomorphically. Here, we determine the electronic and magnetic properties of 3*d*-TM adatoms adsorbed on graphene on Ni(111) based on density functional theory as implemented in the VASP code. We perform a systematic study on the dependence of the exchange interaction across the 3*d*-TM series and take local correlations into account using the DFT+U formalism. We demonstrate the essential influence of the alignment of the adatoms 3d-states with the spin-polarized graphene states on the magnetic coupling with the Ni surface.

[1] Eelbo et al., Phys. Rev. Lett. **110**, 136804, 2013

[2] Wehling et al., Phys. Rev. B **84**, 235110, 2011

HL 76.12 Wed 18:45 WIL C107

Highly spin-polarized Dirac fermions at the graphene-Co interface — •Dmitry Marchenko[1,2], Andrei Varykhalov[1], Jaime Sánchez- Barriga[1], and Oliver Rader[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [2]Physikalische und Theoretische Chemie, Freie Universität Berlin, Berlin, Germany

The interface of graphene with ferromagnets is very interesting for spintronics due to possible use of peculiar graphene electronic structure in transport and spin-filter applications when graphene is used together with nickel or cobalt as ferromagnetic contacts for spin injection and detection [1]. Despite a strong hybridization between graphene and ferromagnetic substrate states the graphene Dirac cone was observed by angle-resolved photoemission without gap between pi and pi* parts [2]. Here we report strong spin polarization of the Dirac cone measured by spin- and angle-resolved photoemission. Wave-vector dependent measurements exclude a Rashba-type spin-orbit contribution to the spin polarization; ferromagnetic origin is verified by reversal of the remanent magnetization. The importance of the spin polarization at the interface for spin filtering is pointed out.

[1] V. M. Karpan et al., Phys. Rev. Lett. 99, 176602 (2007) [2] A. Varykhalov et al., Phys. Rev. X 2, 041017 (2012)

HL 76.13 Wed 19:00 WIL C107

Controlling and understanding the non-linear photoluminescence in graphene on a femtosecond time scale —

•Richard Ciesielski[1], Alberto Comin[1], Matthias Handloser[1], Kevin Donkers[1], Torben Winzer[2], Ermin Malic[2], and Achim Hartschuh[1] — [1]Ludwig Maximilians Universität München & CeNS — [2]TU Berlin

Upon excitation, graphene exhibits nonlinear photoluminescence [1-3] that reflects the charge-carrier population and relaxation around the K-point. We present microscopic measurements on high quality exfoliated graphene samples with a pulsed laser system of ca. 18fs and a broad spectrum centred at 800nm.

Using a pulse shaping setup we can measure and manipulate the incident pulse in amplitude and phase. We find that the PL intensity depends sensitively on the temporal shape of the laser pulse, which we use to study and control the charge-carrier relaxation processes of graphene. Our findings are compared to numerical calculations.

[1] Stöhr, Wachtrup, Phys. Rev. B 82, 121408(R) (2010)
[2] Malic, Winzer, Bobkin, Knorr, Phys. Rev. B 84, 205404 (2011)
[3] Malic, Knorr, John Wiley & Sons (2013)

HL 77: Frontiers of electronic structure theory - Non-equilibrium phenomena at the nano-scale V (organized by O)

Time: Wednesday 16:00–19:15 Location: TRE Ma

Topical Talk HL 77.1 Wed 16:00 TRE Ma

Theory of nonlinear phononics for coherent light-control of solids — •Antoine Georges[1,2,3], Alaska Subedi[2], and Andrea Cavalleri[4] — [1]College de France, Paris, France — [2]Ecole Polytechnique - CPHT, Palaiseau, France — [3]University of Geneva, DPMC, Switzerland — [4]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

The use of light to control the structural and electronic properties of solids is an area of great current interest. We present a microscopic theory [arXiv:1311.0544] for ultrafast control of solids with high-intensity Tera-Hertz frequency optical pulses. When resonant with selected infrared-active vibrations, these pulses transiently modify the crystal structure and lead to new collective electronic properties. The theory predicts the dynamical path taken by the crystal lattice using first-principles calculations of the energy surface and classical equations of motion, as well as symmetry considerations. Two classes of dynamics are identified. In the perturbative regime, displacements along the normal mode coordinate of symmetry-preserving Raman-active mode can be achieved by cubic anharmonicities. This validates the mechanism proposed by Först et al. [Nature Physics 7, 854 (2011)] and explains the light-induced insulator-to-metal transition of manganites reported experimentally by Rini et al. [Rini et al. Nature 449, 72 (2007)]. We also predict a new non-perturbative regime in which ultra-fast instabilities that break crystal symmetry can be induced.

HL 77.2 Wed 16:30 TRE Ma

DFT+Frontier Orbital U — •Emine Kucukbenli and Nicola Marzari — Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne (CH)

Piecewise linearity of the total energy with respect to occupations is not only a fundamental property that should be obeyed by any exact energy functional, but also a starting point to improve approximate functionals that are used in practical applications.

DFT+U enforces piecewise linearity on the Hubbard manifold [1], and it has been shown to greatly improve the accuracy of density-functional theory for transition-metal complexes, thanks to its correction of self-interaction errors [2]. However, it still performs poorly in complexes where significant covalency is present, and intersite corrections (so-called DFT+U+V) have been introduced to improve these challenging cases [3].

Here, we revisit piecewise linearity within the DFT+U and DFT+U+V correction schemes, and explore a novel approach where self-interaction corrections are applied directly to the frontier orbitals. We test this approach on model transition metal complexes, where highly accurate reference results can be established, and on small molecules with varying degrees of covalency.

References: [1] M. Coccoccioni and S. de Gironcoli, Phys. Rev. B 71, 35105 (2005). [2] H. J. Kulik, M. Cococcioni, D. A. Scherlis and N. Marzari, Phys. Rev. Lett. 97, 103001 (2006). [3] V. Leiria Campo Jr and M. Cococcioni, J. Phys. Cond. Matt. 22, 055602 (2010); H. J. Kulik and N. Marzari, J. Chem. Phys. 134, 094103 (2011).

HL 77.3 Wed 16:45 TRE Ma

Quasiparticle self-consistent *GW* method with spin-orbit coupling applied to Bi and HgTe — •Christoph Friedrich, Irene Aguilera, Markus Betzinger, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We present an implementation of the quasiparticle self-consistent (QS) *GW* method where the spin-orbit coupling (SOC) is fully taken into account in each iteration rather than being added *a posteriori*. The implementation is based on the FLAPW method. The SOC gives rise to spin off-diagonal blocks in the Green function G^{SOC} and the self-energy $\Sigma^{\mathrm{SOC}} = iG^{\mathrm{SOC}}W^{\mathrm{SOC}}$. We applied the QS$G^{\mathrm{SOC}}W^{\mathrm{SOC}}$ method to the semimetal Bi, which presents in experiment small electron and hole pockets and a tiny band gap (11-15 meV) at the L point, all of them largely overestimated by LDA (e.g., the gap is 86 meV). The QS$G^{\mathrm{SOC}}W^{\mathrm{SOC}}$ approach predicts a value of the band gap of 8 meV and electron and hole pockets in very good agreement with experiment. The *a posteriori* treatment of the SOC (QSGW+SOC), on the other hand, yields an unphysical result for Bi, predicting it to be a topological insulator with a very large gap at L (260 meV) instead of a trivial semimetal. Similarly, for HgTe, QSGW+SOC reorders the bands in a wrong way and opens a gap at the Γ point in disagreement with experiment. In contrast, the QS$G^{\mathrm{SOC}}W^{\mathrm{SOC}}$ approach yields a qualitatively and quantitatively correct description of the electronic band structure. We acknowledge support from the Helmholtz Association through the Virtual Institute for Topological Insulators (VITI).

HL 77.4 Wed 17:00 TRE Ma

Studies of semiconducting pyrite and marcasite compounds using many-body perturbation theory in the *GW* approximation — •Timo Schena, Gustav Bihlmayer, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, Germany

FeS_2 pyrite and marcasite have recently gained renewed interest as materials for photovoltaic applications, due to their large optical absorption and abundance. Therefore, a reliable description of the fundamental band gap of these compounds within first-principles calculations is desirable. However, common density functional theory (DFT) often suffers from an underestimation of band gaps. This calls for beyond-DFT methods, *e.g.*, the *GW* approximation, which is known to yield gaps in much better agreement with experiment. Although this is widely accepted for "simple" semiconductors, the situation is not well understood for more complicated cases, where the band edges differ in atomic and orbital character. In fact, we observe an uncommon band gap reduction in FeS_2 when applying single-shot *GW* on top of DFT, which might be problematic for photovoltaic applications [1]. In this work, we investigate the effects of the *GW* approximation on a couple of pyrite and marcasite compounds, employing the FLAPW code `FLEUR` and the *GW* code `SPEX` (www.flapw.de). In addition to single-shot *GW*, we also compare to the results of the recently implemented quasi-particle self-consistent *GW* approximation. We gratefully acknowledge funding from BMBF of the NADNuM project 03SF0402A.

[1] T. Schena *et al.* Physical Review B (accepted 2013)

15 min. break

HL 77.5 Wed 17:30 TRE Ma

Probing d-band Quantum Well States in Palladium Nanofilms — •Srijan Kumar Saha[1], Sujit Manna[1], Marek Przybylski[1,2], Valeri Stepanyuk[1], and Jurgen Kirschener[1,3] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, 30-059 Kraków, Poland — [3]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

We present the results of our new study which probes the d-bands

quantum well (QW) states in Pd nanofilms grown on Cu(001) using first-principles density functional theory (DFT) calculations combined with scanning tunneling spectroscopy (STS) experiments. This study reveals that QW states occur in the overlayer films of Pd over a strikingly large film thickness (up to 17 monolayers) and in a large binding energy range (from 0.1 to 3.0 eV below Fermi level), thanks to its distinct and broad 4d-bands. The orbital characters of these states are unambiguously identified by our DFT calculations. Calculations also demonstrate oscillatory multilayer relaxations and d-derived quantum size oscillations in Pd films. The pseudomorphic growth, well-defined interface, and spatially resolved STS allows us to probe individual occupied QW states and extract the accurate dispersion of the (Δ_5-like) d electronic band, as these states are laterally highly localized and give rise to distinct and sharp feature in the tunneling spectra.

HL 77.6 Wed 17:45 TRE Ma

Implementation and analysis of a plane wave and real space pseudopotential method including an efficient spin-orbit coupling treatment tailored to calculate the electronic structure of large-scale semiconductor nanostructures — •Frank Zirkelbach, Pierre-Yves Prodhomme, Jerome Jackson, and Gabriel Bester — Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

The implementation of the *large-scale atomic effective pseudopotential program* to solve the Schrödinger equation of an electronic system is discussed. *Atomic effective pseudopotentials* that are derived from screened local effective crystal potentials of self-consistent density functional theory (DFT) calculations are utilized, which ensure an accurate treatment at reduced computational costs. The capability of describing relevant electronic eigenstates of a quantum dot structure consisting of hundred thousand atoms at an atomistic *ab initio* level comparable to DFT is demonstrated. The possibility to represent the wavefunction and to evaluate parts of the Hamiltonian either in a plane wave or real space basis allows for a coherent analysis of various different approaches. In the fully real space treatment, linear scaling with respect to the system size is achieved. The convergence behavior of the different methods and utilized approximations is shown. Furthermore, an efficient spin-orbit treatment different to previously existing implementations within the pseudopotential formalism is outlined. The accuracy of the method is demonstrated via direct comparison to standard DFT codes.

HL 77.7 Wed 18:00 TRE Ma

Strong Parallelization of Real-Space DFT Calculations — •Andrea Nobile[1,2], Paul Baumeister[1,2], Daniel Wortmann[1], and Stefan Blügel[1] — [1]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungzentrum Jülich and JARA, 52425 Jülich, Germany — [2]Jülich Supercomputing Center, Forschungzentrum Jülich, 52425 Jülich, Germany

The rapid change in modern supercomputing architectures poses a challenge to well established DFT codes. In particular, the increase in raw floating point power obtained through parallelism at different levels is not easily exploitable by using the traditional direct diagonalization methods. We will present our new real-space Projector Augmented Wave (PAW) implementation. The real-space representation of the wave functions, densities and potentials, enables the usage of very flexible boundary conditions and naturally adapts to massively parallel architectures. Parallelism can be exploited in the form of domain decomposition of the three dimensional grid, k-point sampling and bands. The kinetic energy operator, realized as a finite difference stencil, is localized. As a consequence the real-space representation of the Hamiltonian is sparse. This limits the amount of necessary communications and allows an application of the operator to a trial vector in order(N) operations. We will present results about the efficiency of the most numerical intensive parts of the code and we will compare the accuracy of the calculations for reference systems with other established DFT methods.

HL 77.8 Wed 18:15 TRE Ma

Rare Earth Metals in Density-Functional Theory — •Marco Casadei[1], Xinguo Ren[2], Patrick Rinke[1], Angel Rubio[1,3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]University of Technology, Hefei, China — [3]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

The presence of f electrons in the rare earths and their interaction with the s and p electrons give rise to several physical phenomena. One prominent example is the isostructural α-γ phase transition in cerium (Ce). We have shown that density-functional theory (DFT) captures the volume collapse associated with the transition, but only if advanced functionals such as exact exchange plus correlation in the random-phase approximation (EX+cRPA) are used [1]. The volume collapse is understood in terms of a *localization/delocalization* of the f electrons. We then addressed the question: *is the isostructural volume collapse in cerium unique*? By applying DFT, we studied lanthanum (La), praseodymium (Pr) and neodymium (Nd), which undergo several structural changes with pressure. We find that the transitions are already captured at a lower level of DFT (i.e. with (semi)-local functionals) and therefore conclude that f-electrons are not the driving force in this case. Within hybrid functionals, we find only one phase in lanthanum, which has no f-electrons, and more than one stable solution in the fcc crystal for Pr and Nd, as found for Ce. Unlike in Ce, however, there is always one solution that is the most stable, thus no isostructural volume collapse emerges in agreement with experiments. [1] M. Casadei *et al.*, Phys. Rev. Lett. **109**, 14642 (2012).

HL 77.9 Wed 18:30 TRE Ma

Electronic Structure and van der Waals Interactions in the Stability and Mobility of Point Defects in Semiconductors — •Wang Gao and Alexandre Tkatchenko — Fritz-Haber-Institut der MPG, Berlin, Germany

Point defects are abundant in materials, and significantly affect the electronic, optical, and magnetic properties of solids. However, our understanding of the stability and mobility of point defects remains incomplete, despite decades of intensive work on the subject. In the framework of density-functional theory, Perdew-Burke-Ernzerhof functional underestimates formation energies by 0.7 eV due to the electron self-interaction error, while Heyd-Scuseria-Ernzerhof (HSE) functional yields formation energies in better agreement with high-level many-body methods, but often overestimates migration barriers by up to 0.4 eV.

Using HSE coupled with screened long-range vdW interactions [1], we demonstrate that HSE+vdW can simultaneously and accurately describe the formation energies and migration barriers of point defects. The inclusion of vdW interactions significantly changes the transition state geometries, and brings migration barrier into close agreement with experimental values for six different defects. For multiatom vacancies and point defects in heavier semiconductors, vdW interactions play an increasingly larger role [2].

[1] G. X. Zhang, *et al.*, PRL **107**, 245501 (2011); A. Tkatchenko, *et al.*, PRL **108**, 236402 (2012).

[2] W. Gao and A. Tkatchenko, PRL **111**, 045501 (2013).

HL 77.10 Wed 18:45 TRE Ma

Scaling Laws for van der Waals Interactions in Nanostructured Materials — •Vivekanand Gobre and Alexandre Tkatchenko — Fritz Haber Institut der MPG, Berlin

Accurate description of van der Waals (vdW) interactions is crucial for precise prediction of structure and stability of complex materials. VdW forces originate from interactions between fluctuating multipoles in matter and play a significant role in the self-assembly of nanostructured materials. Many models used to describe vdW interactions in nanomaterials are based on a simple pairwise-additive approximation, neglecting the strong electrodynamic response effects caused by long-range fluctuations in matter. We develop and utilize an efficient microscopic method [1,2] to demonstrate that vdW interactions in nanomaterials act at distances greater than typically assumed, and can be characterized by different scaling laws depending on the dimensionality and size of the system. Specifically, we study the behaviour of vdW interactions in single-layer and multilayer graphene, fullerenes of varying size, single-wall carbon nanotubes and graphene nanoribbons. As a function of nanostructure size, the van der Waals coefficients follow unusual trends for all of the considered systems, and deviate significantly from the conventionally employed pairwise-additive picture. We propose that the peculiar van der Waals interactions in nanostructured materials could be exploited to control their self-assembly. [1] Tkatchenko, DiStasio, Car, and Scheffler, PRL (2012); [2] Gobre, Tkatchenko, Nat. Commun. (2013).

HL 77.11 Wed 19:00 TRE Ma

2D nanopatterns of shape-persistent molecular polygons on HOPG — •Stefan-S. Jester, Nina Schönfelder, Eva Sigmund, and Sigurd Höger — Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

Shape-persistent organic molecules with flexible side chains self-assemble at the solution/solid interface to form 2D nanoarchitectures. Scanning tunneling microscopy yields a submolecularly resolved insight into the adsorbate structures. A key issue is how the shape and symmetry of the backbones and their alkyl chain substitution pattern determine the shape and symmetry of the adsorbate patterns. Recently we focused on molecular polygons (triangles, squares, pentagons, and hexagons) with dithiophene corners and phenylene-alkynylene sides.[1] In my talk I will give insight into the relation between Archimedean surface patterns and supramolecular 2D adlayers. [1] S.-S. Jester, E. Sigmund, S. Höger *J. Am. Chem. Soc.* **2011**, *133*, 11062.

HL 78: Quantum dots: Preparation and characterization

Time: Wednesday 16:30–18:45 Location: POT 251

HL 78.1 Wed 16:30 POT 251

Nonvolatile memory characteristics of Ge nanocrystals embedded in TaZrO2 — •David Lehninger[1], Peter Seidel[1], Frank Schneider[1], Volker Klemm[2], Johannes von Borany[3], and Johannes Heitmann[1] — [1]Institut für Angewandte Physik, TU Bergakademie Freiberg, D-09596 Freiberg — [2]Institut für Werkstoffwissenschaft, TU Bergakademie Freiberg, D-09596 Freiberg — [3]Institut für Ionenstrahlphysik und Materialforschung, HZDR, D-01314 Dresden

NVM devices with charge storage in discrete nanocrystals (NCs) offer the chance for better scalability and to operate at lower voltages compared to continuous floating gate (FG) flash devices. Using Ge NCs instead of Si NCs is expected to further improve the memory performance due to the smaller bandgap of Ge compared to Si.

In this work, Ge NCs embedded in a high-k control oxide have been fabricated by magnetron sputtering of Ge-TaZrO2/TaZrO2 layers on a p-type Si-Wafer covered by a 5 nm thermal oxide. The formation of spherically shaped Ge NCs in amorphous TaZrO2 is demonstrated by cross-sectional TEM. C-V measurements exhibit a counter clockwise hysteresis indicating the tunneling of holes through the SiO2 and their subsequent trapping in the Ge NCs. The memory window widens with both, sweep voltage range and programming time. The discharging kinetic is examined by the constant capacity method and shows a long time stabile state after an initial logarithmic decay. It could be shown, that MIS structures comprising Ge NCs in amorphous high-k TaZrO2 show promising NVM characteristics.

HL 78.2 Wed 16:45 POT 251

Atomic structure of InGaAs/GaAs quantum dots in a GaP(001) matrix — •Holger Eisele, Christopher Prohl, Andrea Lenz, Dominik Roy, Gernot Stracke, Andre Strittmatter, Udo W. Pohl, Dieter Bimberg, and Mario Daehne — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin

Due to the comparably low lattice mismatch, GaP is a promising material for the direct integration of optical III-V-semiconductor applications into silicon-based technology. Therefore, the development of epitaxially grown nanostructures—like quantum dots—on GaP(001) substrates for opto-electronic devices is an interesting new task. Furthermore, In(Ga)As/GaP quantum dots are also promising for new nano-memory cells due to an expected high hole localization energy at the quantum dots, as compared with InAs/GaAs quantum dots, resulting in reasonable long storage times. In order to understand the growth and capping of quantum dots in this new material system, we analyzed InGaAs/GaAs/GaP nanostructures on the atomic scale, using scanning tunnelling microscopy (XSTM).

HL 78.3 Wed 17:00 POT 251

Crystallization phenomena of germanium nano crystals in ZrO_2 — •Maximilian Geyer[1], Peter Seidel[1], David Lehninger[1], Volker Klemm[2], Gerhard Schreiber[2], and Johannes Heitmann[1] — [1]TUBAF, Institut für Angewandte Physik — [2]TUBAF, Institut für Werkstoffwissenschaften

Due to the heightened interest of semiconductor nanocrystals in high-κ matrices the crystallization of germanium in ZrO_2 was investigated. Germanium was especially interesting because of its smaller band gap and higher Bohr-radius then silicon and ZrO_2 shows superior high-κ and dielectric properties and is of interest for optical and electrical applications.

All samples were prepared by a co-sputtering process of a superlattice containing pure ZrO_2 and mixed Ge/ZrO_2 layers. First different annealing processes combined with different capping layers to prevent the oxidation of germanium due to the oxygen conductivity of the matrix were tested. A Capping layer of SiO_2 combined with a RTP annealing process gives the best results. Raman and photoluminescence spectroscopy show characteristic peaks after this processing which are connected to nanocrystalline structures.

Furthermore we found that a interface layer of silicon nitride in contrast to the natural silicon oxide transmits the crystal information of our silicon substrate to the layers of our superlattice and makes a continuous crystallization of germanium possible.

Further research will investigate different layer compositions and the possibility of lateral conductivity through the nano crystalline layers.

HL 78.4 Wed 17:15 POT 251

Fabrication of a charge-tunable GaAs/AlGaAs strain-free quantum dot device suitable for single dot spectroscopy — •Fabian Langer, David Plischke, Martin Kamp, and Sven Höfling — Technische Physik and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, University of Würzburg, Am Hubland, D-97074 Würzburg, Germany

Stranski-Krastanov growth has been the method of choice for the fabrication of high-quality self-assembled quantum dots in a variety of material systems. The difference in lattice constants that drives the self-organization of the dots is absent in the GaAs/AlAs material system. Therefore, other approaches like modified droplet epitaxy (MDE)[1] have to be used for producing GaAs QDs on AlGaAs. This process creates QDs without significant material intermixing and allows the investigation of exciton fine-structure splitting or nuclear spin dynamics without the influence of strain or piezoelectric effects. In this contribution we report on the fabrication of a charge-tunable GaAs/AlGaAs QD device containing QDs deposited by MDE. We achieved a QD density in the low 10^9 1/cm^2 range, enabling the use of single dot spectroscopy without any additional patterning. The observed linewidths are as small as 40 μeV. We were able to charge a single QD with up to four electrons in devices with a Schottky gate. The QD character of the photoluminescence (PL) emission was proven by photon antibunching and cross-correlation measurements yielding a $g^{(2)}(0)$ value of 0.05.

[1] Watanabe, K.; Nobuyuki, K.; Gotoh, Y. Jpn. J. Appl. Phys., Vol. 39, L79-L81, 2000

HL 78.5 Wed 17:30 POT 251

GaAs quantum dots in shallow and deep nanoholes fabricated by local droplet etching — •Christian Heyn, Achim Küster, David Sonnenberg, Andreas Graf, Arne Ungeheuer, and Wolfgang Hansen — Institute of Applied Physics, University of Hamburg, D-20355 Hamburg, Germany

We fabricate GaAs quantum dots (QDs) by filling of nanoholes drilled in an AlGaAs substrate utilizing local droplet etching (LDE) [1]. The etching process takes place in a self-assembled fashion during molecular beam epitaxy (MBE) without the need of additional equipment. Using Al droplets as etchant, the nanohole depth d can be varied from less than 10 to more than 100 nm in a controlled fashion. Optical studies of single LDE GaAs QDs show clear excitonic features [2]. Here, we compare the single-dot photoluminescence emission of low-density ($N \simeq 10^7$ cm^{-2}) QDs formed by partial filling of either shallow ($d \simeq$ 10 nm) or deep (d = 70 - 100 nm) holes.

[1] Ch. Heyn, A. Stemmann, T. Köppen, Ch. Strelow, T. Kipp, S. Mendach, and W. Hansen, Appl. Phys. Lett. **94**, 183113 (2009).

[2] Ch. Heyn, Ch. Strelow, and W. Hansen, New Journal of Physics **14**, 053004 (2012).

HL 78.6 Wed 17:45 POT 251

Charge carrier localization by Sb-assisted growth of InAs/GaAs sub-monolayer stacks — •David Quandt, Jan-Hindrik Schulze, Manuel Gschrey, Ronny Schmidt, Sven Rodt,

Andre Strittmatter, Udo W. Pohl, and Dieter Bimberg — Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstraße 36, D-10623 Berlin

Quantum dots (QDs) grown in the sub-monolayer (SML) growth mode result in dense arrays of 3D charge carrier localization centers which enable high-gain active regions in laser devices. InAs/GaAsSML QDs grown by MOVPE typically exhibit very high island densities which, due to lateral electronic coupling, provide only weak carrier localization. Using Sb as additional species during growth of InAs/GaAs SML QDs, the electronic confinement properties can be effectively tuned to strong carrier localization. This is evidenced by spatially resolved cathodoluminescence spectroscopy revealing individual sharp lines in the ensemble luminescence. The amount of supplied Sb controls also the ensemble broadening which is very attractive for mode-locking applications in laser devices.

HL 78.7 Wed 18:00 POT 251

Growth, structure and spectroscopy of $In_{0.50}Ga_{0.50}As$ quantum dots grown by MOVPE on GaP(001) — •Elisa Maddalena Sala, Gernot Stracke, Manuel Gschrey, Christopher Prohl, Andrei Schliwa, Holger Eisele, André Strittmatter, and Dieter Bimberg — Institut für Festkörperphysik, Technische Universität Berlin Hardenbergstr. 36 10623 Berlin, Germany

InGaAs quantum dots (QDs) on GaP have recently attracted great attention for application in nano memory cells and monolithic III/V on silicon photonics. $In_{0.50}Ga_{0.50}As$ QDs on GaP(001) grown by metalorganic vapor phase epitaxy exhibit truncated inverted pyramidal shape and strong indium agglomeration at QD tops. For injection of electrons into the QDs, indirect bandgap of GaP with lowest conduction band states at the X-point has to be taken into account. 8-band k·p theory predicts a QD size- and strain- dependent transition from indirect to direct optical emission. By preparing QD ensemble of ultralow density, detection of luminescence from individual InGaAs/GaP QDs is enabled for the first time. Narrow emission lines with FWHM of 52 μmeV showing no spectral jitter suggest that no electrical active defects are present in the QD vicinity. Temperature-dependent cathodoluminescence investigations allow to study the electronic structure of InGaAs/GaP QDs since thermally induced strain alters the electronic structure of the QDs allowing to research for the transition from indirect-to-direct optical emission.
Towards QD positioning, initial studies on buried stressor formation by selective lateral oxidation of thin AlP layers will be presented.

HL 78.8 Wed 18:15 POT 251

GaN quantum dots grown on AlN by MOVPE — •Farsane Tabataba-Vakili, Konrad Bellmann, Tim Wernicke, Stefan Kalinowski, André Strittmatter, and Michael Kneissl — Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin, Germany

GaN quantum dots (QDs) embedded in an AlN matrix enable single and entangled photon emitters operating at room temperature, which are key elements in quantum information science. Stranski-Krastanow (SK) growth of GaN QDs by metal organic vapor phase epitaxy (MOVPE) is subject to a multi-dimensional parameter space of which we have studied the effects of temperature, V/III ratio, and growth interruption (GRI). Desorption effects have a large impact on surface morphologies. Performing a GRI without ammonia supply transforms two dimensional GaN grown under a high V/III ratio into three dimensional islands with a few nm in height and 50-90 nm in diameter. Narrow emission lines of 10 meV from individual islands are observed in μ-PL experiments. Experiments with different V/III ratios during GaN deposition show that a SK-growth mode transition can be achieved for low V/III ratios during GaN deposition. Thereby, QDs with an average height of 4.5 nm and 26 nm in diameter are obtained at densities of 10^{10} cm^{-2}.

HL 78.9 Wed 18:30 POT 251

Growth and characterisation of InGaN quantum dots on AlGaN-Templates — •Carsten Laurus[1], Timo Aschenbrenner[1], Elahe Zakizadeh[1], Stephan Figge[1], Detlef Hommel[1], JunJun Wang[2], and Ferdinand Scholz[2] — [1]Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee, 28359 Bremen, Germany — [2]Institut für Optoelektronik, Universität Ulm, Albert-Einstein-Allee 45, 89081 Ulm, Deutschland

InGaN quantum dots (QDs) are of great interest to realize single photon emitters. Single photon emission (SPE) up to 50 K was achieved utilizing spinodal phase decomposition for QD formation. In order to improve the confinement of charge carriers in QDs and thus the temperature stability of the emission the introduction of barrier-layers with a higher bandgap energy is reasonable. However, each interface might introduce defects. Using an other template (buffer-layer) material might turns out to be a good compromise. Using InGaN as active layer, AlGaN is a promising material for templates because of its higher bandgap. Samples using GaN- and AlGaN-Templates were grown by MOVPE. For structural analysis by SEM samples without capping layer were used, whereby μ-PL investigations were made with capped samples. Based on SEM data all samples regardless from the template show a meander-like structure of different size in line with the model spinodal decomposition. Furthermore, the capping of InGaN QDs with GaN or AlGaN and its influence on the confinement will be discussed by reference to μ-PL measurements. In addition, sharp μ-PL emission lines could be traced up to 65K for samples grown on AlGaN templates.

HL 79: Transport: Topological insulators II (organized by TT)

Time: Wednesday 16:30–18:30 Location: HSZ 204

HL 79.1 Wed 16:30 HSZ 204

Rashba spin orbit coupling in the Kane-Mele-Hubbard model — •Stephan Rachel — Institut für Theoretische Physik, TU Dresden

Spin-orbit (SO) coupling is the crucial ingredient for topological insulating phases. In particular, the generic emergence of SO coupling involves the Rashba term which fully breaks the SU(2) spin symmetry. As soon as interactions are taken into account, however, many theoretical studies have to content themselves with the analysis of a simplified U(1) conserving SO term without Rashba coupling. We intend to fill this gap by studying the Kane-Mele-Hubbard model in the presence of Rashba SO coupling. We apply the variational cluster approach to determine the interacting phase diagram by computing local density of states, magnetization, single particle spectral function, and edge states.

We find that the Rashba SO coupling drives new electronic phases such as a metallic regime and a "gapless topological insulator phase" which persist in the presence of interactions.

HL 79.2 Wed 16:45 HSZ 204

Conductivity of a generic helical liquid — •Nikolaos Kainaris[1], Igor Gornyi[1,2,4], Sam Carr[3], and Alexander Mirlin[1,2,5] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, Karlsruhe, Germany — [2]Institut für Nanotechnologie, Karlsruher Institut für Technologie, Karlsruhe, Germany — [3]School of physical sciences, University of Kent, Canterbury, UK — [4]A.F. Ioffe Physico-Technical Institute, St. Petersburg, Russia — [5]Petersburg Nuclear Physics Institute, St. Petersburg, Russia

We study the transport properties of a helical Luttinger liquid without S_z symmetry. We focus on the case of long edges of 2D topological insulators and calculate the conductivity in the presence of both interactions and disorder. In the regime where temperature is larger than the frequency of the external field we use a kinetic equation approach to calculate the AC and DC conductivity for weakly interacting fermions. The opposite regime of the AC conductivity is discussed via full bosonization that allows us to treat certain interactions exactly. We find the dependence of the conductivity on temperature, frequency and Fermi energy for different scattering mechanisms and discuss their relevance to transport.

HL 79.3 Wed 17:00 HSZ 204

Influence of a random Rashba spin-orbit coupling on the transport properties of helical liquids — •Florian Geissler, Francois Crepin, and Björn Trauzettel — Theoretische Physik IV, Universität Würzburg, Germany

In a quantum spin Hall system, the edge states are one-dimensional and helical, i.e. their (pseudo) spin degree of freedom and their direction of motion are strongly coupled to each other. This coupling gives rise to protection against elastic backscattering off non-magnetic impurities. Here, we analyze inelastic (two-particle) backscattering in interacting helical liquids in presence of random Rashba spin-orbit coupling. To study this peculiar type of disorder, we bosonize the Hamiltonian and employ a combination of operator product expansion and renormalization group calculations. Thereby, we obtain a consistent set of flow equations for the renormalization of the Luttinger liquid parameters, the disorder strength, and the two-particle backscattering. Finally, we discuss the corrections to the conductance at finite temperature stemming from this type of disorder.

HL 79.4 Wed 17:15 HSZ 204

Generic Helical Liquids: the effect of rotation of the spin-quantization axis — •Alexia Rod[1], Thomas L. Schmidt[2], and Stephan Rachel[1] — [1]Institut für Theoretische Physik, TU Dresden — [2]Department of Physics, University of Basel

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 rotation of the spin quantization axis with momentum. Its manifestation in real space has, however, remained elusive. Here we consider topological insulator sheets and discs and investigate the non-trivial spin structure of the helical edge states. We further propose how to measure this spin structure and discuss potential applications. [1] T.L. Schmidt, S. Rachel, F. von Oppen, L. Glazman, Phys. Rev. Lett. 108, (2012).

HL 79.5 Wed 17:30 HSZ 204

Hanbury Brown-Twiss and Aharonov-Casher effects in a quantum spin Hall Corbino ring — •Anders Ström[1], Henrik Johannesson[2], and Patrik Recher[1] — [1]Institute for Mathematical Physics, TU Braunschweig, Germany — [2]Department of Physics, University of Gothenburg, Sweden

We study the entanglement production in a quantum spin Hall ring where electrons of different spins are emitted from a biased source and detected in two different grounded detectors. The fermionic Hanbury-Brown Twiss effect gives rise to entanglement in the system, measurable via the current-current correlations between the detectors. The production of entanglement is electrically controlled via the Aharonov-Casher phases arising from the Rashba coupling in the system.

HL 79.6 Wed 17:45 HSZ 204

Proximity induced perfectly conducting channel in 2D-metal topological insulator heterostructures — •Sven Essert, Viktor Krueckl, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

Two-dimensional topological insulators have attracted much attention because of their peculiar edge-state transport features. We investigate how these properties carry over to heterostructures made of topological insulators and materials with extended states which are not topologically classifiable (metallic systems).

We find that the proximity of a topological insulator induces a perfectly conducting channel in the metal which is however not localized along the edge but spanning the whole extended state region. This resembles the perfectly conducting channels predicted in graphene nanoribbons and carbon nanotubes. However, the proximity induced channel is expected to be stable even with short-range disorder which should simplify its observation.

We propose experiments to detect this effect by conductance and shot-noise measurements and also show how the proximity of a topological insulator can be understood in terms of an effective boundary condition.

HL 79.7 Wed 18:00 HSZ 204

Majorana fermions on a hexagonally warped 3D topological insulator in proximity to a superconductor — •Daniel Mendler, Panagiotis Kotetes, and Gerd Schön — Institut für theoretische Festkörperphysik, KIT, Karlsruhe

The recent discovery of topological insulators (TIs) opened new perspectives in the field of topological quantum computing (TQC), in terms of Majorana fermions (MFs). The latter are expected to appear in the vortex cores of artificial topological superconductors (TSCs), engineered from the surface states of a 3D-TI in proximity to a conventional SC. Nonetheless, if time-reversal symmetry is spontaneously broken on the TI surface, the hybrid system supports Majorana fermions without the requirement of vortices. The latter property can be advantageous for the experimental realization of TSCs and facilitate the implementation of TQC protocols. In this work, we investigate the above scenario for the hexagonally warped Dirac itinerant surface states of Bi2Te3, which demonstrate enhanced tendency towards the spontaneous formation of magnetism due to Fermi surface nesting. We perform a complete classification of the accessible spin density wave order parameters in the presence of a repulsive Hubbard-like interaction and retrieve the hierarchy of magnetic phase transitions which can occur in the particular system. For the dominant magnetic instability, we investigate the conditions which favor proximity induced SC on the magnetic TI surface. We explicitly demonstrate the emergence of MFs in this system and propose methods for their manipulation.

HL 79.8 Wed 18:15 HSZ 204

Unconventional s- and p-wave proximity effect in topological insulator/superconductor structures — •Tkachov Grigory — University of Wuerzburg

Currently, much effort is being put into understanding unconventional superconductivity in topological insulators (TIs). This contribution addresses a microscopic theory of the proximity effect in three-dimensional TIs coupled to an *s*-wave superconductor. In agreement with earlier results [1] we demonstrate that the induced superconductivity is a mixture of singlet *s*-wave and triplet *p*-wave components [2]. Their interplay depends on several factors, such as the position of the Fermi level, excitation energy, and external magnetic fields, among others. We also discuss the role of disorder and applications of the theory to recent experiments on HgTe-based TIs [3,4].

This work was supported by the German Research Foundation (DFG), Grant No TK60/1-1.

[1] T. D. Stanescu, J. D. Sau, R. M. Lutchyn, and S. Das Sarma, Phys. Rev. B **81**, 241310(R) (2010).
[2] G. Tkachov, Phys. Rev. B **87**, 245422 (2013).
[3] L. Maier, J. B. Oostinga, D. Knott, C. Brüne, P. Virtanen, G. Tkachov, E. M. Hankiewicz, C. Gould, H. Buhmann, and L. W. Molenkamp, Phys. Rev. Lett. 109, 186806 (2012).
[4] J. B. Oostinga, L. Maier, P. Schüffelgen, D. Knott, P. Leubner, C. Brüne, G. Tkachov, H. Buhmann, and L. W. Molenkamp, Phys. Rev. X **2**, 021007 (2013)

HL 80: Transport: Carbon nanotubes (organized by TT)

Time: Wednesday 16:30–18:30 Location: HSZ 304

HL 80.1 Wed 16:30 HSZ 304

Revealing the carbon nanotube quantum dot fine structure by transport spectroscopy — •Daniel R. Schmid[1], Alois Dirnaichner[1,2], Magdalena Marganska[2], Peter L. Stiller[1], Milena Grifoni[2], Andreas K. Hüttel[1], and Christoph Strunk[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

Transport spectroscopy on an ultra-clean carbon nanotube quantum dot allows us to measure the level spectrum of the very first electron above the band gap, which can be understood by an underlying minimal Hamiltonian. This includes curvature induced spin-orbit coupling and KK'-mixing terms. The sample orientation in an external magnetic field can be adjusted from perpendicular to parallel alignment with the nanotube axis. Magnetic fields up to 17 T enable us to get an insight on the full dispersion of the first longitudinal modes.

HL 80.2 Wed 16:45 HSZ 304

Valley-mixed states and energy splitting as a finite size effect in chiral carbon nanotubes — •Magdalena Marganska, Piotr Chudzinski, and Milena Grifoni — Institute for Theoretical Physics, University of Regensburg, Regensburg, Germany

The two main degrees of freedom of an electron in a carbon nanotube (CNT) are valley and spin. The electronic spectra obtained in transport experiments on CNT quantum dots in parallel magnetic field often show an anticrossing of spectral lines assigned to the opposite valleys. One source of this phenomenon could be the disorder, with impurity induced scattering. However, we show that this effect can be reproduced also in ultraclean CNTs, where it is caused solely by the presence of the boundaries. It is therefore a finite size effect, not an inherent property of the CNT. We identify the nanotube chirality class which supports this phenomenon and analyze its dependence on the CNT parameters and on the distance from the charge neutrality point.

HL 80.3 Wed 17:00 HSZ 304

Large scale *ab initio* study of extended metal-CNT contacts — •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, Germany — [2]Center for Advancing Electronics Dresden, TU Dresden, Germany — [3]Dresden Center for Computational Materials Science, TU Dresden, Germany

In experimental samples of carbon nanotube transistors (CNT-FETs) the electrical contact and current inflow occur along relatively long portion of a CNT embedded into a metal. Only very few theoretical studies were done with geometries and materials close to realistic ones. The most common simplified approaches are using the models of point-like or very slightly embedded contacts.We perform large-scale modeling of extended metal-CNT contacts by density functional theory accompanied by Green function method in order to elucidate electrical properties of realistic metal-CNT contacts. We have obtained smooth shrinking of the band gap inside embedded portion of a semiconductor nanotube and induced by the metal doping of the embedded and free-standing part of a CNT. It causes geometry and material dependent behavior of the transmission coefficient and density of states along a CNT. We also analyze the electrostatic potential and charge redistribution and formulate an ab initio based effective transport model to calculate the current-voltage characteristics of large scale CNT-FETs.

HL 80.4 Wed 17:15 HSZ 304

A carbon nanotube in the strong coupling regime: Fabry-Perot interference in a ballistic electron wave guide. — •Alois Dirnaichner[1], Miriam del Valle[2], Andreas Hüttel[1], Christoph Strunk[1], and Milena Grifoni[2] — [1]Institute of Experimental and Applied Physics Regensburg — [2]Institute for Theoretical Physics Regensburg

We present low-temperature measurements of transport through a ultra clean suspended carbon nanotube with strong coupling to the leads. The sample exhibits strikingly high conductance and little reflection at the interfaces between tube and metal, as can be seen from pronounced Fabry-Perot interference patterns in the conductance. The measurements are compared to theoretical results obtained from a scattering matrix calculation where the reflection at the contacts is treated as a perturbation. Furthermore, we discuss the evolution of the patterns in a magnetic field perpendicular to the nanotube axis.

HL 80.5 Wed 17:30 HSZ 304

Signatures of quanta of 1D collective modes in inelastic co-tunneling through a metallic carbon nanotube. — Daniel Steininger[1], •Piotr Chudzinski[2], Amit Kumar[1], Martin Gaim[1], Milena Grifoni[2], Andreas K. Hüttel[1], and Christoph Strunk[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

We report low temperature transport properties of an individual single wall carbon nanotube contacted to superconducting leads. Coulomb diamonds with sharp elastic and inelastic co-tunneling features at applied bias voltages of $2\Delta/e$ and $(2\Delta+\delta)/e$ (with the BCS gap Δ), respectively, are observed. Higher order transport processes generate subgap features at bias voltage Δ/e via the Andreev reflection process. In contrast to previously reported co-tunneling spectra [1], the elastic/in-elastic co-tunneling features we observe are horizontal lines on the bias-gate voltage plane (no bending effect) and do not display any effect related to even and odd electron occupancy of the quantum dot. The in-elastic part has a rich internal structure consisting of several equidistant sub peaks. We analyze various possibilities for the occurrence of such harmonic spectrum. Among these are vibrational excitations of the carbon lattice or the many body bosonic modes that are expected from the Tomonaga-Luttinger liquid description of single wall carbon nanotubes.
[1] Phys. Rev. B 79, 134518

HL 80.6 Wed 17:45 HSZ 304

Fingerprints of thermal quasiparticle excitations in CNT-superconductor hybrid junctions — •Sebastian Pfaller[1], Andrea Donarini[1], Markus Gaass[2], Andreas K. Hüttel[2], Thomas Geiger[2], Christoph Strunk[2], and Milena Grifoni[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute for Exp. and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

We present a study of a electronic transport through a carbon nanotube quantum dot coupled to superconducting contacts. By increasing the temperature above 300mK additional transport features are observed in the stability diagrams. They appear as lines in the Coulomb blockade region, and are attributed to sequential tunneling of thermally excited quasiparticles. Whenever two of these lines cross at zero bias, a conductance peak is observed. In particular, we observe two of these peaks in the vicinity of the charge degeneracy point. The nature of these lines as well as their temperature dependence can be explained by a transport theory based on a generalized master equation approach to lowest order in the tunnel coupling [1].
[1] S. Pfaller *et al.* Phys. Rev. B **87**, 155439 (2013)

HL 80.7 Wed 18:00 HSZ 304

Fine structure of the Kondo resonance in carbon nanotube quantum dots — Daniel R. Schmid[1], Sergey Smirnov[2], Magdalena Margańska[2], Alois Dirnaichner[1], Peter L. Stiller[1], Milena Grifoni[2], •Andreas K. Hüttel[1], and Christoph Strunk[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

Ultraclean carbon nanotubes enable spectroscopy of the unperturbed quantum mechanical properties of electronic states in transport experiments with a high degree of precision. This applies to the case of opaque tunnel barriers between nanotube and leads and, e.g., the excitation spectrum of one or two electrons trapped in the quantum dot as well as to the case of many electrons and strong coupling to the leads.

Manybody correlations in carbon nanotubes with a quadruplet of both spin and valley (K-K') degenerate quantum states can give rise to the so-called SU(4) Kondo effect. We demonstrate a highly regular carbon nanotube quantum dot, where SU(4) symmetry is broken by intrinsic both spin-orbit interaction and valley mixing. This leads to a characteristic Kondo peak in differential conductance at zero bias along with satellite peaks at finite bias. The evolution of these peaks is

strikingly different at finite perpendicular and parallel magnetic fields. We demonstrate how their combined spin and orbital origin and their evolution at finite magnetic fields can be understood in detail in terms of the discrete symmetries of the carbon nanotube Hamiltonian.

HL 80.8 Wed 18:15 HSZ 304

Theory of the Kondo effect in carbon nanotube quantum dots with broken SU(4) symmetry — •Sergey Smirnov[1], Magdalena Margańska[1], Daniel R. Schmid[2], Alois Dirnaichner[2], Peter L. Stiller[2], Andreas K. Hüttel[2], Christoph Strunk[2], and Milena Grifoni[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

We develop an effective low energy field theory for the Kondo effect in a quantum dot where the original four-fold degeneracy of the dot level is partially removed. The SU(2) Keldysh effective action approach [1,2] is generalized to the case of the broken SU(4) Anderson model with spin and orbital degrees of freedom. The theory is valid in the strong and weak coupling regimes as well as in the crossover. It provides universal differential conductance with the scale having the correct limiting behavior for the SU(2) and SU(4) cases. As an application to a physical system, we explore the Kondo effect in a quantum dot made of a carbon nanotube with strong spin-orbit interaction and valley mixing. The symmetry properties of the carbon nanotube Hamiltonian are exploited to identify the structure of the Keldysh effective action. We further investigate in detail the Kondo resonance and its behavior in perpendicular and parallel magnetic fields and compare it with recent experiments on the Kondo effect in ultraclean carbon nanotubes.

[1] S. Smirnov and M. Grifoni, Phys. Rev. B 87, 121302(R) (2013).
[2] S. Smirnov and M. Grifoni, New. J. Phys. 15, 073047 (2013).

HL 81: Poster: Energy materials incl. photovoltaics

Time: Wednesday 17:00–20:00 Location: P1

HL 81.1 Wed 17:00 P1

Plasmonic enhanced photocurrent on GaN and TiO_2 films decorated with Au-NPs — •Verena Hintermayr, Jacek Stolarczyk, and Jochen Feldmann — Photonics and Optoelectronics Group, Physics Department and Center for NanoScience (CeNS), LMU München, Germany

Utilization and storage of solar energy can be achieved by its direct conversion to chemical energy using photocatalysis. Thereby the energy of the photons is used to run chemical reactions like water splitting. These photocatalysts are usually wide band semiconductors and only utilize a small percentage of the solar irradiance. In order to sensitize them to visible light a combination of wide band gap semiconductors and metal nanoparticles is used. The plasmon decay in the nanoparticle leads to the generation of hot electrons which are then injected into the neighbouring semiconductor and drive the reduction reaction.

We investigate the dependency of the photocurrent measured on GaN and TiO_2 films on the Au nanoparticle decoration of the samples. To be able to measure the generated photocurrent for both systems suitable finger structures were defined using optical lithography. In both cases the Au nanoparticles were spin coated on the semiconductor in a further processing step. In the measurements of the GaN and TiO_2 films decorated with Au nanoparticles a plasmon-enhanced photocurrent by producing hot carriers even at energies below the semiconductor band gap can be observed.

HL 81.2 Wed 17:00 P1

3D nano-architectures for next generation solar water splitting devices — •Stefan Bösemann, Liaoyong Wen, Yang Xu, Min Zhou, and Zhibing Zhan — Ilmenau University of Technology, Institute of Physics & IMN MacroNano (ZIK), Prof. Schmidt-Str. 26, 98693 Ilmenau (Germany)

Solar energy is one of the major forms of renewable energy. Various solar water splitting concepts have been regarded as a feasible and cost-effective realization of an artificial analogy to photosynthesis. Unfortunately, the stringent requirements for the physical and chemical properties make it difficult to find suitable photoelectrodes able to perform solar energy conversion efficiently and inexpensively. Devices built from 3D ordered nano-architectures offer a number of advantages over those based on thin film technology, such as larger surface and reaction area to collect more sunlight and to improve the efficiency of solar water splitting. Innovations in 3D nano-architectured photoelectrodes offer potential breakthroughs in this field by taking the advantages correspondingly physical processes. Herein, with the assistance of various fabrication techniques and different templates, including anodic aluminum oxide (AAO) and polystyrene colloidal templates, photoelectrodes with different 3D structures have been achieved and applied in solar water splitting. For example, we have constructed 3D quaternary macro-mesoporous architectures, which showed improved solar energy conversion efficiency. Meanwhile, we also realized a tandem structure, which facilitate the hydrogen and the oxygen evolution at the same time in one single device.

HL 81.3 Wed 17:00 P1

Hierarchical NiMoO4@MnO2 core-shell heterostructured nanowire arrays on Ni foam as high-performance supercapacitor electrodes — Yaoguo Fang[1,2], Kin Mun Wong[1], Gerhard Wilde[2], and •Yong Lei[1] — [1]Ilmenau University of Technology, Institute of Physics & IMN MacroNano (ZIK) Prof. Schmidt-Str. 26, 98693 Ilmenau (Germany) — [2]Institute of Materials Physics and Center for Nanotechnology, University of Muenster, Wilhelm-Klemm-Str. 10, Muenster 48149, Germany

Supercapacitors, also known as electrochemical capacitors, have been considered as one of the most promising energy storage devices because of their many advantages, including high power density, faster charge and discharge processes, living cycle lifetime, compared the conventional capacitors. Recently, research has been particularly focused on MnMoO4, and NiMoO4 because of their superior electrochemical properties, abundant resources and environmental friendliness. In this work, we design and fabricate novel hierarchical NiMoO4@MnO2 core-shell heterostructured nanowire arrays on the nickel foam, which were used as the working electrodes to fabricate high performance supercapacitors. The NiMoO4 nanowires are "core" and ultrathin MnO2 film are "shell" structures. This structure shows attractive electrochemical behavior as electrode materials for supercapacitors. The findings exhibit the importance and great potential of metal molybdate based binary oxides in the development of high performance energy storage systems.

HL 81.4 Wed 17:00 P1

Black-silicon solar cells — •Philipp Assum, Svetoslav Koynov, and Martin Stutzmann — Walter Schottky Institut , Technische Universität München, Am Coulombwall 4, D-85748 Garching, Germany

Avoiding optical losses is a key issue for the improvement of photovoltaic solar cells. Therefore black nano-textured surfaces are a prospective possibility since they almost completely suppress reflection in the whole range of silicon absorption. Furthermore an enhancement of absorption occurs in thin solar cells due to light trapping effects.

The present work focuses on the application of black-silicon nanotextures to actual solar cells. Common approaches first perform the black nano-texture etch process followed by the formation of the emitter. This is due to the fact that the black etch process is problematic on heavily doped emitter layers which are commonly used for present solar cells. In contrast this work presents a new approach where the sequence of processes is changed. First a deep but weakly doped emitter is created. Subsequently a modified black etch process, which is feasible on the doping level of the emitter, is performed. Self-doping grid contacts are applied to form highly doped regions just in vicinity of the contact which is called the selective emitter concept.

Initial results will be reported in comparison with results concerning "black" solar cells produced by the common approach in which the black etch process precedes the emitter formation.

HL 81.5 Wed 17:00 P1

Nanoparticles with high pressure core structures and Si-ZnS nanocomposites: New Paradigms to Improve the Efficiency of MEG Solar Cells — •Stefan Wippermann[1], Marton Vörös[2], Balint Somogyi[3], Adam Gali[3], Dario Rocca[4], Francois Gygi[2], Gergely Zimanyi[2], and Giulia Galli[2] — [1]Max-Planck-Institute

for Iron Research, Düsseldorf — [2]University of California, Davis — [3]Budapest University of Technology and Economics — [4]Universite de Lorraine, Nancy

The efficiency of nanoparticle (NP) solar cells may substantially exceed the Shockley-Queisser limit by exploiting multi-exciton generation. However, (i) quantum confinement tends to increase the electronic gap and thus the MEG threshold beyond the solar spectrum and (ii) charge extraction through NP networks may be hindered by facile recombination. Using ab initio calculations we found that (i) Si and Ge NPs with exotic core structures such as BC8 exhibit significantly lower gaps and MEG thresholds than particles with diamond cores, and an order of magnitude higher MEG rates. (ii) We also investigated Si NPs embedded in a ZnS host matrix and observed complementary charge transport networks, where electron transport occurs by hopping between NPs and hole transport through the ZnS-matrix. Such complementary pathways may substantially reduce recombination, as was indeed observed in recent experiments. We employed several levels of theory, including DFT with hybrid functionals and GW calculations.

HL 81.6 Wed 17:00 P1

Optimizing binary profiles for metallic solar cell back-plane reflectors — •Jan Marc Stockschläder and Erich Runge — Institut für Physik and Thüringer Landesgraduiertenschule für Photovoltaik PhotoGrad, Technische Universität Ilmenau, 98693 Ilmenau

Coupling light to the active medium of a solar cell is a crucial point for high efficiency. Structured substrates have been proposed to scatter light more efficiently into the absorber. Thin geometries are particularly attractive because they have the potential for low-cost fabrication. In acoustics, so-called Galois scatterer are often used because they scatter equally into every available scattering order[1]. However for solar cells, it matters whether scattering orders correspond to long or short path ways in the absorber. Taking this into account, we present a simple criterion as a basis for educated guesses for the absorption enhancement of a particular scattering profile. We compare the results of FDTD simulations and our heuristic estimate for Galois scatters and numerous structures of the same period length.

[1] T. J. Cox , P. D'Antonio, and M. Schroeder, *Acoustic Absorbers and Diffusers: Theory, Design and Application*, JASA **117**, 3345 (2005)

HL 81.7 Wed 17:00 P1

Time-Resolved Single-Photon Counting Measurements of GaAs Nanowires for Photovoltaics — Rami Naklah[1], •Peter Kleinschmidt[1,2], Matthias Steidl[1], Sabine Nieland[2], Christian Koppka[1], Alexander Lawerenz[2], Werner Prost[3], and Thomas Hannappel[1,2] — [1]TU Ilmenau, Germany — [2]CiS Forschungsinstitut, Erfurt, Germany — [3]Universität Duisburg-Essen, Germany

Recent progress in the development of nanowire-based solar cells has led to devices which demonstrate efficiencies of 13,8 % using axial InP nanowires [1]. On the other hand, radial nanowires consisting of a GaAs core-shell structure [2] allow separation of the direction of charge carrier transport from that of the incident light, resulting in less stringent requirements on transport properties. However, surface recombination may have an impact on device performance. We have established a measurement setup which allows to measure time-resolved photoluminescence with high spatial resolution enabling the investigation of luminescence from nanowires with a typical length of a few microns and a typical diameter of 100 nm. While we are able to map the luminescence signal of homogeneously doped nanowires (deposited on sapphire substrates from solution), our measurements indicate charge carrier lifetimes on the order of 10 ps or less. We investigate the influence on lifetimes of TCO layers deposited wet-chemically or by ALD in order to evaluate their passivation properties.

[1] J. Wallentin et al, Science 339, 1057 (2013)
[2] C. Gutsche et al, Adv. Funct. Mater. 22, 929 (2012)

HL 81.8 Wed 17:00 P1

Surface passivation of Si by ZnO doped Al_2O_3 — •Thomas Schneider[1], Johannes Ziegler[1], Alexander N. Sprafke[1], and Ralf B. Wehrspohn[1,2] — [1]Institute of Physics Martin-Luther-Universität Halle-Wittenberg, Heinrich Damerow-Str. 4, 06120 Halle, Germany — [2]Fraunhofer Institute for Mechanics of Materials IWM, Walter-Hülse-Str. 1, 06120 Halle, Germany

The lifetime of the minority charge carriers in thin, high quality Si wafers is mainly limited by surface recombination processes[1]. Thin dielectric layers of Al_2O_3 deposited on the Si surface are known to provide a excellent surface passivation. In this work, ZnO is incorporated into thin Al_2O_3 films and the influence of the ZnO to Al_2O_3 ratio on the passivation quality is studied. The films are deposited by means of thermal atomic layer deposition on p-type Si. Different numbers of ZnO cycles are incorporated into an approximately 10 nm thick Al_2O_3 layer. The passivation quality is determined by lifetime measurements with the QSSPC method. For a certain ratio of ZnO in the Al_2O_3 an increase of the lifetime of the minority charge carriers occurred, indicating a enhanced passivation of the Si surface.

[1] A.G. Aberle, Prog. Photovolt: Res. Appl. 8(5), 473 (2000). doi:10.1002/1099-159X(200009/10)8:5⟨473::AID-PIP337⟩3.0.CO;2-D

HL 81.9 Wed 17:00 P1

Influence of a SiO_2 interlayer on AL_2O_3 passivated silicon wafers — •Johannes Ziegler[1], Thomas Schneider[1], Alexander N. Sprafke[1], and Ralf B. Wehrspohn[1,2] — [1]Institute of Physics Martin-Luther-Universität Halle-Wittenberg, Heinrich Damerow-Str. 4, 06120 Halle, Germany — [2]Fraunhofer Institute for Mechanics of Materials IWM, Walter-Hülse-Str. 1, 06120 Halle, Germany

Silicon surfaces are exellently passivated by Al_2O_3 due to the chemical passivation of recombination active dangling bonds by saturation, as well as field effect passivation generated by a high density of fixed negative charges in the Al_2O_3. Therefore, it is used to reduce parasitic charge carrier recombination in silicon solar cells [1]. However silicon tends to form a layer of SiO_2 on its surface. In most cases, Al_2O_3 is deposited on an Si/SiO_2 interface [2]. Thus the thickness and growing conditions of the SiO_2 interlayer influences the passivation quality of the $Si/SiO_2/Al_2O_3$ passivation stack. The influence of differently wet-chemically grown SiO_2 interlayers in such passivation stack is investigated by effective minority carrier lifetime measurements.

[1] F. Werner, B. Veith, D. Zielke, L. Kühnemund, C. Tegenkamp, M.Seibt, R. Brendel, J. Schmidt, J. Appl. Phys. 109, 113701 (2011).doi:10.1063/1.3587227
[2] V. Naumann, M. Otto, C. Hagendorf, R.B. Wehrspohn, J. Vac. Sci.Technol., A 30, 04D106 (2012). doi:10.1116/1.4704601

HL 81.10 Wed 17:00 P1

Opto-electronic properties of physical vapor deposited Bi_2S_3 on the mm- and μm-scale — •Hendrik Sträter[1], Sebastian ten Haaf[2], Rudolf Brüggemann[1], Gerhard Jakob[2], Niklas Nilius[1], and Gottfried Bauer[1] — [1]Carl von Ossietzky Universität Oldenburg, Institut für Physik, D-26111 Oldenburg — [2]Johannes Gutenberg Universität Mainz, Institut für Physik, D-55099 Mainz

Bismuth sulfide (Bi_2S_3) is a non-toxic n-type semiconductor with a band gap of $E_g = 1.3\,\text{eV}$ and thus a potential candidate for thin film solar cells. We present a temperature dependent photoluminescence (PL) study on the mm-scale and a laterally resolved PL study on the μm-scale and determine in both cases the opto-electronic properties of a physical vapor deposited Bi_2S_3 film. We find a splitting of quasi-Fermilevels (QFL) of $\mu = 650\,\text{meV}$ and an optical band gap of $E_{opt} = 1.3\,\text{eV}$ at room temperature. Although only stoichometric Bi_2S_3 can be found in the film, laterally resolved maps of the PL yield, QFL-splitting and optical band gap show modulations in the local properties most likely due to different crystal orientations of the Bi_2S_3 grains.

HL 81.11 Wed 17:00 P1

Drive Level Capacitance Profiling on CIGS-based Thin Film Solar Cells — •Lisa Paller[1,2], Felix Daume[1,2], Andreas Rahm[1], and Marius Grundmann[2] — [1]Solarion AG, Leipzig (Zwenkau) — [2]Institut für Experimentelle Physik II, Universität Leipzig

For the efficient conversion of solar energy into electrical energy, a high density of mobile charge carriers within the solar cell device is required. The density of defects and their energetic position within the band gap play a decisive role in the generation of such electron hole pairs. These defect properties have been studied on $CuIn_{1-x}Ga_xSe_2$-based thin film solar cells by means of drive level capacitance profiling (DLCP). The variation of the sample temperature and the frequency of the applied AC voltage during DLCP allowed an estimation of the ionization energy of the defects.

We compare DLCP and the strongly related capacitance voltage profiling (CV) in order to point out advantages and disadvantages of both techniques. In the literature an overestimation of the carrier densities acquired via CV-measurements is reported . In order to verify the meaning of these results for our samples, CV measurements have been performed and the resulting doping profiles have been compared to

the ones obtained from DLCP. In addition to high efficiencies a large lifetime of the solar cell devices is desirable. Therefore the samples have been artificially aged by a damp heat treatment and the defect properties have been investigated again via the two aforementioned capacitance profiling techniques.

HL 81.12 Wed 17:00 P1

Accuracy comparison for different methods of extraction of parameters of CIGS solar cells — •Jose Fabio Lopez Salas, Jan Keller, and Ingo Riedel — Laboratory for Chalcogenide Photovoltaics, Energy and Semiconductor Research Laboratory, University of Oldenburg

The Shockley equation describes the current density in a solar cell resulting from a voltage bias. Especially the temperature dependent ideality facotr n and saturation current density J_0 are usually evaluated to understand the fundamental physical loss mechanisms of solar cells, such as the localization of dominant recombination paths. If these parameters are not properly derived, the Shockley equation may not reflect the real current-voltage (IV) characteristics which leads to misinterpretations of internal electrical losses. In this work a number of methods for extraction of the mentioned parameters are applied to different CIGS solar cells and are compared. The accuracy of the parameters is compared for the cases of light, dark, temperature-dependent and intensity-dependent measurements, while the mean square error of the corresponding fits serves as the quality indicator. The objective is to find a reliable method for extraction of parameters of CIGS solar cells which yields the best possible reproduction of their real IV behaviour and to quantify the inaccuracy of each approach.

HL 81.13 Wed 17:00 P1

Impact of light soaking and dark annealing on the electronic properties and transient photoluminescence of Cu(In,Ga)Se2 thin-film photovoltaic solar cells and absorbers. — •Viktor Gerliz, Stephan Heise, Jörg Ohland, Jürgen Parisi, and Ingo Riedel — Carl von Ossietzky University of Oldenburg, Germany

Continuous light soaking (LS) at elevated temperature and dark annealing (DANN) can significantly affect the performance of Cu(In,Ga)Se2 (CIGSe) thin film solar cells. LS at T=90°C under white-light illumination results in improved cell performance due to evident increase of the open circuit voltage and doping concentration. The long-term dark annealing of devices reduces this effect while swapping between meta-stable and relaxed states appears to be more or less reversible. It can be anticipated that both conditioning procedures affect the recombination dynamics of the minority carriers. To investigate such dependence we performed time-resolved photoluminescence measurements (TRPL) using the time-correlated single-photon counting (TCSPC) technique. In this contribution we discuss the progressive change of the photoluminescence decay characteristics as obtained for light-soaked and annealed CIGSe solar cells and CIGSe/CdS heterostructures.

HL 81.14 Wed 17:00 P1

Development of an automated process for chemical bath deposition (CBD) of thin CdS films under inert-gas atmosphere — •Marcus Dressler, Christine Chory, Jan Keller, Ulf Mikolajczak, Jürgen Parisi, and Ingo Riedel — Energy and Semiconductor Research Lab, Dept. of Physics, Univ. of Oldenburg, 26111 Oldenburg

$Cu(In_{1-x}Ga_x)Se_2$ (CIGSe) thin film solar cells are commonly exposed to air prior to the deposition of the n-type buffer layer (e.g. CdS). To avoid atmospheric degradation of the CIGSe surface during the device fabrication process chain we develop an automated technique for chemical bath deposition (CBD) of CdS thin films which is to be performed in a nitrogen glove box. To establish CdS thin films as an in house reference for the future development of alternate buffer materials the scope of this master thesis is to develop a well-defined and reproducible CdS-CBD process which has to be integrated into the automated baseline device fabrication process. In this contribution we present first results of chemical bath deposited CdS films on glass and CIGSe thin films. This poster will particularly focus on the optical and morphological characterization of CdS films manually processed under ambient conditions with the aim to identify promising synthesis-parameters like bath temperature, concentration of reagents and deposition time. While the optical transmission is of crucial importance to minimize parasitic absorption of the buffer layer in completed solar cells we also investigated the film roughness and coverage of the substrate as obtained for different process recipes. These investigations have been carried out by laser-scanning, atomic-force and scanning-electron-microscopy.

HL 81.15 Wed 17:00 P1

Electronic structure of Cu/In/Ga/Se-containing semiconductors — Juliana Srour[1], Fouad El Haj Hassan[1], •Andrei Postnikov[2], Michael Yakushev[3], and Tatyana Kuznetsova[4] — [1]Lebanese University, Beirut, Lebanon — [2]University of Lorraine, Metz, France — [3]Strathclyde University, Glasgow, UK — [4]Institute of Metal Physics, Yekaterinburg, Russia

Semiconductors based on the chalcopyrite-type $CuInSe_2$ (1-1-2) are promising for applications in photovoltaics, not least because their properties are not much deteriorated by the presence of typical point defects and deviations from stoichiometry. For tuning of electronic characteristics, indium is sometimes used in isoelectronic substitution by gallium. Such 1-1-2 compounds belong to a larger family of ternary phases, including notably 1-3-5 and 1-5-8 as particularly stable ones, which do often appear in practical synthesis. The structure of these phases can be generally derived from the zincblende one, with different substitutions on the cationic sublattice and a possible inclusion of ordered defects; however, some details of structures are still subject to debate. The 3-component region of the phase diagram, on its side of binary In-Se, borders to InSe (or, correspondingly, GaSe) semiconductors of not zincblende type (double-layer structure with cation-cation bonds). Different packing of layers gives rise to several polytypes. We study electronic structure of some representative binary and ternary compounds from first principles, using several flavours of exchange-correlation potentials, in order to test the impact of the latter on the band structure and on comparison with available experimental spectra.

HL 81.16 Wed 17:00 P1

Optical, Structural and Surface Properties Te added CIGSeTe Thin Films — •songül fiat[1], Emin Bacaksiz[2], Michael Kompitsas[3], and Güven Çankaya[4] — [1]Dumlupinar University — [2]Karadeniz Technical University — [3]National Hellenic Research Foundation — [4]Yildirim Beyazit University

The aim of this work was to study the dependence of the optical, structural and morphological properties of CuIn0.7Ga0.3(Se(1-x)Tex)2 (briefly CIGSeTe) thin films for three different stoichiometries (for x=0.0 x=0.4 and 1.0). The films have been deposited onto soda lime glass (SLG) substrates by the e-beam evaporation technique. The films showed high absorption and revealed optical band gaps ranging from 1,21-1,11 eV for x=0 and 1,15-1,09 eV for x=0.4 from as deposited to highest annealing temperature 525 °C and as last 1.05-1.00 eV from as deposited to highest annealed temperature 600 °C for x=1.0 amounts. The linear dependence of the lattice parameters as a function of Se and Te contents was examined. X-ray diffraction analyses showed that the films had the single phase chalcopyrite structure. The lattice parameters (a and c) varied linearly with the increase in Te content x from x=0.0 to x= 1.0. AFM maps have been analysed. and the relative elemental composition present in the deposited CIGSeTe films have been measured by using energy dispersive X-ray analysis (EDX).

HL 81.17 Wed 17:00 P1

Photo electric converters (Photovoltaic) and the solar energy power systems — •Ia Trapaidze, Gela Goderdzishvili, Rafiel Chikovani, and Tamaz Minashvili — Dep. of Physics, Georgian Technical University, 77 Kostava Ave. IV block, 0175, Tbilisi, Georgia

Renewable energy sources, such as wind, solar, hydro and geothermal energies, attract increasing attention in the world. Photo electric converters (PV) play an important role in Renewable Power generation. Numerous studies have been recently conducted regarding problems of Photovoltaics.

In this article we discuss physical concepts of Photovoltaics, new materials and structures used in fabrication of PV, constructers types, parameters and all technology of manufacturing. For developing of photovoltaics is very important to use cascaded and concentrating system. In cascaded systems vast amount of solar radiation is converted into electric energy through several cascades, which is the reason of increasing efficiency of photovoltaics. In the article we pay particular importance to the improvement of Photovoltaics parameters. We also discuss principles of design of solar energy power systems based on PV.

HL 82: Poster: Surfaces, interfaces and heterostructures (with O)

Time: Wednesday 17:00–20:00 Location: P1

HL 82.1 Wed 17:00 P1

Waveguide Quantum Electrodynamics - Nonlinear Physics at the Few-Photon Level — Tobias Sproll[1], Christoph Martens[1], •Michael Schneider[1], Peter Schmitteckert[2], and Kurt Busch[1,3] — [1]Max-Born-Institut, Max-Born-Str. 2A, 12489 Berlin, Germany — [2]Institut für Nanotechnologie, Karlsruher Institut für Technologie (KIT), 76344 Eggenstein-Leopoldshafen, Germany — [3]Humboldt-Universität zu Berlin, Institut für Physik, AG Theoretische Optik und Photonik, Newtonstr. 15, 12489 Berlin, Germany

The transport of few photons in 1D structures coupled to a fermionic impurity gives rise to a set of non-linear effects, induced by an effective interaction due to Pauli blocking such as photon bunching and the formation of atom-photon bound states.
We analyze a specific example of such systems, namely a 1-D waveguide coupled to a 2-level system, for the case of one and two-photon transport. Therefore we have developed a general theoretical framework, which contains analytic approaches originating in methods of qutantum field theory, like path integrals and Feynman diagrams as well as powerful numerical tools based on solving the time-dependent Schrödinger equation.
Owing its generality, our approach is also applicable to more involved setups, including disorder and dissipation as well as more complicated impurities such as driven and undriven 3-level systems.

HL 82.2 Wed 17:00 P1

Defect states and band bending effects at c-Si(111)/a-SiN:H interfaces — •Leif Eric Hintzsche[1], Changming Fang[1], Gerald Jordan[1], Martijn Marsman[1], Machteld Lamers[2], Arthur Weeber[2], and Georg Kresse[1] — [1]University of Vienna, Faculty of Physics and Center for Computational Materials Science, Sensengasse 8/12, A-1090 Vienna, Austria — [2]ECN Solar Energy, P.O. Box 1, 1755 ZG Petten, Netherlands

High performance solar cells based on crystalline silicon (c-Si) still play a major role in the photovoltaic market, and amorphous silicon nitride (a-SiN:H) often serves as anti-reflection coating (ARC) and passivation layer on top of those cells. The passivation properties are, thereby, strongly influenced by electronic defect states at the interface. In present study, these defects have been investigated by using ab intio molecular dynamics. We prepared 900 different c-Si/a-SiN:H structures and classified the most important defect types at the interface. Afterwards, we examined their energetic and spacial localization, and their band structure. We generally find higher defect concentrations at the interface, which are dominated by occupied, localized states in the a-SiN part and unoccupied, delocalized states in the c-Si part. While the former are mainly localized at under-coordinated Si atoms, the latter have rather inherited the character of the c-Si conduction band. We argue that this difference is a strong evidence for the band bending effect at the c-Si/a-SiN:H heterojunction.

HL 82.3 Wed 17:00 P1

Influence of surface treatment on NV centers in diamond — •Stefan Borgsdorf[1], Lina Elbers[1], Aniela Scheffzyk[1], Daniel Laumann[1], Christian Klump[1], Andreas Kaivas[1], Ulrich Köhler[1], Dieter Suter[2], and Frederico D. Brandao[2] — [1]Experimentalphysik IV, AG Oberflächen, Ruhr-Universität Bochum — [2]Experimentelle Physik IIIA, TU Dortmund

Color centers in diamond, especially NV centers, are practical single photon emitters due to RT operation and candidates for applications in quantum computing. We present a setup for low energy implantation of NV centers near the surface possibly allowing electrical addressing. Furthermore, we survey the influence of different surface and bulk treatments on the diamond and its NV centers. To purify the diamonds we reduced the amount of natural NV centers in optical grade diamonds by heating up to 1500 °C in hydrogen. The luminous intensity could be reduced down to 1/8. The optical grade diamonds were used for first implantations with N15 in discrete lines. Further, electronic grade diamonds will be applied. To control the charge state of the NV centers, the surface was terminated by Hydrogen or Fluorine via a H2- and a CF4-Plasma, respectively. HREELS and AFM measurements were executed to study the surface after plasma treatment. Likewise, the influence of optical transparent passivation layers on the intensity and charge state are object of interest. Finally a UHV chamber is modified to implant directly under UHV conditions and to allow in situ spectroscopic access to the diamond samples.

HL 82.4 Wed 17:00 P1

Investigation of Charge Transport across GaN-Pt Interfaces by Conductive Atomic Force Microscopy — •Sebnem Tuncay, Andrea Winnerl, Rui Nuno Pereira, and Martin Stutzmann — Walter Schottky Institut, Technische Universität München, Germany

GaN-based semiconductors have attracted great attention for applications including optoelectronics, high-power, high-frequency electronics and biosensing. Besides that, GaN-Pt systems have a considerable potential for future applications in photocatalysis and photoelectrochemical processing. For the latter applications charge transport across interfaces between GaN and metals or electrolytes are of central importance.

In this context, we investigate the charge transport across GaN-Pt interfaces. For sample preparation we use spin-coating in order to deposit Pt nanoparticles on n-type or p-type GaN layers. Using atomic force microscopy and scanning electron microscopy, we image the surface morphology of GaN layers grown on sapphire substrates and characterize the spatial distribution of Pt nanoparticles on such GaN surfaces. Conductive atomic force microscopy enables us to measure and map currents between the Pt nanoparticles and the GaN surface. The current-voltage characteristics of Pt nanoparticles on GaN show Schottky behaviour. Comparing the current-voltage characteristics measured on Pt nanoparticles and directly on the GaN surface is used to understand details of the charge transport across GaN-Pt interfaces.

HL 82.5 Wed 17:00 P1

Impact of high temperature annealing on Pd/GaN(0001) contact morphology — •Justyna Pers[1], Miłosz Grodzicki[2], Piotr Mazur[3], Stefan Zuber[4], and Antoni Ciszewski[5] — [1]Institute of Experimental Physics, University of Wrocław, pl. Maksa Borna 9, 50-204 Wrocław, Poland — [2]Institute of Experimental Physics, University of Wrocław, pl. Maksa Borna 9, 50-204 Wrocław, Poland — [3]Institute of Experimental Physics, University of Wrocław, pl. Maksa Borna 9, 50-204 Wrocław, Poland — [4]Institute of Experimental Physics, University of Wrocław, pl. Maksa Borna 9, 50-204 Wrocław, Poland — [5]Institute of Experimental Physics, University of Wrocław, pl. Maksa Borna 9, 50-204 Wrocław, Poland

Metal/GaN junction is the necessary part of each modern electronic and optoelectronic devices based on GaN; on the one hand as the ohmic contact for communication, and on the other as Schottky contacts in active devices or diodes. This report concerns Pd layers deposited under ultrahigh vacuum conditions onto n-type GaN(0001) crystals kept at room temperature. Combined surface techniques as XPS, UPS, STM and LEED were used to investigate physicochemical properties of the Pd/GaN(0001) contacts. The obtained Pd films have a grainy morphology beginning from the earliest stage of growth. Electron affinity of the clean n-GaN surface amounts to 3.1 eV. The work function of the Pd film of mean thickness of 1 nm is equal to 5.3 eV. The Schottky's barrier height of the Pd/GaN(0001) junction has the value to 1.60 eV. After heating at 800°C of the Pd/GaN interface, the formation of Pd-Ga alloy is observed.

HL 83: Poster: Graphene (with MA/O)

Time: Wednesday 17:00–20:00 Location: P1

HL 83.1 Wed 17:00 P1

Semi-empirical phonon calculations for graphene on different substrates — •Henrique Miranda, Alejandro Molina-Sanchez, and Ludger Wirtz — Physics and Materials Science Research Unit, UNIVERSITÉ DU LUXEMBOURG, Luxembourg

We investigate the graphene-substrate interaction via changes in the phonon dispersion of graphene. Ab-initio calculations on these systems are of high computational cost due to the non-commensurability of the unit cells of graphene and the substrate. This leads to the formation of Moiré patterns with accordingly large supercell sizes. We use a semi-empirical force constant model for the calculation of phonons of graphene on different metallic and insulating substrates. The interaction of graphene with the substrate is described via suitably chosen spring constants. The phonon dispersion in the primitive unit cell of graphene is obtained via an "unfolding procedure" similar to the ones used for the discussion of ARPES (angular resolved photo-emission spectroscopy) of graphene on incommensurate substrates.

HL 83.2 Wed 17:00 P1

Bilayer graphene: topological phases and entanglement spectrum — •Sonja Predin and John Schliemann — Institute for Theoretical Physics,University of Regensburg, D-93040 Regensburg, Germany

We present a calculation of the entanglement spectrum of fermions in bilayer graphene. In particular, a non-trivial topological order of the Abelian phase of the time-reversal symmetry breaking d-wave state is studied. We show that the entanglement spectrum is gapped, additionally we show that edge excitations in the entanglement spectrum form doublet Dirac fields around every K point.

HL 83.3 Wed 17:00 P1

Ultrafast dynamics and photoluminescence of hot carriers in graphene — •Thomas Danz, Andreas Neff, Reiner Bormann, Sascha Schäfer, and Claus Ropers — IV. Physical Institute, University of Göttingen, 37077 Göttingen, Germany

The ultrafast dynamics of optically excited carriers in graphene can be monitored by pump-probe spectroscopy [1,2]. Furthermore, it was recently shown that the thermalization of hot carriers leads to photoluminescence at wavelengths far away from the exciting pump [3,4]. Here, we present the implementation of an experimental setup which combines transient spectroscopy with sub-15-fs temporal resolution with hot carrier photoluminescence detection under the same excitation conditions. With this approach, we aim at a comprehensive picture of the ultrafast carrier response and the disentanglement of the timescales underlying different relaxation pathways. First experimental results will be presented.

[1] J. M. Dawlaty *et al.*, Appl. Phys. Lett. **92**, 042116 (2008)
[2] M. Breusing *et al.*, Phys. Rev. B. **83**, 153410 (2011)
[3] C. H. Lui *et al.*, Phys. Rev. Lett. **105**, 127404 (2010)
[4] W. Liu *et al.*, Phys. Rev. B. **82**, 081408 (2010)

HL 83.4 Wed 17:00 P1

Electron spin resonance of ion-irradiation induced single vacancies on monolayer graphene characterized by scanning tunneling spectroscopy — •Sven Just[1], Stephan Zimmermann[2], Vladislav Kataev[2], Marco Pratzer[1], Bernd Büchner[2], and Markus Morgenstern[1] — [1]II. Physikalisches Institut B, RWTH Aachen — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden

Single vacancies with densities of $0.003/\mathrm{nm}^2 - 3/\mathrm{nm}^2$ are prepared on HOPG and on single layer graphene on SiO_2 produced by chemical vapour deposition using Ar ions with 50 eV kinetic energy. The vacancies exhibit a peak at E_F in scanning tunneling spectroscopy, which survives 3 h of air exposure, afterwards a small broadening of the peak is observed. Electron spin resonance shows a peak corresponding to g = 2.0022, if the defect density is above $0.3/\mathrm{nm}^2$, and a peak width of 10 G with an anisotropy below 0.5 G between in-plane and out-of-plane magnetic field. The peak width hardly depends on temperature, while the peak intensity decreases with increasing temperature in the range of 4 K - 20 K.

HL 83.5 Wed 17:00 P1

Enhancing the Raman signal of graphene on SiC(0001) by using a solid immersion lens in *top-down* geometry — •Felix Fromm[1], Martin Hundhausen[2], Michl Kaiser[3], Julia Krone[1], and Thomas Seyller[1] — [1]TU Chemnitz, Institut für Physik — [2]FAU Erlangen-Nürnberg, Lehrstuhl für Laserphysik — [3]FAU Erlangen-Nürnberg, Lehrstuhl für Werkstoffwissenschaften

We present a study of epitaxial graphene by recording Raman spectra from the backside through the silicon carbide (SiC) substrate. In that *top-down* geometry we profit from the fact, that the graphene layer emits approximately 96 % of the Raman intensity into the SiC [1]. However, we only observe an intensity enhancement of approximately a factor of 4 compared to the conventional *top-up* geometry. This is because the solid angle of detection is decreased by refraction at the SiC/air interface and is limited by the total internal reflection. To further improve the detection efficiency, we use a high refractive index solid immersion lens (SIL) made of cubic zirconia combined with a suitable immersion liquid. By that, the angle of total internal reflection, as well as the solid angle of detection are increased. We eventually observe an increase of the detected Raman intensity towards the *top-up* geometry to a factor of 25. As an additional advantage, the background signal of the two-phonon Raman modes of the SiC is suppressed to a large extent.

[1] F. Fromm et al., New J. Phys. 15, 113006 (2013)

HL 83.6 Wed 17:00 P1

Growth of graphene on 6H-SiC(0001) under ammonia/argon atmosphere — •Christian Raidel, Felix Fromm, Samir Mammadov, Martina Wanke, and Thomas Seyller — TU Chemnitz, Insitut für Physik, Germany

In this work we investigated the nitrogen incorporation into epitaxial grown monolayer graphene by using ammonia as process gas within argon flow during thermal decomposition of SiC. The growth parameters as temperature and ammonia concentration were studied by various surface sensitive methods as XPS, LEED, RAMAN, AFM, and STM. ARPES shows that the ammonia grown graphene shows more p-type doped graphene than undoped graphene on SiC(0001). Due to the dissociation of ammonia during the growth process etch pits are produced. Vacancy associated nitrogen incorporation was observed by XPS and STM.

HL 83.7 Wed 17:00 P1

Characterization and transfer of 2D dichalcogenides produced by anodic bonding — •Philipp Nagler, Gerd Plechinger, Christian Schüller, and Tobias Korn — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany

Atomically thin MoS_2 and WS_2 structures have attracted growing attention as promising 2D semiconductors. As monolayers, both materials exhibit a direct bandgap and therefore are suitable candidates for future opto-electronical devices. We produced singlelayer MoS_2 and WS_2 by means of anodic bonding. In this process, the material is bonded by electrostatic forces on a borosilicate glass substrate. Compared to mechanical exfoliation, this technique usually yields larger flakes. Anodic bonded MoS_2 flakes were characterized by Raman and photoluminescence (PL) spectroscopy. Performing low-temperature PL measurements, we observed similar behaviour as in SiO_2-supported MoS_2. Furthermore, PL measurements for anodic bonded WS_2 are presented. By applying the wedging transfer technique, we transferred anodic bonded monolayer WS_2 from the glass to a SiO_2 substrate. Additionally, using this method, heterostructures consisting of various 2D materials could be produced and characterized.

HL 83.8 Wed 17:00 P1

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

Graphene consists of carbon atoms, which are arranged in a two-dimensional honeycomb lattice. It has unique electronic properties, which can be examined in high quality samples [1]. These are often

prepared by mechanical exfoliation on a silicon wafer with silicon dioxide on top. This substrate has a strong influence on the transport properties due to charge traps and surface roughness [2]. To reduce these effects or to produce novel complexe layersystems, graphene sheets can be stacked by a transfer methode e. g. onto other substrates or one upon the other to fabricate twisted flakes. The latter has been done and was under examination with magnetotransport measurements. Graphene is exfoliated on a thin PMMA layer, which can be detached from the silicon wafer. This layer is then placed on another graphene mono- or bilayer flakes. The samples were characterized at low temperatures and in dependence of a magnetic field. Magnetic field independent oscillations could be observed in a multilayer system.

[1] K. S. Novoselov et al. Science **306**, 666 (2004)
[2] P. Barthold et al. NJP **13**, 0433020 (2011)

HL 83.9 Wed 17:00 P1

Twisted graphene bilayers, folded via atomic force microscope — •Johannes C. Rode, Dmitri Smirnov, Christopher Belke, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover

Naturally occurring double-layer graphene consists of two hexagonal lattices in Bernal stacking. We investigate the folding of single-layer graphene via atomic force microscope (AFM) and the electronic properties of thusly created bilayers. The crystal lattices of these are twisted against each other which affects the interlayer coupling, giving rise to interesting electronic properties like a screening effect and reduced Fermi velocities at higher twist angles. Furthermore, the influence of a moiré-superlattice or twist induced van-Hove-singularities can be expected at lower twist angles. Our samples are obtained by micromechanical cleavage of natural graphite and placed on a silicon substrate with a top layer of silicon dioxide. The atomic force microscope then serves as a tool to mechanically manipulate the sample by programmed tip movements. We show AFM-induced folding of graphene on a μm-scale which can afterwards be contacted via e-beam lithography. Magnetotransport measurements over the folded areas show interesting signatures like multiple origins of landau fans in the charge carrier concentration.

HL 83.10 Wed 17:00 P1

The Effect of the Chemical Potential of Graphene on THz Detection — •Markus Göthlich[1], Fathi Gouider[1], André Müller[2], Yuri B. Vasilyev[3], and Georg Nachtwei[1] — [1]Institut für Angewandte Physik, Technische Universität Braunschweig, Mendelssohnstraße 2, D-38106 Braunschweig — [2]Physikalisch Technische Bundesanstalt, Bundesallee 100, D-38116 Braunschweig — [3]A.F.Ioffe Physical Technical Institute, RU-194021 St.Petersburg, Russia

One particular fact about graphene is its remarkable Landau quantization $E_n = \mathrm{sgn}(n)\sqrt{\Delta^2 + 2\hbar e v_F^2 |n|B}$ with n being the Landau level (LL) index. This would allow a transition at 2.4 THz (corresponding to an energy of about 10 meV) to happen at a magnetic field as low as 0.2 T. But theoretical investigations show the opening of a bandgap and a high chemical potential in epitaxial graphene on Si-face SiC due to graphene–substrate interactions. On the other hand our calculations—based on Gusynin et al. Phys. Rev. Lett. 98, 157402 (2007)—show that at high chemical potential the photoresponse can only be observed at higher magnetic fields of some Tesla. Gating is difficult due to the insolating behaviour of SiC substrate on the one hand and THz intransparency of top gates on the other hand. Therefore our aim is to design a new sample geometry that allows the manipulation of the chemical potential of the graphene while not blocking the THz radiation before reaching the detector.

HL 83.11 Wed 17:00 P1

Gate-controlled STM study of magnetic impurities on a graphene surface — •Paul Punke[1], Christian Dette[1], Roberto Urcuyo[1], Christopher Kley[1], Sören Krotzky[1], Rico Gutzler[1], Marko Burghard[1], Soon Jung Jung[1], and Klaus Kern[1,2] — [1]Max-Planck-Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany — [2]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

Graphene has been regarded as an ideal material for post silicon electronic application due to its unique electronic properties. To realize a field effect transistor for logic applications out of graphene, there has been a lot of effort to understand the gating effect on the charge-carrier-density-dependent properties of graphene, such as electronic scattering, spin based phenomena and collective excitations. We have designed a gatable low temperature scanning tunneling microscope (STM) by adding contacts to the sample holder. To prepare the gate-tunable graphene devices, we use graphene grown by chemical vapor deposition (CVD), transferred with or without a supporting layer of polymethylmethacrylate (PMMA) or polystyrene (PS), on an insulating layer of SiO2 or hexagonal boron nitride (h-BN) on SiO2. We also grow the graphene on h-BN directly on Ni substrate by CVD method. The quality of these samples will be compared by means of optical microscopy, atomic force microscopy (AFM), Raman spectroscopy and STM. Finally, we will present the gate-controlled electronic structure of graphene.

HL 83.12 Wed 17:00 P1

Ion Implantation of Graphene - Toward IC Compatible Technologies — •H. Hofsäss[1], U. Bangert[2,3], W. Pierce[2], D. M. Kepaptsoglou[3], Q Ramasse[3], R Zan[1], M. H. Gass[3,4], J.A. van den Berg[5], C. Boothroyd[6], and J Amani[1] — [1]II. Physikalisches Institut, Georg-August-Universität Göttingen, Göettingen, Germany — [2]School of Materials, The University of Manchester, Manchester, United Kingdom — [3]SuperSTEM Laboratory, Daresbury, United Kingdom — [4]AMEC, Walton House, 404 The Quadrant, Birchwood, United Kingdom — [5]School of Computing, Science and Engineering, University of Salford, Salford, United Kingdom — [6]Ernst Ruska-Centre for Microscopy and Spectroscopy, Juelich Research Centre, Juelich, Germany

Doping of graphene via ultra low energy ion implantation could open possibilities for fabrication of nanometer-scale patterned graphene-based devices as well as for graphene functionalization compatible with large-scale integrated semiconductor technology. Using advanced electron microscopy/spectroscopy methods, we show for the first time directly that graphene can be doped with B and N via ion implantation of mass selected ions at energies of 20 - 30 eV and that the retention is in good agreement with predictions from calculation-based literature values. Atomic resolution high-angle dark field imaging (HAADF) combined with single-atom electron energy loss (EEL) spectroscopy reveals that for sufficiently low implantation energies ions are predominantly substitutionally incorporated into the graphene lattice with a very small fraction residing in defect-related sites.

HL 84: Poster: Electronic structure theory / Carbon (other than graphene) / Si, Ge, and SiC / III-V semiconductors (other than nitrides)

Time: Wednesday 17:00–20:00 Location: P1

HL 84.1 Wed 17:00 P1

Analytic evaluation of the electronic self-energy in the *GW* approximation for two electrons on a sphere — •Arno Schindlmayr — Department Physik, Universität Paderborn, 33095 Paderborn, Germany

The *GW* approximation for the electronic self-energy is a very important tool for the quantitative prediction of excited states in solids. However, its mathematical exploration has been hampered by the fact that it must, in general, be evaluated numerically even for very simple systems. Here I describe a nontrivial continuum model, consisting of two interacting electrons on the surface of a sphere, and show that a completely analytic derivation of the *GW* self-energy, in the absence of self-consistency, is possible in this case. In contrast to lattice Hubbard models with the same property, the electron dynamics are governed by the normal long-range Coulomb potential instead of a short-range onsite interaction, the strength of the correlation can be controlled by a natural physical parameter, the sphere radius, and the infinite Hilbert space of one-particle states is not truncated. Therefore, the analytic expression for the self-energy can be used to study the convergence of the energy gap between the highest occupied and the lowest unoccupied quasiparticle orbital with respect to the total number of states included in the spectral summations. The obtained asymptotic formula shows that the truncation error is dominated by a term proportional to the cutoff energy to the power $-3/2$, which is compatible with earlier numerical results for band gaps in real materials.

HL 84.2 Wed 17:00 P1

Defect energy levels: Hybrid density functional theory vs. many-body perturbation theory — •Wei Chen and Alfredo Pasquarello — Chaire de Simulation à l'Echelle Atomique (CSEA), Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

We establish a consistent description of the thermodynamic charge transition levels of localized point defects through hybrid density functional theory and many-body perturbation theory. Three point defects are presented in this work, including a color center (a fluorine vacancy) in lithium fluoride, an oxygen interstitial in silicon oxide, and a carbon split interstitial with ⟨100⟩-orientation in cubic silicon carbide. The choice of the defects spans atomically localized defects in both ionic insulators and covalent semiconductors. The hybrid-functional calculations are performed using the PBE0 and the range-separated HSE functionals. The G_0W_0 calculations are performed on top of PBE eigenvalues and eigenstates. We find that the total-energy difference method using (hybrid) density functionals yields remarkably compatible charge transition levels relative to the higher level G_0W_0 approach, provided the electronic structures are aligned with respect to the electrostatic potential. We highlight the importance of the finite-size effect, the delocalization error, and the choice of the calculation path in the G_0W_0 scheme of the defect level calculation. Our results substantiate the need of a correct description of the band edges in the prediction of defect energy levels.

HL 84.3 Wed 17:00 P1

Depth-Localization of Nitrogen-Vacancy-Centers in Diamond with Subwavelength-Accuracy — •Andreas Häussler and Fedor Jelezko — Institut für Quantenoptik, Universität Ulm, Albert-Einstein-Allee 11, 89081 Ulm , Germany

Nitrogen-Vacancy (NV) color centers in diamond are interesting candidates for several applications, e.g. magnetic sensing in solid state. In certain cases it is crucial to know the exact position of the center below the surface.

In our work, we use a simple confocal microscope and measure both the reflected light from the surface and the emitted light of the NV to determine the depth of the color center. Suitable calibration measurements and statistical evaluation of the data can then lead to a much higher precision than the point spread function of the microscope down to nanometer accuracy.

HL 84.4 Wed 17:00 P1

Peapods on NV-centers in diamond for quantum computing — •Fabian Fritz[1,5], Christian Spudat[2], Lothar Houben[3,5], Nicolas Wöhrl[4], Claus M. Schneider[1,4], and Carola Meyer[1,5] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, Germany — [2]Fraunhofer ENAS Chemnitz, Germany — [3]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Jülich, Germany — [4]University Duisburg-Essen and CeNIDE, Faculty of Physics, Germany — [5]JARA - Fundamentals of Future Information Technologies

The electron spin of an endohedral fullerene like $N@C_{60}$ is very well shielded from the environment showing a long spin coherence time and thus resembles a good quantum bit. The read-out of an individual electron spin remains a challenge but can be achieved by coupling the spin of the $N@C_{60}$ to an NV-center in diamond. In order to couple several quantum bits, the $N@C_{60}$ molecules have to be aligned in a one-dimensional chain. This can be accomplished by filling the $N@C_{60}$ into carbon nanotubes (CNTs), forming so-called peapods. To form such a quantum register, peapods have to be fabricated and placed on diamond substrates.

We present growth of CNTs directly on a diamond surface using chemical vapor deposition (CVD). For the peapod synthesis we use solvent filling instead of vapor filling, since the $N@C_{60}$ fullerenes are thermally instable. Peapods are synthesized using different solvents and characterized using high-resolution transmission electron microscopy. The most promising solvent to prevent residues in the CNTs is supercritical CO_2 due to the small-sized molecules.

HL 84.5 Wed 17:00 P1

Magnetotransport in carbon nanotube networks functionalized with tetranuclear metal complexes — •Marlou Slot[1,4], Michael Schnee[1,4], Claire Besson[1,2,4], Fabian Fritz[1,4], Robert Frielinghaus[1,4], Lothar Houben[1,3,4], Christopher Nakamoto[1,4], Paul Kögerler[1,2,4], Claus M. Schneider[1,4], and Carola Meyer[1,4] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, Germany — [2]Institut für Anorganische Chemie, RWTH Aachen, Germany — [3]Ernst Ruska-Centre, Forschungszentrum Jülich, Germany — [4]JARA - Fundamentals of Future Information Technologies

Carbon nanotubes (CNTs) exhibit outstanding electronic and spin transport properties. These properties can be manipulated by chemical functionalization. We present CNT networks, grown by chemical vapor deposition, to which tetranuclear cobalt(II), manganese(II) and zinc(II) coordination complexes are attached. In contrast to commonly used van der Waals bonding, where the molecular orientation with respect to the CNT is arbitrary, we fix the angle between CNT and complex using covalent functionalization. Since the chemical route is based on carboxylate ligand exchange, oxidation of the CNTs before the functionalization is required. Raman spectroscopy is used to optimize the oxidation with respect to the desired density of carboxylate groups and the resistance of the CNT network. Magnetotransport measurements at temperatures down to 3 K show a resistance increase towards lower temperatures and a negative magnetoresistance. The underlying transport mechanism and the effect of the functionalization with magnetic complexes on the magnetoresistance are analyzed.

HL 84.6 Wed 17:00 P1

Quantum transport in functionalized carbon nanotubes — •Michael Schnee[1,3], Robert Frielinghaus[1,3], Claire Besson[1,2,3], Paul Kögerler[1,2,3], Claus M. Schneider[1,3], and Carola Meyer[1,3] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institut für Anorganische Chemie, RWTH Aachen, 52074 Aachen, Germany — [3]JARA - Fundamentals of Future Information Technologies

Carbon nanotubes are a promising material with regard to future nanoelectronic applications due to their exceptional mechanical and electronic properties. Moreover, the transport properties can be altered by attaching molecules to the CNTs. Thus, electronic transport experiments on functionalized CNTs can be used to study CNT-molecule interactions.

In this work we present experiments conducted on CNTs covalently functionalized with tetramanganese coordination complexes. The functionalization procedure is very versatile and manganese can be exchanged with several other metals.

The CNTs are cooled down to a temperature of T=25mK using a dilution refrigerator. First results of quantum transport experiments

on functionalized CNTs suggest a quantum dot size similar to the designed device length. This indicates that the electron wave function is only weakly disturbed and coherence is not destroyed by the covalent bonding of a small number of molecules. Therefore, quantum transport spectroscopy can be used to study the interactions between CNTs and the attached molecules.

HL 84.7 Wed 17:00 P1

study of electrical and mechanical properties of single walled carbon nanotubes — •Maryam Youhannayee[1], Mathias Getzlaff[1], and Hossein Golnabi[2] — [1]Heinrich Heine Universität Düsseldorf — [2]Sharif university of technology

In this research, using the single-band tight-binding approach and the energy dispersion relation, variation of band gap energy due to the effect of uniaxial stress on the zigzag and armchair single wall carbon nanotubes has been investigated analytically. The obtained results show that in all the zigzag carbon nanotubes, the band gap behaves linearly with increasing the uniaxial stress and one can observe a transition from semiconducting to metallic. In case of zigzag nanotubes with small diameter we have critical point which in that point critical break happens. The armchair carbon nanotubes are disable in response to the uniaxial stress and their metallic behavior is retained.

This research also investigates the electromechanical coupling in single-walled carbon nanotubes. In the model system, the extra electric charge of nanotubes is assumed to be uniformly distributed between carbon atoms. The electrostatic interactions between charged carbon atoms are calculated using the Coulomb law. It is shown that the classical electrostatics is computationally efficient. I studied a simplified electron- lattice model at low charge injection levels and showed that the electromechanical actuation of SWNTs strongly depends on (N, M). N and M are the chiral index that shows different kind of nano tubes. The effects of charge injection (electron and hole), tube diameter on longitudinal, radial and torsional angle change have been examined.

HL 84.8 Wed 17:00 P1

I-V characterisation of a-Si/c-Si heterojunctions — •Patrick Thoma, Evelyn T. Breyer, Ovidiu D. Gordan, and Dietrich R. T. Zahn — Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

As pure crystalline silicon solar cells have limited light absorption efficiency due to their indirect band gap requiring thick absorption layers manufactured in an energy intensive production process, research tries to find new cheaper and more efficient systems for energy harvesting. One promising approach is the use of so called heterojunction solar cells, consisting of different semiconducting material layers which have advantages like complementary absorbance of light in various wavelength regions and lower production cost. The heterojunction of amorphous and crystalline silicon combines a favorable absorption characteristic for the solar spectrum and could reduce the amount of silicon used due to overall thinner films. For sample preparation, thin layers of amorphous silicon (a-Si) were prepared by magnetron sputtering in high vacuum on HF-etched p-type crystalline silicon (c-Si). During the sputtering process deposition parameters like temperature, hydrogen flow rate and film thickness of the amorphous film were varied. Using ohmic Nickel-Chromium back and front contacts, the samples were investigated by temperature dependent I-V characterisation and measurements under illumination using a solar simulator. Especially the influence of hydrogen flow rate on the current voltage (I-V) characteristics, barrier heights and thermal activation energies are shown in relation with cell efficiencies.

HL 84.9 Wed 17:00 P1

Electronic and optical properties of amorphous Ge nanocrystals in a crystalline Si matrix — •Moritz Laubscher[1], Sebastian Küfner[1], Jürgen Furthmüller[1], Peter Kroll[2], and Friedhelm Bechstedt[1] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas 76019, USA

Embedded Ge nanocrystals have been discussed as promising elements for novel optoelectronic devices, because of their luminescence and charge rentention properties. The low dimensionality, together with the heterojunctions formed by the nanocrystals and the matrices, lead to (unique) quantum-confined electronic states and therefore new tunable electronic and optical properties. In contrast to the well investigated embedded c-NC, amorphous Ge nanocrystalls have not been studied in an *ab-initio* framework. Usually, Ge NCs show quantum confinment effects, e.g. size-depended photoluminescence. The Ge/Si interfaces most likely build a type II heterostructure. It is not known how amorphousness together with quantum confinment and the interface between NCs and matrices effect electronic structure and therefore optical properties. In this study we use a algorithm analogue to the WWW-algorithm in order to generate embedded amorphous nanocrystals and the density functional theory with the Tran-Blaha approximation to simulate the electronic and optical properties near the fundamental gap with quasiparticle corrections. We discuss optical properties and possible photoluminescence by calculating optical dipole matrix elements.

HL 84.10 Wed 17:00 P1

Comparison of melting properties reproduced by the MOD Tersoff potential in diamond silicon structures with experimental values. — •Robert König, Vladimir Lipp, Dmitriy S. Ivanov, and Martin E. Garcia — Universität Kassel, Institut für Physik, Heinrich-Plett-Straße 40, 34132 Kassel, Germany

Abstract

Inspite of being one of the most widely used interatomic potentials for silicon, the Tersoff potential showed some discrepancies for the description of the melting properties for diamond silicon. In order to clear this issue Sakai et al. improved the Tersoff potential through changes in the angular dependent term. The improved potential was named the MOD Tersoff potential. Using classical Molecular Dynamics the properties of the MOD Tersoff potential at the melting point were computed in two ways. First the equilibrium melting temperature was determined from a sequence of liquid-crystal coexistence simulation performed at different pressures. In the second part, other properties like the volume of melting and the enthalpie of melting were found from another sequence of constant pressure and constant temperature simulations where the interatomic distance and the energy per atom were computed as a function of temperature. The results showed good agreement with their experimental values published in literature.

HL 84.11 Wed 17:00 P1

Cathodoluminescence and Electron Beam Induced Current Study on Grain Boundaries in Silicon — •Markus Nacke[1], Matthias Allardt[1], Paul Chekhonin[2], Ellen Hieckmann[1], and Jörg Weber[1] — [1]TU Dresden, IAP/ Halbleiterphysik — [2]TU Dresden, ISP/ Metallphysik

Temperature dependent cathodoluminescence (CL) and room temperature electron beam induced current (EBIC) measurements have been used to investigate the optical behaviour and electrical activity of grain boundaries (GBs) in silicon. Electron backscatter diffraction (EBSD) was applied for a comprehensive characterization of the structural properties of the GBs including the misorientationaxis and -angle as well as the crystallographic orientation of the GB plane. It was found that the panchromatic CL contrast of $\Sigma 3$ large-angle GBs depends strongly from the hkl-type of the GB plane. The results are in agreement with EBIC investigations on coherent and incoherent twins in Si. D1 emission (0.812 eV) was detected at a small-angle GB (SA-GB). Other D-lines were not observed. Mono- and pan-CL investigations performed in the temperature range from 4.5K to 50K revealed a complex CL contrast behaviour of the SA-GB. Cross-correlation (CC-) EBSD was applied to analyze the relationship between the strain field of the SA-GB and the spatial D1 emission distribution. CC-EBSD results indicate that the crystal lattice is locally expanded at the SA-GB.

HL 84.12 Wed 17:00 P1

Electrical characterization of femtosecond laser sulfur doped silicon — •Arne Ahrens[1], Philipp Saring[1], Anna Lena Baumann[2], Stefan Kontermann[2], Wolfgang Schade[2], and Michael Seibt[1] — [1]IV.Physikalisches Institut, Georg-August Universität Göttingen, Friedrich Hund Platz 1, 37077 Göttingen, Germany — [2]Frauenhofer Heinrich Hertz Institute, Am Stollen 19B, 38640 Gosslar, Germany

Femtosecond (fs) laser pulse irradiation in sulfur hexaflouride atmosphere is a versatile tool to modify optical and electrical properties of silicon. Structuring of the surface and sulfur doping beyond the solubility limit (hyperdoping) enhance optical absorption in the subbandgap and in the visible range which is attributed to surface structuring and the introduction of deep levels, respectively. Especially the sub-bandgap absorption makes such material a promising candidate for intermediate band solar cell applications, especially if impurity bands form due to a Mott transition [1]. In case of p-type silicon substrates, sulfur hyperdoping also leads to the formation of a buried

pn-junction which has recently been studied by means of cross-section transmission electron microscopy (TEM) and electron-beam induced current (EBIC) [2] as well as capacitance-voltage (CV) and SIMS measurements [3]. In this work, we apply EBIC, temperature-dependent CV- and deep-level transient spectroscopy (DLTS) to study deep levels which are introduced by the irradiation with fs laser pulses accompanied by careful TEM analyses. [1] M. Winkler et al., Phys. Rev. Lett. 106, 178701 (2011). [2] P. Saring et al., Appl. Phys. Lett. 103, 061904 (2013) [3] K.-M. Guenther et al., Appl. Phys. Lett. 102, 202104 (2013)

HL 84.13 Wed 17:00 P1

How to explain laser induced Si–>SiO2 electron injection at front and rear interfaces of a Si membrane? — •Per-Christian Heisel[1], Wolfgang Paa[1], and Herbert Stafast[1,2] — [1]Institute of Photonic Technology, Albert-Einstein-Str. 9, 07745 Jena — [2]Faculty of Physics & Astronomy, Max-Wien-Platz 1, 07743 Jena

Electrical field induced second harmonic generation (EFISH) is well known for Si/SiO2 interfaces and typically measured in reflection [1]. EFISH in transmission was first shown with an external field applied to a 100 microns thick MOS structure [2]. The first comparison of EFISH in reflection and transmission was shown recently [3,4] using a 10 microns thick, naturally oxidized Si membrane. The rear EFISH signal (transmission) rises much faster than the front signal (reflection) and yields a larger steady state value. These findings essentially originate from differences in the laser induced electron injection from Si to SiO2. Their explanation is approached by different models like e. g. the image force model.

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[4] G. P. Nyamuda et al., Appl. Phys. B 104, 735 (2011)

HL 84.14 Wed 17:00 P1

Coherent Transport in GaAs/InAs Core/Shell Nanowires — •Patrick Zellekens[1,2], Fabian Haas[1,2], Tobias Wenz[1,2], Natalia 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 Institute - 9, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA - Fundamentals of Future Information Technology

GaAs/InAs core/shell nanowires are very interesting objects for studying magnetic flux dependent quantum transport phenomena, due to the fact that the low bandgap InAs shell forms a cylindrical tube-like conductor around the high bandgap GaAs core. This allows the emergence of phase coherent transport phenomena, i.e. (h/e) flux-periodic conductance oscillations. In this contribution, we present magneto-transport measurements of GaAs/InAs core/shell nanowires at various temperatures in a magnetic field applied parallel to the wire axis. The magneto conductance of the core/shell nanowires revealed pronounced h/e-periodic oscillations, which can be attributed to electronic transport via angular momentum states. In a more detailed analysis higher harmonic $h/2e$ periodic oscillations were also resolved. In nanowires comprising a small core diameter of 70nm the h/e oscillations are visible at temperatures up to 50 K, indicating a large energetic separation of successive angular momentum states. These findings are supported by gate-dependent universal conductance fluctuation measurements, which show thermal stability of phase coherent transport up to 40 K.

HL 84.15 Wed 17:00 P1

Properties of exciton-polariton gap-solitons in a two-dimensional lattice — •Edgar Cerda-Mendez[1], Dimitryi Krizhanovskii[2], Sergei Gavrilov[3], Klaus Biermann[1], Maurice S. Skolnick[2], and Paulo Santos[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]University of Sheffield, Sheffield, United Kingdom — [3]Institute of Solid State Physics, Chernogolovka, Russia

Exciton-polaritons are bosonic quasi-particles that result from the strong coupling of photons and quantum well excitons in a semiconductor microcavity (MC). While the small mass arising from the photonic component allows polaritons to form condensates at low densities and high temperatures, the repulsive excitonic interactions provide a strong nonlinearity. The periodic spatial modulation of the MC creates an artificial band structure with energy gaps and negative dispersion. Due to the nonlinearity, spatially self-localized polariton states, known as gap solitons (GSs), may appear within the energy gaps when the kinetic energy contribution due to localization of polaritons with a negative mass compensates their repulsive interaction energy. In this work, we show that the properties of polariton condensate GSs are well described by a simple variational approach to solve the Gross-Pitaevskii equation. The GSs form in an (Al,Ga)As-based MC where a 2D tunable lattice is created by surface acoustic waves. We calculated the metastable states in the square lattice. The model predicts the observed real and k-space profiles of the GS as well as the dependence of its coherence length and optical threshold power with the lattice amplitude.

HL 84.16 Wed 17:00 P1

Growth of GaAs nanowires on GaAs (111)B substrates induced by focused ion beam — •Rüdiger Schott, Sven Scholz, Dirk Reuter, Arne Ludwig, and 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 samples fascinating structural properties. Heterostructures of highly lattice mismatched materials can be combined without dislocations and the growth metastable phases, unattainable in bulk materials like wurtzite GaAs, can be made. We present focused ion beam (FIB) induced molecular beam epitaxy (MBE) grown single GaAs nanowires on GaAs (111)B substrates from site selectively deposited Au seeds. Structural and optical properties of the nanowires are investigated by secondary electron microscopy (SEM), transmission electron microscopy (TEM) and photoluminescence spectroscopy (PL).

HL 84.17 Wed 17:00 P1

Epitaxial growth of heterostructures on GaAs (111)A and GaAs (111)B substrates — •Julian Ritzmann, Arne Ludwig, Rüdiger Schott, Dirk Reuter, and Andreas D. Wieck — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Universitätsstr. 150, D-44780 Bochum, Germany

Heterostructures on (111)-oriented GaAs substrates are known for possibly high light emitting efficiency and tunable electron spin lifetimes by suppressing the Dyakonov-Perel relaxation. This offers a wide range for new and unique devices in the field of spintronics and -optics. The growth by molecular beam epitaxy on these surfaces is however rather challenging and only a limited range of growth parameters leads to structures of high crystal quality.
In this work we present the capabilities of MBE-grown AlGaAs and GaAs layers on (111)A and (111)B GaAs substrates without miscut. The samples exhibit reduced surface roughness and good electrical properties shown by atomic force and scanning electron microscopy and van-der-Pauw Hall measurements.

HL 84.18 Wed 17:00 P1

Photo-modulated reflection spectroscopy of Ga(AsBi) bulk and quantum well structures — •Jan Kuhnert, Peter Ludewig, Kerstin Volz, and Sangam Chatterjee — Philipps-Universität Marburg, Marburg, Germany

Bismuth-containing structures based on GaAs are promising candidates for semiconductor lasers operating at telecom wavelength. By an incorporation of about 10% bismuth, this desired wavelength of 1550nm is reached. In this system the reduction of band gap is due to shifting of the valence bands rather than the conduction band. Besides the influence on the band gap, the spin orbit coupling is increased and the gap between the valence bands is increased[1]. This way, losses due to auger processes are reduced and high temperature efficiency is increased.To quantify the influence of bismuth concentration, we investigated multiple Ga(AsBi)/GaAs bulk samples with different Bi concentrations by room temperature photo-modulated reflection spectroscopy. In addition, to characterize confinement effects, a set of multi quantum well structures is investigated using the same technique. [1] Appl. Phys. Lett. 91, 051909, (2007)

HL 84.19 Wed 17:00 P1

Temperature-dependent external quantum efficiency of Ga(AsBi) — •Philipp Vlacil, Nils Rosemann, Peter Ludewig, Kerstin Volz, and Sangam Chatterjee — Philipps-Universität Marburg, Marburg, Germany

Dilute bismuth-containing alloys of GaAs have recently gained a lot of interest due to the large band gap reduction of about 60meV per percentage of bismuth. This large bowing shifts the Band gap of the alloy

towards the telecom wavelength for concentrations of about 10%. This band gap shift is a consequence of modifications to the valence bands rather than the conduction bands, which are shifted, e.g. when In or N are incorporated. Additionally, the spin orbit coupling is increased and the shift of the split-of valence band is significantly increased[1], inhibiting hole-related Auger recombination processes. Nevertheless, the rather large covalent radius of bismuth induces significant disorder effects in such alloys. To quantify these, we investigated two sets of Ga(AsBi)/GaAs bulk and multiple quantum well (MQW) samples with different Bi concentrations by temperature-dependent absolute photoluminescence spectroscopy using an integrating sphere mounted inside a closed-cycle cryostat. The temperature dependence of the luminescence is used to quantify disorder. [1] Appl. Phys. Lett. 91, 051909, (2007)

HL 84.20 Wed 17:00 P1

The influence of growth parameters on the phase composition and defect structure of InAs nanowires — •Anton Davydok[1,2], Andreas Biermanns-Föth[1], Emmanouil Dimakis[3,4], Lutz Geelhaar[3], and Ullrich Pietsch[1] — [1]Universität Siegen,Siegen, Germany — [2]Im2np, Marseille, France — [3]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [4]Helmholtz-Zentrum Dresden-Rossendorf (HZDR)

We presented the results of X-ray investigation of MBE grown InAs nanowires (NWs) onto silicon (111) substrate. It was found that InAs NWs preferentially grow in wurtzite phase but may contain a large number of stacking faults (SF). The aim of this work was to investigate the influence of various growth parameters as temperature, In-flux, V/III ratio etc.) on the structural phase composition. The density of SF has been evaluated from the FWHM of the (10i5) wurtzite Bragg reflection which is particularly sensitive to SF inclusions, followed by numerical simulations using a model of a statistical distribution of SF in an ensemble of many nanowires. It has been found that nearly independent from the choice of growth parameters a low SF density is found in the initial phase of NW growth. With increasing growth time the increase of SF density can be described by a function SF_den=A*exp(-L/d)+m, with A=0.37, d=-752 and m=0.41. The SF density increases fast in the beginning but saturates for longer growth time.

HL 84.21 Wed 17:00 P1

Self-assembled growth of InxGa1-xAs quantum dots on GaP by gas-source molecular-beam epitaxy — •Shabnam Dadgostar[1], Fariba Hatami[1], W. Ted Masselink[1], Jan Schmidtbauer[2], and Torsten Boeck[2] — [1]Departmant of physics, Humboldt university of Berlin. Newtonstr. 15, 12489 Berlin. Germany. — [2]Leibniz- Institute für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Germany

The InGaAs/GaP heterosystem is expected to be type I, suggesting its use for light emission. We have used gas-source molecular-beam epitaxy to grow InxGa1-xAs (x= 0.3, 0.5) quantum dots on GaP (100) substrates; the lattice mismatch is 6.0 and 7.4 %, x=0.3 and x=0.5. For a coverage of 2 monolayers of In0.3Ga0.7As deposited at 0.4 ML/s, however, AFM indicates the formation of high density of In0.3Ga0.7As quantum dots. Their density is 1.2 e11 cm-2, with average diameter and height of 12.5 nm and 2.5 nm, respectively. For In0.5Ga0.5As deposited under the same conditions, however, AFM measurements show evolution of large islands with diameter of 95 nm and height of 20 nm. The critical thickness for transition from two-dimensional to three-dimensional growth was determined by AFM results and it was found less than 1.5 and 1.3 monolayers for In0.3Ga0.7As and In0.5Ga0.5As respectively.

HL 84.22 Wed 17:00 P1

Structural properties of AlGaP films on GaP grown by gas-source molecular-beam empitaxy. — •Shabnam Dadgostar[1], Emad Hameed Hussein[1], W. Ted Masselink[1], Fariba Hatami[1], Jan Schmidtbauer[2], and Torsten Boeck[2] — [1]Departmant of physics, Humboldt university of Berlin. Newtonstr. 15, 12489 Berlin. Germany. — [2]Leibniz- Institute für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Germany

High-Q photonic crystal cavities with working range in visible wavelengths can be realized based on GaP membranes. Such membranes can be prepared as a single crystal using gas-source molecular-beam epitaxy with a sacrificial layer of AlGaP. High quality factor of photonic crystal cavity is limited by crystal quality of GaP membrane which depends on AlGaP sacrificial layer crystal quality. We have studied the effects of growth temperature and PH3 flux on the crystal quality of AlGaP layer. For our applications we used AlGaP structures with thickness of 1.0 μm and Al content of 85%. Both high-resolution x-ray diffraction and AFM measurements indicate that dislocation and oval-defects are minimized for growth temperature of 490oC and PH3 flux of 2.7 sccm.

HL 85: Organic light emission

Time: Thursday 9:30–10:45 Location: POT 006

HL 85.1 Thu 9:30 POT 006

OLED Lifetime Limitation by its Intrinsic Emission Characteristics — •Mustapha Al-Helwi[1,2,3], Jonathan Helzel[2], Johannes Reinker[2], Hans-Hermann Johannes[2], Ute Heinemeyer[1], and Wolfgang Kowalsky[2] — [1]BASF SE, Ludwigshafen, Germany — [2]Technische Universität Braunschweig, Brunswick, Germany — [3]Innovation Lab GmbH, Heidelberg, Germany

Organic light Emitting Diodes (OLEDs) already have efficiencies comparable to current commercial light sources. However, the chemical degradation of the materials during operation is still a major obstacle for the development of economically feasible devices. Thus investigating the mechanisms of the degradation origin is highly important. In this study we focus on the blue phosphorescent OLED. We introduce a differentiating lifetime measurement setup for probing of material stability toward different stress mechanisms. We identify the instability of fac-tris(N-diphenyl-benzimidazole-carbene)iridium(III): (Ir(dpbic)3), a hole transport material, towards high energetic exciton-polaron interaction. A sophisticated OLED spectrum measurement indicates the emission of UV photons with intensities strongly correlated to the device lifetime. Underpinned with polaron spectra, we signify our aging hypothesis: UV photons are generated by (Ir(dpbic)3) and absorbed by its positive polarons leading to the degradation of the molecule and hence to the limitation of the device lifetime.

HL 85.2 Thu 9:45 POT 006

Electroluminescence of Tamm states in a hybrid OLED/microcavity structure — •Stefan Meister, Robert Brückner, Daniel Kasemann, Hartmut Fröb, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden, Germany

We implemented an organic light emitting diode (OLED) into a high quality microcavity consisting of two distributed Bragg reflectors (DBRs). The OLED is composed of seven different layers. In order to electrically contact the active region it is inevitable to implement two metal layers. The high absorption coefficient of metal, however, limits the thickness and the positioning of these layers inside the microcavity.

Therefore simulations based on the transfer matrix algorithm are performed and the structure of the OLED is optimized to maximize the resulting quality factor of the microcavity.

After designing a suitable structure, the complete sample is realised and both electrically and spectroscopically investigated. Evaluating an electroluminescent spectra clearly shows emission from coupled resonances, so called Tamm states exhibiting quality factors of at least 800.

In summary it is possible to get electroluminescence from an OLED in a microcavity with quite high quality factors.

HL 85.3 Thu 10:00 POT 006

OLED - a light emitting thermistor? — •Axel Fischer[1], Thomas Koprucki[2], Klaus Gärtner[2], Daniel Kasemann[1], Björn Lüssem[1], Karl Leo[1], Annegret Glitzky[2], and Reinhard Scholz[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden — [2]Weierstraß-Institut (WIAS), Mohrenstraße 39, 10117 Berlin

For lighting applications, OLEDs need much higher brightness than for displays, causing substantial self-heating. Recently, it has been shown

that the temperature-activated transport in organic semiconductors favors thermal runaway and the occurrence of negative differential resistance (NDR) [1]. Here, we show by experiment and simulation that OLEDs produce such a strong electrothermal feedback that S-shaped NDR occurs similar to a thermistor device [2] but with the difference that the OLED comes along with a laterally extended crossbar architecture. Self-heating combined with the sheet resistance of the transparent electrode produces regions with declining voltage across the organic layers under rising voltage applied to the contacts. Interestingly, a part of these regions shows decreasing currents. Then, the current density becomes extremely inhomogeneous because regions with increasing and decreasing currents can occur at the same time, leading to strong local variations in luminance. [1] A. Fischer, P. Pahner, B. Lüssem, K. Leo, R. Scholz, T. Koprucki, K. Gärtner, and A. Glitzky, Phys. Rev. Lett. **110**, 126601 (2013) [2] A. Fischer, T. Koprucki, K. Gärtner, M. L. Tietze, J. Brückner, B. Lüssem, K. Leo, A. Glitzky, and R. Scholz, subm. to Adv. Funct. Mater. (2013)

HL 85.4 Thu 10:15 POT 006

Photolithographic structuring of organic electroluminescent devices with state-of-the-art efficiency — •Simonas Krotkus[1], Fabian Ventsch[1], Daniel Kasemann[1], Alexander A. Zakhidov[2], Simone Hofmann[1], Karl Leo[1], and Malte C. Gather[1,3] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Straße 1, 01069 Dresden, Germany — [2]Fraunhofer Research Institution for Organics, Materials & Electronic Devices COMEDD, 01109 Dresden, Germany — [3]School of Physics & Astronomy, University of St Andrews, North Haugh, St Andrews, KY16 9SS, Scotland, UK

Photolithography is a well-established patterning technique used in various applications, including color filter structuring for LCD displays. However, its use in pixel patterning for organic light-emitting diode (OLED) screens to date is rather limited, due to the use of organic or water-based solvents, etchants and photoresists, which are known to be detrimental to the OLEDs. Thus, structuring via shadow mask is used instead, which has its limitations in the high resolution patterning as well as the scalability to the large area substrates.

To address the incompatibility between organic semiconductors and the processing steps of the conventional photolithography, we utilize a double resist approach. It consists of a fluoropolymer as a lift-off layer in combination with a traditional photoresist/solvent process to allow pattern transfer. The lift-off step is performed in hydrofluoroether solvents, which are shown to be compatible with state-of-the-art OLED technology.

HL 85.5 Thu 10:30 POT 006

Inorganic nanolaminate-encapsulation for organic light emitting diodes — •Aarti Singh[1], Frederik Nehm[2], Hannes Klumbies[2], Uwe Schröder[1], Lars Müller-Meskamp[2], Christoph Hossbach[3], Matthias Albert[3], Karl Leo[2], and Thomas Mikolajick[1] — [1]Namlab GmbH, Nöthnitzerstr 64, 01187 Dresden, Germany — [2]Institut für Angewandte Photophysik, TU Dresden, George-Bähr-Straße 1, 01069 Dresden — [3]Institut für Mikroelektroniktechnik, Nöthnitzerstr 64, 01187 Dresden

TiO2/Al2O3 and HfO2/Al2O3 multilayer of 20-100 nm total thickness have been tested for their diffusion barrier properties as direct encapsulation on organic light emitting diodes (OLEDs) and as indirect barrier layers on flexible PPET substrates. The different atomic layer deposition (ALD) process precursors, individual layer thickness and the total thickness of the nanolaminate stack were varied to evaluate optimum parameters that yielded best protection for OLEDs and resulted in lowest transmission rates for water. Water vapour transmission rates deduced out of electrical Ca test measurement reflect that the thin single layers (approx. 2 nm) in multilayer film stacks prove to be the best encapsulation layers in TiO2/Al2O3 system. WVTR values of 4x10-5 g/m2/day have been measured at 38°C, 90 RH in 20 nm thick ALD single layers deposited at 80°C. Luminescence measurements on OLEDs/Glass will be presented. The measurements are in accordance with the results of WVTR measurements and show that nanolaminates with thin single layers in the range of 0.5-1nm protect OLEDs better and longer than nanolaminates with thick single layers.

HL 86: Photonic crystals and cavities

Time: Thursday 9:30–11:15 Location: POT 051

HL 86.1 Thu 9:30 POT 051

Transverse Mode Localization in Three-Dimensional Deterministic Aperiodic Structures — •Michael Renner[1] and 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

We study the propagation of light in three-dimensional deterministic aperiodic structures fabricated by Dip-in direct-laser-writing. This fabrication technique enables us to investigate previously inaccessible thick polymer structures containing more than 100 elements of the underlying aperiodic sequence along the vertical direction. We employ one general construction scheme derived from the square Fibonacci tiling to obtain structures of different lattice spectral types, namely pure-point (Fibonacci sequence), singular-continuous (Thue-Morse) and absolute-continuous (Rudin-Shapiro). Characteristic reflectance spectra confirm the presence of the desired spatial correlations in the fabricated samples. By measuring the effective width of an incoherent beam traversing structures of different heights we deduce sub-diffusive behavior for all sequences in the near-infrared spectral range. The slowest broadening is observed for Rudin-Shapiro structures for which we find exponentially decaying lateral mode profiles indicating the existence of localized states.

HL 86.2 Thu 9:45 POT 051

The impact of nanoperforation on persistent photoconductivity and optical quenching effects in suspended GaN nanomembranes — •Olesea Volciuc[1], Tudor Braniste[2], Ion Tiginyanu[2], Marion Stevens-Kalceff[3], Jakob Ebeling[1], Timo Aschenbrenner[1], Detlef Hommel[1], Veaceslav Ursaki[4], 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]School of Physics, University of New South Wales, Sydney NSW 2052, Australia — [4]Institute of Applied Physics, Academy of Sciences of Moldova, Chisinau 2028, Moldova

GaN being ≈ 15-nm thick membranes and nanoperforated in an ordered fashion were fabricated using direct writing of negative charges by focused ion beam and subsequent photoelectrochemical etching of GaN epilayers. The characterization of the photoelectrical properties shows that both continuous and nanoperforated membranes exhibit pronounced persistent photoconductivity (PPC) which can be optically quenched under excitation by 546-nm radiation via impurity levels. We found that optical quenching of PPC occurs also under relatively intense intrinsic excitation of nanoperforated membranes by 355-nm radiation at temperatures T ¡ 100 K. The results are explained by taking into account strong surface localization of charge carriers in nanoperforated membranes and UV-induced reactions occurring at the surface states under intense intrinsic excitation.

HL 86.3 Thu 10:00 POT 051

ZnO based two-dimensional photonic crystal resonators. — •Sandro Hoffmann, Marcel Ruth, Thomas Zentgraf, and Cedrik Meier — University of Paderborn, Experimental Physics & CeOPP, Warburger Str. 100, 33098 Paderborn.

With emission in the UV region, ZnO is a promising material system for photonic resonator based devices. In particular, photonic crystals (PhCs) have the potential for realizing high quality resonators and waveguides.

The fabrication of fully undercut ZnO based photonic crystal membranes is presented in this talk. Initially, the ZnO is grown by plasma assisted molecular beam epitaxy (MBE) on a dry oxidized SiO_2 layer on top of a Si(111) substrate and is subsequently covered with SiO_2 via chemical vapor deposition (CVD). Thereafter, the heterostructure is patterned by electron beam lithography and reactive ion etching, followed by wet etching in a KOH solution. Additionally, high tem-

perature rapid thermal annealing (RTA) is used in order to enhance the photoluminescence (PL) of the ZnO layer. Measurements of a H3 cavity by cw excitation and two-photon absorption result in resonances within the photonic band gap for TE-polarization between 2.9 eV and 3.2 eV. Finite-differences time-domain (FDTD) simulations support the experimental data. Providing emission in the UV region and photonic waveguiding, this is essential for the realization of numerous applications, including quantum information and photonic circuits.

HL 86.4 Thu 10:15 POT 051

Photonic Crystal Grating Couplers for Quantum Applications — •Janik Wolters[1], Andreas W. Schell[1], Carlo Barth[1], Jürgen Probst[2], Max Schoengen[2], Bernd Löchel[2], and Oliver Benson[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, AG Nano-Optik, Newtonstraße 15, 12489 Berlin — [2]Helmholtz Zentrum Berlin, Institut Nanometeroptik und Technologie, Albert-Einstein-Str. 15, 12489 Berlin

Photonic crystals [1] are a promising platform for integrated quantum networks. In recent years, coupling of single emitters to photonic crystal cavities as first step towards such systems has been demonstrated [2].

Additional key ingredients are efficient photon guiding and coupling to the far-field. The latter is crucial since it forms the interface between photonic chips and the macroscopic measurement environment.

We present our latest results on the design and characterization of efficient grating couplers with large directivity and small footprint, as well as their integration into photonic networks.

[1] J. Wolters, et al., Thermo-optical response of photonic crystal cavities operating in the visible spectral range. Nanotechnology 24, 315204 (2013).

[2] J. Wolters, et al., Enhancement of the zero phonon line emission from a single nitrogen vacancy center in a nanodiamond via coupling to a photonic crystal cavity. Applied Physics Letters 97, 141108 (2010).

HL 86.5 Thu 10:30 POT 051

Thermo-optical response of photonic crystal cavity resonances — •Niko Nikolay[1], Janik Wolters[1], Max Schoengen[2], Andreas Schell[1], Jürgen Probst[2], Bernd Löchel[2], and Oliver Benson[1] — [1]Nano-Optics, Institute of Physics, Humboldt-Universität zu Berlin, Newtonstraße 15, D-12489 Berlin, Germany — [2]Institute for Nanometre Optics and Technology, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Albert-Einstein-Straße 15, D-12489 Berlin, Germany

Two-dimensional photonic crystal cavities are promising candidates for scalable integrated optical devices. Hence, they have increasing importance for quantum optics, photonics and sensing applications [1,2]. We focus on thermo-optical effects in photonic crystal slab resonators made of gallium phosphide. The thermal shift of the resonance wavelength and the underlying change of the refractive index are explored. An increased Q-factor is observed at low temperatures. Our results are the first systematic study of these properties over the wide temperature range between 5 and 300 K at a wavelength of about 605 nm [3]. In addition, experimental studies and theoretical analysis of thermo-optical switching of visible light by local heating of ultra-small attoliter volumes are discussed.

[1] Vahala, Nature 424, 839-846 (2003), doi:10.1038/nature01939

[2] Wolters et al., APL 97, 141108 (2010), doi:10.1063/1.3499300

[3] Wolters et al., Nanotech. 24, 315204 (2013), doi:10.1088/0957-4484/24/31/315204

HL 86.6 Thu 10:45 POT 051

Phononic Crystal Waveguides in GaAs — •Golnaz Azodi and James Stotz — Queen's University, Kingston, Canada

Surface acoustic waves (SAWs) provide a unique platform to create dynamically modulated semiconductor nanostructures for use in quantum information processing. The use of plane wave SAWs is the most practical and have been applied to a number of different quantum systems. However, as the complexity of a quantum system increases, the acoustic energy may be required to be delivered locally. In leveraging the tremendous success of photonic crystals, the use of phononic crystals enables the creation of phononic waveguide cavities to control the delivery of the acoustic modulation. To this end, we will discuss the development and recent results of fabricating phononic crystal waveguides on GaAs. While an unusual platform for SAW devices, GaAs is a rich platform for quantum systems, and it uniquely balances the demands for such hybrid systems. We will present FDTD modelling of the devices, and discuss the limitations that are placed on the design of the waveguides. To measure the effectiveness of the phononic crystal waveguides, we can image the SAW using a Sagnac interferometer, which provides a spatial mapping of the SAW as it travels through the waveguide structures.

HL 86.7 Thu 11:00 POT 051

Influence of the number of ZnSe QWs on the light-matter interaction in 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, Institute of Solid State Physics, University of Bremen, P.O. Box 330440, 28334 Bremen, Germany — [2]Semiconductor Epitaxy, Institute of Solid State Physics, University of Bremen, P.O. Box 330440, 28334 Bremen, Germany

The strong light-matter coupling in semiconductor microcavities (MCs) exhibits a high potential to realize novel types of optoelectronic devices such as thresholdless lasers based on polariton lasing. In order to operate such devices at elevated temperatures, high oscillator and high coupling strengths are required. For this purpose II-VI semiconductors with large excitonic binding energies are advantageous. The coupling strength can be enhanced by increasing the number of quantum wells (QWs) and by optimizing the amplitude of the cavity field at the QW position. We investigate binary ZnSe QW-based microcavities with different numbers of QWs and cavity thicknesses. The samples are characterized by micro-reflectivity and micro-photoluminescence measurements at different temperatures. The distributed Bragg reflector (DBR) stopband is centered at about 2.78eV. The QW emission can be tuned into resonance with the cavity mode by changing the sample temperature. Measurements show, that both are in resonance at about 200K. By increasing the number of QWs, a tendency to reach the strong coupling regime can be observed.

HL 87: Invited Talk Tobias Korn (with TT)

Time: Thursday 9:30–10:00 Location: POT 081

Invited Talk HL 87.1 Thu 9:30 POT 081

Time-resolved optical spectroscopy of 2D dichalcogenides — •Tobias Korn, Gerd Plechinger, Philipp Nagler, and Christian Schüller — Institut für Experimentelle und Angewandte Physik, Universität Regensburg

Recently, atomically thin layers of transition-metal dichalcogenides, such as MoS_2 and WS_2, have attracted a lot of attention. Like graphene, they can be prepared from bulk crystals by mechanical exfoliation. Unlike graphene, these materials are semiconductors with large bandgaps, and a transition from indirect to direct gap occurs for single layers. Spin and valley degrees of freedom in these structures are coupled, and can be directly addressed via optical excitation. We will demonstrate preparation and optical characterization of single-layer dichalcogenides, heterostructures built from different two-dimensional crystals, and large-area MoS_2 films. Deposition of single-layer MoS_2 on viscoelastic substrates allows us to apply local biaxial strain and subsequently vary the bandgap. We observe large valley polarization effects in our structures in photoluminescence experiments under near-resonant excitation. Photocarrier dynamics are investigated using time-resolved photoluminescence and picosecond pump-probe spectroscopy techniques.

HL 88: Graphene-like materials: Silicene, MoS_2 and relatives (with DY/MA/O/TT)

Time: Thursday 10:00–12:30 Location: POT 081

HL 88.1 Thu 10:00 POT 081

Many-body effects in 2D hexagonal semimetals and semiconductors — •Tineke Stroucken, Johanna Grönqvist, and Stephan W. Koch — Department of Physics and Material Sciences Center, Philipps University Marburg, Renthof 5, D-35032 Marburg, Germany

Recently, a variety of graphene-analogues materials like h-BN, silicene or transition-metal dichalcogenides have been fabricated. Similar to graphene, these novel material systems display exciting new physical properties, distinct from their bulk counterparts.

Owing to the symmetry of the hexagonal lattice, band edge carriers are described by massive Dirac Fermions. Typically, the Fermi-velocity is in the range of $c/300$ or below. This yields effective fine structure constants $\alpha = e^2/\epsilon\hbar v_F \gtrsim 2/\epsilon$, implying prominent Coulomb interaction and relativistic effects. Particularly, $\alpha \gtrsim 1$ indicates an excitonic instability of the noninteracting ground state.

In this presentation, we discuss conditions for strong Coulomb coupling in 2D hexagonal crystals and identify experimentally observable signatures signaling an excitonic ground state. To this end, the gap equations are solved self consistently with the polarization function, which depends on the interacting band structure.

[1] T. Stroucken *et al.*, Phys. Rev. B 84, 205445 (2011)
[2] J. H. Grönqvist *et al.*, EPJ B 85, 12 (2012)
[3] T. Stroucken *et al.*, Phys. Rev. B. 87, 245428(2013)
[4] T. Stroucken *et al.*, Appl. Phys. Lett. 103, 163103 (2013)

HL 88.2 Thu 10:15 POT 081

Single and Multi-Layer Silicene: Growth, Properties and Perspectives — •Patrick Vogt[1], Thomas Bruhn[1], Andrea Resta[2], Paola De Padova[3], and Guy Le Lay[2] — [1]Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany — [2]Aix-Marseille University, CNRS- PIIM UMR 7345, F-13397 Marseille Cedex 20, France — [3]Instituto di Struttura della Materia, Consiglio Nazionale delle Ricerche -ISM, via Fosso del Cavaliere, 00133 Roma, Italy

Silicene, a new silicon allotrope with a graphene-like honeycomb structure, has recently attracted considerable interest, because its topology confers to it the same remarkable electronic properties as those of graphene, with the potential advantage of being easily integrated in current Si-based nano/micro-electronics offering novel technological applications.

We will discuss the epitaxial formation of single layer silicene on Ag substrates and its structural and electronic properties [1-2]. Based on these results we will look at the growth of silicene multi-layers which can be explained by stacking of single silicene sheets [3-4]. Different experimental techniques are used to investigate atomic structure and electronic properties of this layered system and to discuss its similarities to graphite.

1) Vogt, P. et al., Phys. Rev. Lett. 108, 155501 (2012).
2) Avila, J. et al., J. Phys.: Condens. Matter 25, 262001 (2013).
3) De Padova, P.; Vogt, et al. Appl. Phys. Lett. 102, 163106 (2013).
4) Resta, A. et al., Sci. Rep. 3, 2399 (2013).

HL 88.3 Thu 10:30 POT 081

Optical and vibrational properties of MoS2 — •Ludger Wirtz[1], Alejandro Molina-Sanchez[1], and Kerstin Hummer[2] — [1]Physics and Materials Science Research Unit, University of Luxembourg — [2]Faculty of Physics, University of Vienna, Austria

Monolayer MoS2 is currently receiving a lot of attention as a potential alternative to graphene. Its band gap of about 2eV (depending on the dielectric environment) makes it a suitable candidate for thin-film electronics. The optical and vibrational properties of mono-layer, few-layer, and bulk are seemingly straightforward to calculate. Nevertheless some surprises occur: the phonon dispersion displays an anomalous Davydov splitting and the optical absorption spectra display a rich structure of excitonic peaks in the band-gap and in the continuum of interband transitions. We give a short review of the state-of-the art and discuss recent advances in the understanding of the influence of the substrate on the vibrations and electronic excitations.

HL 88.4 Thu 10:45 POT 081

Carrier- and valley dynamics of singlelayer MoS_2 — •Gerd Plechinger[1], John Mann[2], Christian Schüller[1], Ludwig Bartels[2], and Tobias Korn[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany — [2]Chemistry, Physics, and Materials Science and Engineering, University of California, CA 92521 Riverside, USA

Consisting of an only 0.7 nm thin S-Mo-S sheet and offering a direct bandgap at the K-points in the Brillouin zone, singlelayer MoS_2 represents a promising semiconductor material for flexible and transparent optoelectronic applications. By means of chemical vapor deposition (CVD), large-area films (several mm^2) of singlelayer MoS_2 can be produced. These were characterised by photoluminescence and Raman spectroscopy. In order to investigate the carrier dynamics, we performed pump-probe measurements in the spectral range of the optical transitions in singelayer MoS_2. Helicity-resolved PL measurements have demonstrated an efficient valley polarisation of the K^+ or K^- valley at near-resonant excitation. We probe these valley dynamics with Kerr spectroscopy and find a biexponential decay of the valley polarisation with decay times of a few tens of ps and a few hundreds of ps at low temperatures.

Coffee break (15 min.)

HL 88.5 Thu 11:15 POT 081

Photocurrent studies on semiconducting MoS2 — Marina Hoheneder, •Eric Parzinger, Alexander Holleitner, and Ursula Wurstbauer — Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, 85748 Garching

The current interest in transition metal dichalcogenides is stimulated by their peculiar electrical and optoelectrical properties and their potential for novel device applications. We investigate the semiconductor MoS2, which shows a crossover from an indirect to a direct bandgap semiconductor by thinning it down to a monolayer. We prepare MoS2 samples through micromechanical exfoliation and characterize the thin flakes with Raman spectroscopy. We further study photocurrent generation of single and few layer MoS2 in dependence of wavelength and power of the exciting light. We gratefully acknowledge financial support by BaCaTec.

HL 88.6 Thu 11:30 POT 081

Resonant Inelastic Light Scattering on MoS_2 — •Bastian Miller, Eric Parzinger, Alexander Holleitner, and Ursula Wurstbauer — Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, 85748 Garching (Germany)

Two-dimensional layered 'van-der Waals' materials are of increasing interest for fundamental research due to their peculiar band-structure.

We utilize inelastic light scattering - a contactless and extremely versatile tool - to study phonon excitation spectra of mono- and fewlayer MoS_2. The phonon modes are unique fingerprints of the material properties and are sensitive to defects, strain, doping and the number of MoS_2 -layers.

We observe signatures of multistep scattering processes involving phonon-phonon, electron-phonon as well as electronic excitations under resonant conditions, where the incoming or outgoing light meets the energy of a fundamental optical transition of the system.

HL 88.7 Thu 11:45 POT 081

The effect of substrate and environment on the elementary excitations of MoS_2 — •Eric Parzinger[1], Marina Hoheneder[1], Bastian Miller[1], Anna Cattani-Scholz[1], Alexander Holleitner[1], Joel W. Ager[2], and Ursula Wurstbauer[1] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, 85748 Garching (Germany) — [2]Joint Center for Artificial Photosynthesis, Lawrence Berkeley National Laboratory, One Cyclotron Road, Berkeley, California 94702 (United States)

The novel two-dimensional layered 'van-der Waals' material Molybdenum disulfide (MoS_2) is investigated using inelastic and resonant light scattering - a contactless and extremely versatile tool - to study phonon and electronic excitations. In particular, we focus on the influence of different supporting materials (SiO_2, sapphire and SAMs of organic molecules) as well as various environmental conditions (ambient, vacuum and water) on the low energy excitations of MoS_2. We find that both, different substrate and environment give rise to a significant modification of the most prominent Raman modes, whereas a monolayer is most effected by the environmental conditions. We gratefully acknowledge financial support by BaCaTec.

HL 88.8 Thu 12:00 POT 081

Spin-orbit coupling, quantum dots, and qubits in transition metal dichalcogenides — •Andor Kormanyos[1], Viktor Zolyomi[2], Neil Drummond[2], and Guido Burkard[1] — [1]Universität Konstanz — [2]Lancaster University

We derive an effective Hamiltonian describing the dynamics of electrons in the conduction band of transition metal dichalcogenides (TMDC) in the presence of perpendicular electric and magnetic fields. We discuss both the intrinsic and Bychkov-Rashba spin-orbit coupling (SOC) induced by an external electric field. We identify a new term in the Hamiltonian of the Bychkov-Rashba SOC which does not exist in III-V semiconductors. We point out important differences in the spin-split conduction band between different TMDC compounds. A significant consequence of the strong intrinsic SOC is an effective out-of-plane g-factor for the electrons which differs from the free-electron g-factor $g \simeq 2$. Using first-principles calculations, we give estimates of the various parameters appearing in the theory. Finally, we consider quantum dots (QDs) formed in TMDC materials and derive an effective Hamiltonian allowing us to calculate the magnetic field dependence of the bound states in the QDs. We find that all states are both valley and spin split, which suggests that these QDs could be used as valley-spin filters. We explore the possibility of using spin and valley states in TMDCs as quantum bits, and conclude that, due to the relatively strong intrinsic SOC in the conduction band, the most realistic option appears to be a combined spin-valley (Kramers) qubit at low B fields.

HL 88.9 Thu 12:15 POT 081

Analytical approach to excitonic properties of MoS2 — •Gunnar Berghäuser and Ermin Malic — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We present an analytical investigation of the optical absorption spectrum of monolayer molybdenum disulfide (MoS2). Based on the density matrix formalism [1], our approach gives insights into the microscopic origin of excitonic transitions, their relative oscillator strength, and binding energy [2]. We show analytical expressions for the carrier-light coupling element, which contains the optical selection rules and well describes the valley- selective polarization in MoS2 . In agreement with experimental results, we find the formation of strongly bound electron-hole pairs due to the efficient Coulomb interaction. The absorption spectrum of MoS2 on a silicon substrate features two pronounced peaks at 1.91 eV and 2.05 eV corresponding to the A and B exciton, which are characterized by binding energies of 420 meV and 440 meV, respectively. Our calculations reveal their relative oscillator strength and predict the appearance of further low-intensity excitonic transitions at higher energies. The presented approach is applicable to other transition metal dichalcogenides and can be extended to investigations of trion and biexcitonic effects.

[1] E. Malic and A. Knorr, Graphene and Carbon Nanotubes: Ultrafast Optics and Relaxation Dynamics, 1st ed. (Wiley-VCH, Berlin, 2013).

[2] Gunnar Berghäuser and Ermin Malic, arXiv:1311.1045 (2013)

HL 89: Metamorphic structures: Bringing together incompatible materials I (Focus session with DF)

This session is devoted to the challenge to epitaxially combine materials, which differ strongly in their basic properties like lattice constant or symmetry and hence seem to be incompatible. It shall provide a discussion forum about understanding, how such material combinations can be grown with high yield, i.e. low defect densities in the final active region, in order to realize device structures of a given material system on a substrate of another system. Examples where such combinations are needed are materials, where adequate substrates are not available, like In-rich GaInN structures for green light emitting devices on GaN, or complex device structures like multi-junction solar cells requiring the combination of incompatible layers.

Organizers: Ferdinand Scholz, Universität Ulm, and Andreas Hangleiter, TU Braunschweig.

Time: Thursday 9:30–13:00 Location: POT 251

Topical Talk HL 89.1 Thu 9:30 POT 251

Metamorphic III-V-on-IV structures and its application to optoelectronic devices — Yoshiaki Nakano, •Masakazu Sugiyama, and Takuo Tanemura — Department of Electrical Engineering and Information Systems, University of Tokyo, Japan

There has been a considerable interest to combine merits of different III-V semiconductors with group IV-based materials and devices. One obvious example is the integration of InGaAs FETs with Si MOSFETS for enhancing CMOS performance. Another example is the "silicon photonics" where III-V materials are integrated on silicon substrates to have them perform light emission and control functions. Such integration is brought about by either heteroepitaxy or wafer bonding. The former is regarded better in terms of manufacturablity but in general more difficult than the latter, and therefore, its applicability has been limited. In this talk, our trial of integrating III-nitrides and III-phosphides/arsenides on silicon and germanium by metal-organic vapor phase epitaxy and wafer bonding is reviewed, together with its application to light emitting, controlling, and receiving devices, includ-

ing micro lasers on Si and multi-junction solar cells.

Topical Talk HL 89.2 Thu 10:00 POT 251

Two types of buffer layer for the growth of GaN on highly lattice mismatched substrates and their impact on the development of sustainable systems — Tadashi Mitsunari[1], Koji Okuno[1], Yoshio Honda[1], Shigeyasu Tanaka[2], and •Hiroshi Amano[1,3] — [1]Department of Electrical Engineering and Computer Science, Nagoya University — [2]EcoTopia Science Institute, Nagoya University — [3]Akasaki Research Center, Nagoya University

There are two types of buffer layer for the growth of commercially available GaN-based blue LEDs on a sapphire substrate. One is the low-temperature deposited AlN or GaN buffer layer and the other is the sputter-deposited AlN buffer layer. In both cases, deposition condition, thickness and the annealing condition are critical for the fabrication of high performance blue LEDs. In this presentation, detailed study on the deposition and growth process of the low-temperature deposited AlN buffer layer and the following GaN growth will be discussed. We applied the sputter-deposited AlN buffer layer for the growth of GaN on Si. Details of the quality of GaN on a sputter-deposited AlN layer will be shown.

HL 89.3 Thu 10:30 POT 251

Influence of the substrate quality on the structural properties of short-period GaN/AlGaN superlattices grown by MBE — •Felix Schubert[1], Ulrich Merkel[2], Thomas Mikolajick[1,2], and Stefan Schmult[2] — [1]NaMLab gGmbH, Nöthnitzer Straße 64, D-01187 Dresden — [2]Institute of Semiconductor and Microsystems, TU Dresden, Nöthnitzer Straße 64, D-01187 Dresden

Short-period AlGaN/GaN superlattices have been established as versatile test structures to investigate the influence of the GaN substrate quality on the structural properties of AlGaN/GaN heterostructures. Of particular interest are surface roughness, layer accuracy and aluminum mole fraction in the MBE-grown superlattices. A variety of GaN substrates prepared by MBE, MOCVD, HVPE and ammothermal growth was investigated. For the best substrate quality theoretically expected properties like narrow high-order satellite peaks and interface fringes can be recovered from high resolution x-ray diffraction scans of the superlattices.

HL 89.4 Thu 10:45 POT 251

Strain engineering in a-plane GaN - Investigations on anisotropic strain behaviors — •Matthias Wieneke, Martin Feneberg, Michael Winkler, Peter Veit, Armin Dadgar, Jürgen Bläsing, Rüdiger Goldhahn, and Alois Krost — Otto-von-Guericke-Universität Magdeburg, FNW/IEP, Universitätsplatz 2, 39106 Magdeburg

The use of low temperature AlN interlayers (LT AlN) is a successful technique to prevent crack formation in thick c-plane GaN films, but also to reduce the density of basal plane stacking faults in semipolar GaN. Here, we studied the impact of LT AlN on a-plane GaN films grown by metal-organic vapor-phase epitaxy on 2-inch r-plane sapphire substrates. The curvature increases during the growth of tensely-strained a-plane GaN buffer layers, while it decreases after inserting LT AlN. However, an increasing asphericity evaluated by a 3-spot-curvature measurement indicates an anisotropic strain relaxation. Consequently, after cooling-down various ex-situ X-ray diffraction (XRD) measurements reveal an increase in compressive strain along the in-plane GaN m-direction, while it marginally decreases along the in-plane GaN c-direction for layers with a LT AlN interlayer. The non-biaxial strain behavior mirrors in energy shifts of the characteristic photoluminescence features which is compared to the results of 4-band **k·p** theory. Furthermore, XRD and transmission electron microscopy measurements exhibit a degradation in the crystalline quality of GaN layers grown on LT AlN interlayer.

HL 89.5 Thu 11:00 POT 251

Growth and characterization of non- and semipolar AlInN and possibilities for relaxed buffer layer engineering — •Ernst Ronald Buss[1], Uwe Rossow[1], Heiko Bremers[1], Tobias Meisch[2], Ferdinand Scholz[2], and Andreas Hangleiter[1] — [1]Institute of Applied Physics, TU Braunschweig, Germany — [2]Institute of Optoelectronics, Ulm University, Germany

The different a/c-ratios of group-III-nitrides open the possibility of strain engineering for relaxed buffer layers of AlInN in non- and semipolar GaN based structures. In this contribution, we present the very first results on low pressure MOVPE grown AlInN on semipolar $(11\bar{2}2)$ GaN templates, m-plane GaN templates, as well as m-plane pseudo-bulk GaN substrates. AlInN layers exhibit a macroscopic tilt due to the activation of basal plane slip for all non-c-plane orientations. For the m-plane case we will show that there is no shear of the unit cells of the different layers of the sample. Growth rates and indium incorporation efficiencies of m-plane and $(11\bar{2}2)$ oriented material could be estimated to be similar and the same as on c-plane GaN. While c- and m-plane AlInN shows extreme roughening with increasing layer thickness, $(11\bar{2}2)$ AlInN does not. Furthermore, we will present first experiments demonstrating a proof of concept of the specific relaxation of AlInN in different in-plane directions for $(11\bar{2}2)$ orientation. Depending on the indium content we are able to initiate relaxation only in $[1\bar{1}00]$ direction for 18% of indium, or $[11\bar{2}\bar{3}]$ direction for 28% of indium, respectively. All these results make AlInN quite promising for relaxed buffer layers and strain engineering for further growth.

Coffee break (15 min.)

Topical Talk HL 89.6 Thu 11:30 POT 251

Development of High Performance Semipolar GaN-based Blue and Green Lasers: Control of Stress Relaxation — •James Speck — UCSB Materials Department, Santa Barbara, CA USA

Nonpolar and semipolar GaN-based emitters have demonstrated low droop for LEDs and high performance for laser diodes. In this talk, we present two approaches to high performance blue and green laser diodes: the first using intentionally relaxed InGaN buffer layers for (11-22) oriented laser diodes and the second using selective area growth for (20-21) laser diodes.

For the relaxed (11-22) lasers we used strain compensated AlGaN/InGaN superlattice electron/hole blocking layers on intentionally relaxed InGaN buffer layers. Using this design, lasing at 447 nm was achieved with a threshold currentdensity of 7.2 kA/cm2, which is remarkably lower than previous results. Furthermore, wedemonstrate a 497 nm aquamarine-emitting semipolar (11-22)laser diode under pulsed operation.

For the coherent (20-21) lasers we used limited area epitaxy to minimize the misfit dislocation (MD) formation by preventing pre-existing TDs from entering a patterned mesa. Significant MD formation was suppressed by at least a factor of four for Al0.1Ga0.9N/GaN superlattices, enabling AlGaN-clad structures similar to those used in c-plane LDs. We then demonstrate AlGaN-clad blue (456 nm) LDs with threshold current density (Jth) of 4.5 kA/cm2 and GaN-clad true green (523 nm) LDs with Jth of 12 kA/cm2.

HL 89.7 Thu 12:00 POT 251

Improved X-ray diffraction simulations taking into account inhomogeneities exceeding the coherence length — •Christoph Berger, Dennis Schmidt, Jürgen Bläsing, Armin Dadgar, and Alois Krost — Otto-von-Guericke-Universität, Magdeburg, Deutschland

In many cases simulated diffraction patterns of semiconductor thin films or superlattices differ significantly from experimental data. The reason is that structural imperfections are often neglected in the simulation model. Indeed, many software packages can include the influence of compositional or thickness variations, but these variations occur on a shorter length scale than the coherence length of the diffractometer and have to be treated by dynamical theory. Including these influences often does not improve the simulation result. Due to the large area that is usually probed by the X-ray beam, one has to take into account structural variations larger than the coherence length as well, for instance lateral gradients across the wafer. These variations can be described by a sum of the diffracted intensity from the different parts of the specimen. In our method, a series of ideal simulations, each multiplied with a weighting factor, is summed up by a MATLAB routine that minimizes the deviation between the measurement and the sum of the weighted ideal simulations. The distribution of the weighting factors enables the estimation of the lateral variation width within the sample and the fit between simulated and experimental data is significantly improved.

HL 89.8 Thu 12:15 POT 251

Interactions between dislocations and overgrown v-shaped defects in GaN epitaxial layers — Phillip Weidlich[1], Michael Schnedler[1], Holger Eisele[2], Rafal E. Dunin-Borkowski[1], and •Philipp Ebert[1] — [1]Peter Grünberg Institut, Forschungszentrum

Jülich GmbH, 52425 Jülich, Germany — [2]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany

Due to the lack of large bulk substrates, most group III-nitride epitaxial layers have to be deposited on lattice-and thermal-mismatched substrates. The mismatch induces high dislocation concentrations. A variety of methods were invented to reduce the dislocation concentration in epitaxial GaN. Their common principle is the introduction of interfaces or inclined growth facets, which influence the line directions of threading dislocations. Inclined growth facets are also introduced by one of the most common extended defect in GaN layers, so called v-shaped defects. Therefore, we investigate the interactions between dislocations and v-shaped defects by mapping the spatial distribution and projected line directions of dislocations intersecting a cross-sectional (10-10) cleavage plane of GaN epitaxial layers using STM. The data is correlated with the spatial positions of v-shaped defects. The dislocations are found to be bent away from the inclined semipolar facets of v-shaped defects, due to a strain-induced repulsive interaction. The dislocation distribution is characterized by agglomerations and intersecting bundles of dislocations with parallel projected line directions, stabilized by many-body effects in the repulsive strain interactions.

HL 89.9 Thu 12:30 POT 251

Optical and structural investigations of the effect of barrier growth on GaInN quantum well structures — •Fedor Alexej Ketzer, Heiko Bremers, Torsten Langer, Uwe Rossow und Andreas Hangleiter — Institut für Angewandte Physik, Technische Universität Braunschweig

We study the influence of the growth of the barriers in GaInN multiple quantum wells (MQW) on structural and optical parameters of the wells. Therefore several MQWs were grown via low pressure MOVPE. Because the growth with H_2 as carrier gas is known to impede the incorporation of indium but is necessary during the growth of other layers, and therefore present in the reactor and structure, we investigate the effects of H_2 on the structure. We compare MQWs with different additional H_2 buffer gas flows during barrier growth with our reference samples with N_2 carrier gas. The growth parameters for the wells of all samples remain unchanged and lead to a nominal thickness of 2 nm with an indium content of 18 %. While the well thickness and indium content determined by photoluminescence do not differ for the reference samples without and the samples with H_2 buffer gas, the data of high resolution X-ray diffraction contradicts at a first glance. Here we see a drastically lower effective indium content of 7 %. This can only be explained by a strong inhomogeneity of the quantum wells and that only a small fraction of the quantum well area remains after growth. The influence of these inhomogeneities on the optical parameters and the internal quantum efficiency is discussed in detail.

HL 89.10 Thu 12:45 POT 251

Metamorphic growth of UV-B LEDs on $Al_{0.5}Ga_{0.5}N$ on AlN/Sapphire by MOVPE — •Johannes Enslin[1], Frank Mehnke[1], Martin Guttmann[1], Christoph Reich[1], Jens Rass[1,2], Tim Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Univerät Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Gustav-Kirchhoff-Str. 4, 12489 Berlin, Germany

For AlGaN-based LEDs emitting in the UV-B spectral region between 280 nm and 320 nm relaxed buffer layers enable pseudomorphic growth of the multiple quantum well active region. In our contribution we present a study of the effects of various superlattice designs on pseudomorphic growth. The superlattice consists of 80 periods of AlN and GaN layers. We found that the thickness of the GaN layer and the relative AlN to GaN layer thicknesses (i.e. AlN/GaN ratio) are crucial for the relaxation process. 4.5 μm thick $Al_{0.5}Ga_{0.5}N$ with an AlN/GaN ratio of one exhibits high densities of pits and cracks. LEDs grown on this layer show no luminescence most likely due to these defects. UV-B LEDs grown on templates with AlN/GaN ratios $\leq$ 0.4 exhibit fewer pits and no cracks, but show only poor luminescence. A smooth morphology was obtained for GaN thicknesses $\leq$ 2 nm and AlN/GaN ratios between 0.4 and 0.8. XRD scans show a distinct superlattice reflection. Reduced densities of pits and cracks indicate metamorphic growth. The optical emission power obtained from 305 nm LEDs grown on those layers reaches values up to 2.3 mW at 60 mA.

HL 90: Low-dimensional systems: Topological order (organized by TT)

Time: Thursday 9:30–13:15 Location: HSZ 204

HL 90.1 Thu 9:30 HSZ 204

Silicene and germanene as topological insulators: ab-initio approach — •Lars Matthes and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Silicene is a two-dimensional honeycomb lattice formed by silicon atoms and shares many properties of graphene, e.g. massless Dirac electrons at the Fermi level. In silicene the effect of spin-orbit interaction (SOI) is enhanced due to its buckled structure. Furthermore, by means of tight-binding calculations including SOI the emergence of topologically protected edge states has been predicted in silicene (and also germanene) nanoribbons [1] for zigzag and armchair edges, turning these crystals into topological insulators.

In this talk we study, whether or not silicene and germanene are topological insulators in a real simulation. We employ density-functional theory for the simulation of germanene nanoribbons. The band structures of ribbons of several widths as well as zigzag and armchair edges with hydrogen passivation are presented. The presence of topologically protected states is discussed versus edge shape, edge magnetization, ribbon width, and strength of spin-orbit interaction. The validity of results of the tight-binding model is critically discussed.

[1] M. Ezawa and N. Nagaosa, Phys. Rev. B 88, 121401(R) (2013)

HL 90.2 Thu 9:45 HSZ 204

First-principles Fermi surface characterization of doped PbTe — •Boris Sangiorgio, Michael Fechner, and Nicola Spaldin — ETH Zürich, Department of Materials, CH-8093 Zürich, Switzerland

Doped PbTe has raised increased interest because of its peculiar properties. In particular, it shows enhanced thermoelectricity, topological insulator behaviour and a charge Kondo effect, depending on the dopant atom. Here we investigate the nature of the Fermi surface in hole-doped PbTe using first-principles calculations. We begin by comparing recent experimental characterizations of the Fermi surface by means of effective masses, band offsets and de Haas-van Alphen frequencies with results from density functional theory (DFT). We find that the values of these properties depend strongly on the choice of exchange-correlation functional and identify functionals that give good agreement with experiment. Our results indicate appropriate methodologies for first-principles studies of doped-PbTe, and give insights into the origin of the charge Kondo effect.

HL 90.3 Thu 10:00 HSZ 204

Conductance of flat bands with long range Coulomb interactions — •Wolfgang Häusler — Institut für Physik, Universität Augsburg, D-86135 Augsburg

Dispersionless ("flat") electronic bands can arise throughout the Brillouin zone in certain multipartite lattices, besides ordinary dispersing bands. In such a flat band, hoppings between atomic orbitals interfere destructively which then leads to localization, a phenomenon denoted as "caging" of carriers. As a consequence, the system is insulating at zero temperature even when this band is partly filled, provided all other bands are either empty or completely filled.

One may ask whether long range Coulomb interactions can alter this situation and cause finite conductivity. In the absence of kinetic energy, flat band carriers tend to Wigner crystallize. Here, this general observation is analyzed for the two-dimensional case specifically for the Sutherland or $\mathcal{T}_3$–lattice where a conductivity is found, depending non-trivially on the carrier density at small flat band fillings.

HL 90.4 Thu 10:15 HSZ 204

Fluctuation-Induced Topological Insulators — •Sebastian Riese and Stephan Rachel — Institut für Theoretische Physik, TU Dresden

We consider interaction-induced topological insulators as paradigms for systems which are dominated by the interplay of a topological band structure and electron-electron correlations. In particular, we ex-

tend the previous work about fluctuation-induced topological phases. We show that the fluctuation-induced Chern insulator phase can be reduced to the non-interacting model with an additional mass-term which depends on the parameters of the self-energy. Then we generalize this idea to the spinfull case of time-reversal invariant topological insulators. We show that his phase is stable with respect to spin-mixing in the band structure and in the self-energy. Implications for realistic interacting Hamiltonians are discussed.

HL 90.5 Thu 10:30 HSZ 204

Topological phase transition in the Kitaev-Ising ladder — Amir Mohammad-Aghaie[1], Reza Haghshenas[1], and •Abdollah Langari[1,2] — [1]Department of Physics, Sharif University of Technology, P.O.Box 11155-9161, Tehran, Iran — [2]Max-Planck-Institut fuer Physik komplexer Systeme, 01187 Dresden, Germany

We have studied the Kitaev-Ising model on a ladder geometry using iDMRG algorithm. We find a quantum phase transition between the Kitaev and Ising phases whenever the ratio of Ising to Kitaev coupling is exactly equal to 1/2. The divergence in the von-Neumann entropy and the change of degeneracy in the entanglement spectrum justifies the symmetry protected topological phase (SPT) transition. We investigate the robustness of the SPT phase in the presence of cluster terms which preserve/break the symmetry of the model. We also discuss the effect of Ising terms on the legs of ladder in addition to the rhombic interaction, which leads to frustration for the antiferromagnetic interactions.

HL 90.6 Thu 10:45 HSZ 204

Entanglement Spectra of Interacting Fermions in Quantum Monte Carlo Simulations — Fakher F. Assaad[1], Thomas C. Lang[2], and •Francesco Parisen Toldin[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [2]Department of Physics, Boston University, U.S.A.

In a recent article T. Grover introduced a simple method to compute Renyi entanglement entropies in the realm of the auxiliary field quantum Monte Carlo algorithm [1]. Here, we further develop this approach and provide a stabilization scheme to compute higher order Renyi entropies and an extension to access the entanglement spectrum [2]. The method is tested on systems of correlated topological insulators.

[1] T. Grover, Phys. Rev. Lett. 111, 130402 (2013)
[2] F. F. Assaad, T. C. Lang, F. P. Toldin, arXiv:1311.5851

HL 90.7 Thu 11:00 HSZ 204

Topological insulators with arbitrarily tunable entanglement scaling — •Jan Carl Budich[1], Jens Eisert[2], and Emil Johansson Bergholtz[2] — [1]Department of Physics, Stockholm University, SE-106 91 Stockholm, Sweden — [2]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

We elucidate how Chern and topological insulators fulfill an area law for the entanglement entropy. By ex- plicit construction of a family of lattice Hamiltonians, we are able to demonstrate that the area law contribution can be tuned to an arbitrarily small value, but is topologically protected from vanishing exactly. We prove this by introducing novel methods to bound entanglement entropies from correlations using perturbation bounds and complement this approach by an intuitive understanding. These insights have a number of important consequences. The non-universality implies that the entanglement scaling cannot be used as a faithful diagnostic of topological insulators. The existence of arbitrarily weakly entangled topological insulators opens up possibili- ties of devising correlated topological phases in which the entanglement entropy is small and which are thereby numerically tractable, specifically in tensor network approaches.

15 min. break.

Topical Talk HL 90.8 Thu 11:30 HSZ 204

Density Matrix Renormalization Group: Probing the Topology of Quantum States — •Frank Pollmann — Max-Planck-Institute for the Physics of Complex Systems, Dresden, Germany

Matter occurs in various phases with different properties. Usually these phases are characterized in terms of symmetry breaking. A major discovery in the 1980s was the quantum Hall effect which forms a new kind of "topological" order. This order represents exotic phases with unusual properties and cannot be understood in terms of symmetry breaking. Since then, a growing number of instances of topological phases has accumulated, and important applications – not least topological quantum computers – have been proposed, but a characterization and classification of these new phenomena has been slow to emerge. In parallel, DMRG has arrived as a powerful numerical method with extensions to two dimensional systems and time-dependent phenomena. I will show how to use DMRG to develop new frameworks that help to understand topologically ordered systems. For example, it is now possible to extract characterizing properties of the anyonic excitations directly from the ground state of fractional quantum Hall systems. This approach further makes contact with "measurable" quantities (Hall viscosity) and field theories (central charge at critical points). Other remarkable examples are symmetry protected topological phases in one-dimensional systems for which DMRG provides a complete characterization.

HL 90.9 Thu 12:00 HSZ 204

Excitation statistics distinguish topologically ordered phases — •Siddhardh Morampudi[1], Curt von Keyserlingk[2], and Frank Pollmann[1] — [1]Affiliation: Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [2]Affiliation: Rudolf Peierls Centre for Theoretical Physics, 1 Keble Road, Oxford, OX1 3NP, United Kingdom

We investigate the characterization of topologically ordered phases and phase transitions between them. Topological order is a kind of order which cannot be characterized by the traditional approach of Landau's symmetry breaking theory and local order parameters. It is known to arise in diverse systems ranging from the well known fractional quantum hall systems to highly frustrated systems like the Heisenberg antiferromagnet on the Kagome lattice. The lack of local order parameters makes it difficult to uniquely identify a topologically ordered phase and to investigate phase transitions between them.

We consider two topologically ordered phases and use exact diagonalization to look at behaviour of various quantities as we move between them. We find that the usual methods of identifying a topologically ordered phase fail to uniquely distinguish these two phases. We then extract the braiding statistics of the excitations in the phases and use it as a non-local order parameter to distinguish the two phases, finding a first-order transition between them. Finally, we discuss how the approach could easily be generalized to other topologically ordered systems.

HL 90.10 Thu 12:15 HSZ 204

Detection of symmetry enriched topological phases — •Ching-Yu Huang[1], Xie Chen[2], and Frank Pollmann[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Department of Physics, University of California, Berkeley, California, USA

Topologically ordered systems in the presence of symmetries can exhibit new structures which are referred to as symmetry enriched topological (SET) phases. We introduce simple methods to detect the SET order directly from a complete set of topologically degenerate ground state wave functions. In particular, we first show how to directly determine the characteristic symmetry fractionalization of the quasiparticles from the reduced density matrix of the minimally entangled states. Second, we show how a simple generalization of a string order parameter can be measured to detect SET. The selection rules will get a characterization of SET. This way is more physical, and can be used by other methods, e.g., quantum Monte Carlo methods or potentially measured experimentally. We demonstrated the usefulness of this approach by considering first a spin-1 model on the honeycomb lattice and the resonating valence bond state on a kagome lattice.

HL 90.11 Thu 12:30 HSZ 204

Persisting topological order via geometric frustration — •Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik I, TU Dortmund, Deutschland

We introduce a toric code model on the dice lattice which is exactly solvable and displays topological order at zero temperature. In the presence of a magnetic field, the flux dynamics is mapped to the highly frustrated transverse field Ising model on the kagome lattice. This correspondence suggests an intriguing disorder by disorder phenomenon in a topologically ordered system implying that the topological order is extremely robust due to the geometric frustration. Furthermore, a connection between fully frustrated transverse field Ising models and topologically ordered systems is demonstrated which opens an exciting physical playground due to the interplay of topological quantum order and geometric frustration.

HL 90.12 Thu 12:45 HSZ 204

Kondo holes in topological Kondo insulators — •Pier Paolo Baruselli and Matthias Vojta — Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

The interplay between strong correlations and topology is a fast-developing and fascinating subject in the field of condensed matter.

Recently, the existence of topological Kondo insulators has been proposed [1]. In these materials the insulating behavior arises from strong correlations, that is from the Kondo screening of localized moments via conduction electrons, while non-trivial topology emerges from the structure of the hybridization between the local-moment and conduction bands.

We present a study of the physics of Kondo holes, i.e., missing local moments, in such topological Kondo insulators, using a self-consistent real-space mean-field theory. Kondo holes induce in-gap states which, for Kondo holes at or near the surface, hybridize with the topological surface state. In particular, we investigate the surface-state quasiparticle interference (QPI) induced by a dilute concentration of surface Kondo holes. We find that most QPI features can be interpreted by taking into account the shape of two-dimensional Fermi surface, together with the absence of backscattering characterizing Dirac cones in topological insulators. However, deviations from this simple picture arise: for example, the real part of the substrate Green's function and of the scattering matrix cannot be neglected in several cases.

[1] M. Dzero, K. Sun, V. Galitski, and P. Coleman, Phys. Rev. Lett. 104, 106408 (2010)

HL 90.13 Thu 13:00 HSZ 204

Topological entanglement entropy at quantum critical points — •Johannes Helmes and Simon Trebst — Institut für Theoretische Physik, Universität zu Köln, Germany

It is increasingly appreciated that a precise determination of the entanglement entropy of an interacting quantum many-body system can be used to identify the fundamental nature of its ground states. In particular, corrections to the prevalent boundary-law can be used to unambiguously identify topological order – a non-local form of order that eludes a standard characterization via correlation functions.

Here we report results for the entanglement entropy at a family of quantum critical points separating a topologically ordered phase from a conventionally ordered one. In technical terms, we employ large-scale quantum Monte Carlo simulations to study various deformations of the paradigmatic toric code model harboring a Z2 topological quantum spin liquid.

HL 91: Sustainable photovoltaics with earth-abundant materials I (organized by DS)

Energy conversion technologies, especially photovoltaics, exibit enormous growth aiming at extremely high power capacities per year. Therefore nontoxicity, low energy footprint and abundance of the materials used for photovoltaic devices are among the key requirements to a sustainable photovoltaic technology. Binary and ternary oxides and related materials are promising as the key materials to reach these goals. From this point of view copper and zinc based materials like ZnO, ZnS, Cu_2O, $ZnSnN_2$, Cu_2S, Zn_3P_2, $Cu(In,Ga)Se_2$, $Cu_2ZnSn(S,Se)_4$ are of special interest. For instance, the combination of ZnO and Cu_2O has been shown to be one of the promising approaches for next generation photovoltaics. Theoretical predictions promise efficiencies of such solar cells of up to 18%. Recently a breakthrough has been reported demonstrating of ZnO/Cu_2O thin film solar cell with efficiency of ca. 5%. Nevertheless, the fabricated devices are still far from commercial application. Further fundamental investigations are needed in order to understand the relevant materials and device physics in detail and to improve the efficiency of the cells. Progress on the growth of thin films, heterostructures and nanostructures, as well as new fabrication approaches will be discussed. Special attention will be given to the effect of the materials properties on the device efficiency, phenomena at interfaces, band gap alignment and surface passivation. This topical session aims to give an overview over the latest developments in the dynamic field of sustainable photovoltaics with earth abundant materials. (Organizers: Andrey Bakin and Andreas Waag, Technische Universität Braunschweig)

Time: Thursday 9:30–12:45 Location: CHE 91

Invited Talk HL 91.1 Thu 9:30 CHE 91

Photovoltaics with Copper Oxides — •Bruno Meyer — 1. Physikalisches Institut, JLU Giessen

The p-type conducting Copper-oxide compound semiconductors (Cu2O, Cu4O3 and CuO) provide a unique possibility to tune the band gap energies from 2.1 eV to the infrared at 1.40 eV into the middle of the efficiency maximum for solar cell applications. They appear to be an attractive alternative absorber material in terms of abundance, sustainability, and non-toxicity of the elements. Heterostructures with n-type AlGaN and MgZnO will be the basis of the solar cells. We present experimental results on the band offsets between the three copper oxides and the transparent conducting oxides and nitrides. Based on these finding various combinations of thin-film solar-cells are fabricated and compared to each other. The role of intrinsic defects and interface properties are discussed.

Invited Talk HL 91.2 Thu 10:00 CHE 91

Energy band alignment at interfaces of polycrystalline semiconductors for thin film solar cells — •Andreas Klein — Technische Universität Darmstadt, Germany

Thin film solar cells utilizing CdTe or $Cu(In,Ga)Se_2$ chalcogenide semiconductors have reached conversion efficiencies close to or even above 20%, respectively. The device structure of these cells is characterized by a sequence of an ohmic back contact, an unintentionally doped medium-gap chalcogenide as light absorber, a wide-gap chalcogenide buffer layer, and a transparent conducting oxide (TCO) front contact. Critical for high conversion efficiencies of such heterojunction devices is the energy band alignment at the various interfaces, which enable or block current transport. Historically, suitable interface properties have been achieved mainly by empirical device optimization. Photoelectron spectroscopy (PES) can provide detailed information on the chemical and electronic interface properties. This contribution introduces the experimental approach of interface analysis using PES and reviews available experimental data and understanding of interfaces for various thin film solar cells. In addition to interface properties of CdTe, $Cu(In,Ga)Se_2$, metallic back contacts, and TCO front contacts, the challenge of finding new absorber materials and device structures will be particularly addressed.

Invited Talk HL 91.3 Thu 10:30 CHE 91

Use of doped oxides for enhanced performance solar cells — •Judith MacManus-Driscoll — Dept. Materials Science, University of Cambridge, U.K.

ZnO and TiO2 are two of the most commonly used n-type metal oxide semiconductors in new generation solar cells due to their abundance, low-cost and stability. ZnO and TiO2 can be used as active layers, photoanodes, buffer layers, transparent conducting oxides, hole-blocking layers and intermediate layers. Doping is essential to tailor the materials properties for each application. The dopants used and their impact in hybrid solar cells and all inorganic solar cells are presented. In ad-

dition, the advantages, disadvantages and commercial potential of the various low energy fabrication methods of these oxides are presented.

Coffee break (15 min)

Invited Talk HL 91.4 Thu 11:15 CHE 91

Nanowire device concepts for thin film photovoltaics — •Silke Christiansen — Helmholtz Zentrum für Materialien und Energie, Berlin — Max-Planck-Institute for the Science of Light, Erlangen

Aligned silicon nanowire (SiNW) arrays to aim for power conversation efficiencies >>15% are fabricated on multi-crystalline Si layers on glass substrates using reactive ion etching with prior lithographic patterning using densely packed polystyrene (PS) spheres. Diameter, length, density and shape of SiNWs can be controlled and tuned for highest absorptions (close to 90%). Cell concepts with SiNWs are realized: (i) a hybrid organic/inorganic cell using SiNWs as absorber and PEDOT:PSS as a hole conducting polymer; (ii) a semiconductor-insulator-semiconductor (SIS) cell with SiNWs as absorbers, oxide (few Å thick Al2O3 by atomic layer deposition-ALD)) tunneling barriers for charge carrier separation and a transparent conductive oxide (TCO here: Al:ZnO, by ALD). Initial thin film solar cell prototypes reached open-circuit voltages of > 680 mV, short-circuit current densities of even > 35 mA/cm2 and efficiencies >13%. Advanced analytics to improve materials and cells are: (i) electron beam induced current (EBIC) to study charge carrier distributions; (ii) electron backscatter diffraction (EBSD) to study structural quality of the multi-crystalline Si layer; (iii) integrating sphere measurements to study optical properties and (iv) 4-point nano-probing to study electrical properties. Alternative electrodes such as graphene or silver nanowire webs are studied to even further improve the cells.

Invited Talk HL 91.5 Thu 11:45 CHE 91

Core shell ZnO nanowire heterostructures for solar cells — •Vincent Consonni — Laboratoire des Matériaux et du Génie Physique, Grenoble INP - CNRS, Minatec, 3 parvis Louis Néel 38016 Grenoble, France

ZnO nanowires (NWs) have received increasing interest due to their potential applications for instance in photovoltaic devices via core shell heterostructures. The core can be composed of ZnO NWs as electron transporting layer and the shell can comprise an absorbing layer such as a direct band gap semiconductor or a chemical dye in order to form type II heterostructures [1,2]. In this work, the structural properties and electron scattering mechanisms are investigated for SnO2:F thin films acting as front electrodes in nanostructured solar cells made from ZnO NW heterostructures [3]. A special emphasis is made on the formation mechanisms of ZnO NWs in solution by specifically focusing on polarity and crystal orientation effects [4]. Also, the light absorption properties of core shell ZnO NW heterostructures are studied by rigorous coupled wave analysis in order to design nanostructured solar cells. Eventually, several types of solar cells made from core shell ZnO NW heterostructures are fabricated by using different types of absorbing layers and their photovoltaic performances are tested under dark and AM 1.5G standard illumination conditions [1,2].

[1] V. Consonni et al., Appl. Phys. Lett. 98, 111906 (2011). [2] E. Puyoo et al., J. Phys. Chem. C 116, 18117 (2012). [3] V. Consonni et al., Acta Mater. 61, 22 (2013). [4] S. Guillemin et al., J. Phys. Chem. C 117, 20738 (2013).

Invited Talk HL 91.6 Thu 12:15 CHE 91

Potential and challenges of kesterite-type materials for thin film solar cells — •Thomas Unold — Helmholtz-Zentrum Berlin für Materialien und Energie

$Cu_2ZnSn(S,Se)_4$ thin film semiconductors have attracted much interest recently because of their potential application as absorber layers in thin-film solar cells. These kesterite-type materials can be derived from the chalcopyrite semiconductor $CuInSe_2$ by replacing the relatively rare element indium alternatingly with the more abundant elements tin and zinc, which would allow sustainable deployment of this technology on the terawatt scale. The close relation of their crystal structures raises the hope that also for the kesterite materials the excellent optoelectronic properties of their chalcopyrite cousins can be achieved. Although conversion efficiencies of 12% have now been demonstrated for kesterite-type solar cells, this value is still substantially lower than the record efficiencies above 20% for $Cu(In,Ga)Se_2$. One major challenge with kesterite materials lies in the control over defects and secondary phases imposed by the quartenary nature of this semiconductor. Interestingly, solution-based synthesis methods so far have yielded electronically superior material compared to vacuum-based deposition methods, in contrast to previous experience with the synthesis of almost any other inorganic semiconductor.

HL 92: Spintronics II (with MA/O/TT)

Time: Thursday 10:00–12:15 Location: POT 151

HL 92.1 Thu 10:00 POT 151

Magnetotransport in nanostructured InAs-based Heterostructures — •Olivio Chiatti[1], Sven S. Buchholz[1], 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, D-10099 Berlin — [2]FG Wachstum, Institut für Angewandte Physik, Universität Hamburg, D-20148 Hamburg — [3]Dept. of Physics, University at Buffalo, the State University of New York, Buffalo, NY 14260-1500 USA

The control of spin-polarized currents entirely by electrical fields is of great interest in the field of spintronics. The spin-orbit coupling in narrow-gap semiconductors has been identified as a possible tool to this end, because it couples the momentum of an electron to its spin. Nanostructures can be used to filter specific momentum modes and offer the possibility to create and detect spin-polarized currents. [1] Quantum point contacts (QPCs) in nominally symmetric InAs quantum well structures have been reported to generate spin-polarized currents, when asymmetric gate voltages are applied. [2]

We have fabricated Hall-bars and QPCs with in-plane gates in InAs quantum well structures, and performed transport measurements at low temperatures and in high magnetic fields. We investigate the effects of symmetric and asymmetric gate voltages. Here, we present the results of our measurements and discuss their implications for investigations of the spin-orbit coupling in InAs.

[1] Silsbee, *J. Phys.: Condens. Matter* **16**, R179 (2004)
[2] Debray *et al.*, *Nature Nanotech.* **4**, 759 (2009)

HL 92.2 Thu 10:15 POT 151

Acoustic charge and spin transport in GaAs (111)B quantum wells — •Alberto Hernández-Mínguez, Klaus Biermann, and Paulo Santos — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

The special properties of electron spin dynamics in GaAs (111) quantum wells (QWs) have been subject of study during the last years. Recently, it has been experimentally shown that, to first order in the electron wavevector, the in-plane component of the spin-orbit interaction can be suppressed simultaneously for all electrons in the QW just by applying an electric field of a certain amplitude perpendicularly to the QW plane. As a consequence, by tuning the amplitude of the electric field, the spin polarization lifetime of an electron ensemble is varied from a few hundred picoseconds to tens of nanoseconds.

In addition, surface acoustic waves (SAWs) have proved to be an useful tool for the controlled transport and manipulation of electron spins in GaAs QWs: the piezoelectric field accompanying the SAW allows the spatial confinement of electrons and their transport, with the well defined SAW velocity, over distances of several tens of micrometers. In this contribution, we explore the generation of SAWs in GaAs (111) QWs, as well as their combination with vertical electric fields for the acoustic transport of long living electron spins. In this way, we observe acoustic charge transport along 40μm distance, and spin transport around 15 μm.

HL 92.3 Thu 10:30 POT 151

Indirect Excitons Spin manipulation in GaAs/Al$_x$Ga$_{1-x}$As double quantum wells — •Adriano Violante[1], Snežana Lazić[2], Klaus Biermann[1], Rudolph Hey[1], Paulo Santos[1], Kobi Kohen[3], and Ronen Rapaport[3] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]Departamento de Física de Materiales,

Universidad Autónoma de Madrid, Madrid, Spain — [3]Racah Institute of Physics, Hebrew University of Jerusalem, Jerusalem, Israel

A spatially indirect exciton (IX) is a bound state of an electron and a hole localized in different quantum wells (QWs) of a double quantum well structure (DQW). In an IX, the spatial separation of electrons and holes reduces the exchange interaction, thus significantly enhancing the spin lifetime with respect to the direct QW excitons. [1] In this contribution, we show that spin-polarized IXs created using a circularly polarized laser beam diffuse up to distances 15 μm away from the generation point, revealing spatial oscillations of the polarization degree ρ_z. The latter are attributed to the precession of the spin vector in the spin-orbit effective magnetic field B_{SO} as they move away from the excitation spot, which can be modulated both with electric and magnetic fields. The IXs spin transport using acoustic fields is also discussed.

[1] J. R. Leonard, Y. Y. Kuznetsova, S. Yang, L. V. Butov, T. Ostatnick, A. Kavokin, and A. C. Gossard. Nano Lett. 9, 4204-4208 (2009)

HL 92.4 Thu 10:45 POT 151

Time- and space-resolved measurements of spin diffusion in high-mobility GaAs-based 2D electron systems — •Markus Schwemmer[1], Roland Voelkl[1], Tobias Korn[1], Sergey Tarasenko[2], Dieter Schuh[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

Two-dimensional electron systems embedded in (110)-grown, symmetrically doped GaAs/AlGaAs QWs are highly interesting for spintronics. They combine high carrier mobility with long spin dephasing times. Previously, we have studied these systems in different experiments, which either gave temporal or spatial resolution. By using a two-beam Hanle-MOKE method we could observe diffusion lengths of more than 125 μm at low temperatures. As a next step, the experimental setup was modified in order to achieve temporal and spatial resolution with the help of a single pulsed TiSa laser. The main issue is the spectral separation of the pump and the probe beams, which are collinearly focused onto the sample. Due to the broad spectrum of the femtosecond laser pulse, this can be realized using bandpass filters. Besides the mapping of the temporal propagation of the spins via diffusion, this experimental setup should also allow to visualize the evolution of a drifting spin packet. Financial support by the DFG via SFB 689 and SPP 1285 is gratefully acknowledged.

HL 92.5 Thu 11:00 POT 151

Direct measurement of the spin splitting in GaAs quantum wells — •Christoph Schönhuber[1], Matthias Walser[2], Christian Reichl[3], Werner Wegscheider[3], Gian Salis[2], Tobias Korn[1], and Christian Schüller[1] — [1]Universität Regensburg, 93040 Regensburg, Germany — [2]IBM Research-Zurich, 8803 Rüschlikon, Switzerland — [3]ETH Zurich, 8093 Zurich, Switzerland

We investigate the spin splitting in the conduction band of GaAs quantum wells employing Raman scattering experiments. The investigated system consists of a 12-nm-wide (001)-oriented GaAs/AlGaAs QW, which is asymmetrically Si modulation doped to reach a balanced Rashba and Dresselhaus SOI contribution.

The performed measurements on intrasubband transitions reveal a double peak structure for the [11] direction, while in [1-1] direction there is only a single peak. This anisotropic behavior in the spin splitting is probed for a wide range of transfered wavevectors and in good agreement with the prediction for a system with comparable magnitudes of Rashba and Dresselhaus SOI.

HL 92.6 Thu 11:15 POT 151

Hole g-factor anisotropy in coupled GaAs/AlAs quantum wells — •Christian Gradl, Michael Kempf, Dieter Schuh, Dominique Bougeard, Christian Schüller, and Tobias Korn — Universität Regensburg, D-93040 Regensburg, Germany

We performed time-resolved Kerr rotation measurements on undoped [110]- and [113]-grown double quantum well (QW) structures to resolve the spin dynamics of hole ensembles at low temperatures. For these growth directions, a strong anisotropy of the hole g-factor with respect to the in-plane magnetic field direction is theoretically predicted.

Our gated system consists of two QWs with different well widths, which we use for the spatial separation of the optically excited electron-hole pairs. Thus, we are able to create hole ensembles with spin lifetimes of several hundreds of picoseconds in the broader QW without any doping. This also allowed an observation of a strong hole g-factor anisotropy by varying the magnetic field direction in the QW plane. Moreover, our extracted values are in a very good agreement with theoretical predictions.

HL 92.7 Thu 11:30 POT 151

Polarization oscillations in spin-polarized vertical-cavity surface-emitting lasers controlled by multiple excitation pulses — •Henning Höpfner, Markus Lindemann, Nils C. Gerhardt, and Martin R. Hofmann — Photonics and Terahertz Technology, Ruhr-University Bochum, D-44780 Bochum, Germany

Spin-polarized lasers offer many potential advantages over their conventional counterparts, including threshold reduction, polarization control and ultrafast dynamics for increased modulation bandwidth [1].

Upon excitation with circularly polarized light that creates spin-polarized carrier in a vertical-cavity surface-emitting laser (VCSEL), the VCSEL shows oscillations of the circular polarization degree. These polarization oscillations can be much faster than the relaxation oscillations of the carrier-photon system. From calculations based on a rate-equation model we show that these oscillations can be switched on and off in a controlled manner using multiple circularly polarized optical excitation pulses. The results are verified experimentally, showing spin-induced polarization oscillation in conventional, electrically biased VCSELs subject to optical spin injection. We show polarization oscillation bursts with possible modulation frequencies far beyond the device's electrical modulation bandwidth.

[1] Gerhardt et al., Applied Physics Letters 99 (15), 151107 (2011)

HL 92.8 Thu 11:45 POT 151

Spin polarization of electron states in GaAs quantum wells — •Pavel Streda — Institute of Physics ASCR, Praha, Czech Republic

The standard method to establish the spin orientation of electron states, for zinc-blende semiconductors like GaAs, is based on the effective medium approach represented by the Luttinger Hamiltonian. For a two-dimensional electron gas, confined within a potential well, the real eigenfunctions of bound states across the well has been approximated by an envelope function. It leads to the conclusion that along main crystallographic axis, $[1,0,0]$ and $[0,1,0]$, the spin orientation is parallel or antiparallel with velocity directions. This contradicts to the tendency of the spin to be perpendicular to the velocity direction, observed in bulk structures.

The question arises if an envelope function approach, which suppresses the effect of local environment, is not too crude approach for real quantum wells, which are usually wider than ten lattice constants. To answer this question the empirical pseudopotential method has been used to establish energy dispersions and spin expectation values for two-dimensional electron gas confined within quantum wells of the different width. In all cases the tendency of the spin to be perpendicular to the velocity direction has been observed. For wide enough wells the obtained spin structure approaches that given by the bulk GaAs crystal with $k_z = 0$.

HL 92.9 Thu 12:00 POT 151

Spin injection efficiency dependence on MgO tunnel barrier thickness — •Lennart-Knud Liefeith, Tomotsugu Ishikura, Zhixin Cui, and Kanji Yoh — Research Center for Integrated Quantum Electronics, Japan

We study non-local spin valves in inverted InAlAs/InGaAs high-electron mobility transistors on InP(001). On the ferromagnet (FM) side, permalloy electrodes are employed. On the semiconductor (SC) side the electron system resides in a two-dimensional InAs channel. It has been argued that direct FM/SC contacts provide negligible spin polarization in the SC if the transport is diffusive, known as the conductivity mismatch problem[1]. In the ballistic transport regime efficient spin injection is predicted[2]. For devices basing on ballistic transport, a low contact resistance between FM and SC is essential. An strategy to tackle the conductivity mismatch problem is the insertion of a tunnel barrier at the FM/SC interface. We thus study ballistic structures with MgO tunnel barriers of varied thickness. Here we will compare spin injection efficiencies in non-local spin valve structures with either no or a 2 nm-thick MgO tunnel barrier at the FM/SC interface.

[1] G. Schmidt, „Fundamental obstacle for electrical spin injection from

a ferromagnetic metal into a diffusive semiconductor“, Physical Review B 62, R4790 (2000)
[2] M. Zwierzycki, „Spin-injection through an Fe/InAs interface“, Physica Status Solidi A: Applications and Materials Science 1, 25-28 (2003)

HL 93: Frontiers of electronic structure theory - Non-equilibrium phenomena at the nano-scale VI (organized by O)

Time: Thursday 10:30–13:15 Location: TRE Ma

Topical Talk HL 93.1 Thu 10:30 TRE Ma

Localization at the edge of 2D topological insulator by Kondo impurities — •Boris Altshuler[1], Igor Aleiner[1], and Vladimir Yudson[2] — [1]Physics Department, Columbia University, New York, NY 10027, USA — [2]Institute for Spectroscopy, Russian Academy of Sciences,Troitsk, Moscow 142190, Russia

Recent interest to the topological insulators [1] is inspired by the fact that their boundaries host gapless electronic excitations, which are extended and make the system conductive even in the presence of a potential disorder. 1D edge of a 2D topological insulator is predicted to have perfect conductance (2e2/h): right and left moving electrons carry opposite spins and potential disorder cannot flip spins and thus causes neither back-scattering nor the usual 1D localization.

What if there are localized spins coupled to the edge electrons? It turns out that the conductivity is still perfect provided that this coupling conserves the z-projection of the total spin of the impurities and electrons. Magnetic anisotropy violates this conservation and causes the backscattering even at T=0, i.e. an arbitrary small density of the spins with arbitrary weak anisotropy of the coupling leads to Anderson localization of the edge states in long enough samples [3]. The conclusion follows from the mapping of the electron-spin coupling to the well-studied problem [2] of disordered Luttinger liquid.

1. M.Z. Hasan and C.L. Kane, Rev. Mod. Phys. 82, 3045 (2010).
2. T.Giamarchi and H.J.Schulz, Phys. Rev. B 37, 325 (1988).
3. B.L.Altshuler, I.L.Aleiner, V.I. Yudson Phys. Rev. Lett 111, 086401 (2013)

HL 93.2 Thu 11:00 TRE Ma

Multiple Exciton Generation in Si and Ge Nanoparticles with high pressure core structures — •Stefan Wippermann[1], Marton Vörös[2], Dario Rocca[3], Adam Gali[4], Gergely Zimanyi[2], and Giulia Galli[2] — [1]Max-Planck-Institute for Iron Research, Düsseldorf — [2]University of California, Davis — [3]Universite de Lorraine, Nancy — [4]Budapest University of Technology and Economics

Multiple exciton generation (MEG) in semiconductor nanoparticles (NPs) is a promising path towards surpassing the Shockley-Queisser limit in solar energy conversion efficiency. Recent studies demonstrate MEG to be more efficient in NPs than in the bulk, including Si. However, the increased efficiency is observed only on a relative energy scale in units of the gap: quantum confinement (QC) effects believed to be responsible for efficient MEG in NPs, also increase their optical gap, swiftly shifting the MEG threshold beyond the solar spectrum.

We present density functional and many body perturbation theory calculations of the electronic, optical, and impact ionization properties of Si and Ge nanoparticles (NPs) with core structures based on high-pressure bulk Si and Ge phases. Si and Ge particles with a BC8 or ST12 core structure exhibit significantly lower optical gaps and multiple exciton generation (MEG) thresholds, and an order of magnitude higher MEG rate than diamondlike ones of the same size (1).

(1) S. Wippermann et al., Phys. Rev. Lett. 110, 046804 (2013)

HL 93.3 Thu 11:15 TRE Ma

Advanced time-evolution method for optical absorption spectra calculations — •Tobias Sander and Georg Kresse — Computational Materials Physics, University of Vienna, Sensengasse 8/12, 1090 Vienna, Austria

The Green's function formalism from many-body perturbation theory gives access to electronic structure calculation within the quasiparticle picture, as well as provides for calculating optical absorption spectra. Within the traditional ansatz [1], a Bethe-Salpeter like equation for the polarizability is solved. This requires to diagonalize an in general non-hermitian and complex matrix (BSE matrix). Usually, the off-diagonal elements of the BSE matrix are neglected and this is referred to as Tamm-Dancoff approximation. The computational effort can be reduced by using the time-evolution ansatz [2] which avoids the matrix diagonalization. We present a method based on the time-evolution algorithm, that finally avoids storing and diagonalizing the BSE matrix. This leads to a reduction of the scaling w.r.t the system size N from N^5 to N^3. Finally, we present first results for typical systems.

[1] S. Albrecht, L. Reining, R. Del Sole, G. Onida, PRL 80, 4510 (1998)
[2] W. G. Schmidt, S. Glutsch, P. H. Hahn, F. Bechstedt, PRB 67, 085307 (2003)

HL 93.4 Thu 11:30 TRE Ma

New starting point for the calculation of optical properties — •Igor Reshetnyak[1,2] and Lucia Reining[1,2] — [1]Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-DSM, F-91128 Palaiseau, France — [2]European Theoretical Spectroscopy Facility (ETSF)

The Bethe-Salpeter Equation based on Hedin's GW approximation to the self-energy is a powerful approach for describing electron-hole interactions in optical properties and photo-absorption spectra. However, in its current formulation it is both computationally heavy and displays cancellation effects not accounted for analytically. We discuss the sources of these cancellations and the possibility of putting them forward explicitly. We furthermore assess alternative formulations and sets of approximations to the BSE. For each of them we examine its behavior on model systems as well as their computational applicability. Finally we suggest possible directions for further investigations.

HL 93.5 Thu 11:45 TRE Ma

Electron-Energy Loss and Inelastic X-ray Scattering of CuO from First Principles — •Claudia Rödl, Francesco Sottile, Matteo Gatti, and Lucia Reining — Laboratoire des Solides Irradiés, Ecole Polytechnique, CNRS, CEA-DSM, 91128 Palaiseau cedex, France and European Theoretical Spectroscopy Facility (ETSF)

Even though the strongly correlated transition-metal oxide CuO has many fields of application (potential absorber material in photovoltaic devices, pigment in glass and ceramics, building block of cuprate superconductors,...), surprisingly little is known about its electronic excitations from a theoretical point of view. The band gap and all electronic excitations in its vicinity are governed by the intricate interplay between itinerant O $2p$ and localized Cu $3d$ electrons. Complex many-body effects, that are still not well understood nowadays, determine the screening of the electron-electron interaction.

Electron-energy loss and inelastic x-ray scattering experiments yield direct access to the wave-vector- and frequency-dependent loss function $-\operatorname{Im}\varepsilon^{-1}_{\mathbf{GG'}}(\mathbf{q},\omega)$, and, hence, to the screened Coulomb interaction W. We use time-dependent density-functional theory (TDDFT) to calculate the loss spectrum of CuO and discuss the occurring d-d and plasmon excitations. This allows us, by comparing theory and experiment, to assess the quality of the screened Coulomb interaction which is a key quantity for many-body approaches, for instance, GW and Bethe-Salpeter calculations.

HL 93.6 Thu 12:00 TRE Ma

Optical Spectra from Molecules to Solids: Insight from Many-Body Perturbation Theory — •Caterina Cocchi and Claudia Draxl — Humboldt-Universität zu Berlin, Institut für Physik and IRIS Adlershof, Berlin, Germany

The spurious long-range behavior of time-dependent (TD) density functional theory (DFT) is a well known source of error in describing bound excitons in solids. Remarkably, TD-DFT is often able to capture the optical features of isolated systems, even with the most simple exchange-correlation kernels, like the TD local density approximation. With the example of molecular crystals, we aim at solving the puzzle when and why TD-DFT can be relied on. We answer this question by confronting TD-DFT with many-body perturbation theory (GW and

Bethe-Salpeter equation), which is the most accurate methodology to describe optical excitations in solids. Our results are obtained with the all-electron code "exciting" (http://exciting-code.org), where all the quantities entering the two formalisms are treated on the same footing [1]. In-depth analysis allows us to identify the shortcomings of TD-DFT in predicting the excitonic spectra of extended systems and to understand when this methodology is capable of providing correct results.

[1] S. Sagmeister and C. Draxl, Phys. Chem. Chem. Phys. 11, 4451 (2009)

HL 93.7 Thu 12:15 TRE Ma

Relativistic Solar Cells — •Paolo Umari[1], Edoardo Mosconi[2], and Filippo De Angelis[2] — [1]Dipartimento di Fisica e Astronomia, Università di Padova, via Marzolo 8, I-35131 Padova, Italy — [2]Computational Laboratory for Hybrid/Organic Photovoltaics (CLHYO), CNR-ISTM, Via Elce di Sotto 8, I-06123, Perugia, Italy

Hybrid AMX_3 perovskites (A=Cs, CH_3NH_3; M=Sn, Pb; X=halide) have revolutionized the scenario of emerging photovoltaic technologies. Indeed, a rapid evolution led, very recently, up to 15% efficient solar cells. $CH_3NH_3PbI_3$ has so far dominated the field, while the similar $CH_3NH_3SnI_3$ has not been explored for photovoltaic applications, despite the reduced band-gap. Replacement of Pb by the more environment-friendly Sn would facilitate the large uptake of perovskite-based photovoltaics. Despite the extremely fast progress, the materials electronic properties which are key to the photovoltaic performance are relatively little understood. Here we develop an effective GW method incorporating spin-orbit coupling which allows us to accurately model the electronic, optical and transport properties of $CH_3NH_3SnI_3$ and $CH_3NH_3PbI_3$, opening the way to new materials design. The different $CH_3NH_3SnI_3$ and $CH_3NH_3PbI_3$ properties are discussed in light of their exploitation for solar cells, and found to be entirely due to relativistic effects.

HL 93.8 Thu 12:30 TRE Ma

Solar nanocomposites with complementary charge extraction pathways for electrons and holes: Si embedded in ZnS — •Stefan Wippermann[1], Marton Vörös[2], Adam Gali[3], Francois Gygi[2], Gergely Zimanyi[2], and Giulia Galli[2] — [1]Max-Planck-Institute for Iron Research, Düsseldorf — [2]University of California, Davis — [3]Budapest University of Technology and Economics

We propose that embedding silicon nanoparticles (NP) into amorphous, non-stoichiometric ZnS leads to promising nanocomposites for solar energy conversion. Using ab initio molecular dynamics simulations we show that upon high temperature amorphization of the host chalcogenide, sulfur atoms are drawn to the NP surface. We found that the sulfur content may be engineered to form a type II heterojunction, with complementary charge transport channels for electrons and holes, and that sulfur capping is beneficial to lower the nanoparticle gap, with respect to that of NPs embedded in oxide matrices. Our analysis was conducted using density functional theory with local and hybrid functionals and many body perturbation theory at the GW level.

HL 93.9 Thu 12:45 TRE Ma

Ultraviolet photo-emission spectroscopies from Koopmans-compliant functionals — •Ngoc Linh Nguyen[1], Giovanni Borghi[1], Andrea Ferretti[2], Ismaila Dabo[3], and Nicola Marzari[1] — [1]Theory and Simulations of Materials, École Polytechnique Fédérale de Lausanne, Station 12, 1015 Lausanne, Switzerland. — [2]Centro S3, CNR-Istituto Nanoscienze, I-41125 Modena, Italy — [3]Department of Materials Science and Engineering, The Pennsylvania State University, University Park, USA.

We study the photo-electron properties of organic photovoltaic molecules using Koopmans-compliant functionals [1] as well as the Perdew-Zunger self-interaction correction (PZ-SIC) [2] to density-functional theory. A simple method for simulating ultraviolet photoemission spectra (UPS) of molecules has been implemented. It is based on a plane-wave approximation for the final states to account for the spectra intensities. Our calculations show that Koopmans-compliant functionals provide ionization potentials and electron affinities closely comparable with those obtained by many-body perturbation theory (GW). In addition, we find that UPS spectra computed imposing the Koopmans' condition on the PZ-SIC functional are in remarkable agreement with experimental results.

Refs: [1] I. Dabo, A. Ferretti, N. Poilvert, Y. Li, N. Marzari, and M. Cococcioni, Phys. Rev. B 82, 115121 (2010); [2] J. P. Perdew and A. Zunger, Phys. Rev. B 23, 5048 (1981).

HL 93.10 Thu 13:00 TRE Ma

Self-consistent dynamical embedding in real space — •Wael Chibani[1], Xinguo Ren[1,2], Patrick Rinke[1], and Matthias Scheffler[1] — [1]*Fritz Haber Institute of the Max Planck Society, Berlin, Germany* — [2]*Key Laboratory of Quantum Information, USTC, Hefei, China*

Density-functional theory with its local-density (LDA) and generalized gradient approximations (GGA) is known to fail for localized states. To extend *ab initio* approaches to this domain, we have devised an embedding scheme that facilitates the treatment of the physically important part of a system with electronic structure methods, that are computationally too expensive for periodic systems, whereas the rest of the periodic system is treated with computationally less demanding approaches, i.e. LDA/GGA, in a self-consistent manner. Our scheme is based on the concept of dynamical mean-field theory (DMFT) [1]. However, in contrast to the original DMFT formulation for correlated model Hamiltonians, we consider here the unit cell as 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 functionals for simple bulk systems, e.g. Si or NiO. 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. By treating the embedded region with *GW* we were able to improve the band gap using only a small cluster. The effect of self-consistency in *GW* for the embedded region will also be addressed. [1] A. Georges *et al.*, Rev. Mod. Phys. **68**,14 (2006)

HL 94: Invited Talk Yong Lei

Time: Thursday 11:00–11:30 Location: POT 006

Invited Talk HL 94.1 Thu 11:00 POT 006

Template-realized three-dimensional functional nanostructures of semiconductors for high-performance device applications — •Yong Lei — Institute of Physics and IMN, Ilmenau University of Technology, Germany

With the device miniaturization, functional nanostructures become the foundation of modern and future devices. Comparing to planar nanostructures, three-dimensional (3D) nanostructures have extremely large surface areas and high structure densities, hence the realization of 3D nanostructures presents an important task for nanotechnology research. To address this challenging point, template-based 3D nanostructuring techniques with scalable, parallel and fast fabrication processes have been developed in our group. Using these techniques, different 3D semiconductor nanostructures are achieved with advantageous features including perfect regularity of large-scale nanostructure arrays, high density, scalable and parallel fabrication processes, and cost-effectiveness [1], which are highly desirable for device applications. More importantly, the obtained 3D nanostructures have high structural controllability, which makes these 3D nanostructures good systems for investigating and optimizing their physical properties. Using these well-defined semiconductor nanostructures, high performance devices have been realized, mainly for energy-related applications including supercapacitors and solar water splitting devices. These achievements indicate the high potential and importance of the 3D nano-structuring techniques both for basic research and for device applications.

[1] Y. Lei, et al., Chem. Soc. Rev., 40, 1247 (2011).

HL 95: Polaritons

Time: Thursday 11:30–13:00 Location: POT 051

HL 95.1 Thu 11:30 POT 051

Influence of disorder on polariton BEC — •Martin Thunert[1], Alexander Janot[2], Chris Sturm[1], Helena Franke[1], Bernd Rosenow[2], Rüdiger Schmidt-Grund[1], and Marius Grundmann[1] — [1]Universität Leipzig, Fakultät für Experimentelle Physik II, Linnestr. 5, 04103 Leipzig — [2]Universität Leipzig, Fakultät für Theoretische Physik, Brüderstr. 16, 04103 Leipzig

We discuss the impact of disorder effects on the dynamics of exciton-polariton Bose-Einstein condensates (BEC) in a ZnO-based bulk planar microcavity. In contrast to previous experimental work [1], we do not observe significant stabilization of the condensate with increasing polariton density and find even at high excitation powers strong traces of disorder effects in the momentum space intensity distributions. Recent theoretical work shows that disorder destroys the spatial long-range order of a driven quantum condensate [2]. Moreover, the superfluid stiffness of a driven condensate vanishes in the thermodynamic limit and a rigid behaviour is expected over finite length scales only. This indicates that disorder has a significantly pronounced impact on a polariton condensate compared to an equilibrium condensate. We simulate the polariton emission in the momentum space for a large number of disorder realisations. For a condensate phase fluctuation length comparable to the condensate size, our simulations allow us to understand the experimental findings and reproduce its qualitative behaviour for increasing excitation power.

[1] A. Baas *et al.*, Phys. Rev. Lett. **100**, 170401 (2008); [2] A. Janot *et al.*, arXiv:1307.1407 (2013)

HL 95.2 Thu 11:45 POT 051

An electrically driven polariton laser — •Matthias Amthor[1], Arash Rahimi-Iman[1], Na Young Kim[2,3], Julian Fischer[1], Lukas Worschech[1], Martin Kamp[1], Christian Schneider[1], Alfred Forchel[1], Yoshihisa Yamamoto[2,4], and Sven Höfling[1,5] — [1]Technische Physik and Wilhelm-Conrad-Röntgen-Research Center for Complex Material Systems, Universität Würzburg, D-97074 Würzburg, Am Hubland, Germany. — [2]E.L. Ginzton Laboratory, Stanford University, Stanford CA, 94305, USA. — [3]Institute of Industrial Science, University of Tokyo, 4-6-1 Komaba, Meguro-ku, Tokyo 153-8505, Japan. — [4]National Institute of Informatics, Hitotsubashi, Chiyoda-ku, Tokyo 101-8430, Japan. — [5]SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, KY16 9SS, United Kingdom

We report on magneto-optical measurements of an electrically driven GaAs based exciton-polariton light-emitting diode. While using direct current excitation at a temperature of 8K three different regimes occur in the energy-momentum dispersion characteristics. Subject to an applied magnetic field in Faraday configuration, we observe two distinct nonlinearities in the excitation power dependent output characteristics and a characteristic shift of the emission energy. Furthermore the linewidth shows a drop at the first threshold, which is a sign for the buildup of temporal coherence, and continously decreases to the resolution limit in the photonic regime. Additionally, we prove the conservation of the strong coupling regime above the first threshold and its loss above the second threshold by investigating the Zeeman splitting.

HL 95.3 Thu 12:00 POT 051

Determination of operating parameters for a GaAs-based polariton laser — •Johannes Schmutzler[1], Franziska Wishahi[1], Marc Assmann[1], Jean-Sebastian Tempel[1], Sven Höfling[2], Martin Kamp[2], Alfred Forchel[2], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, D-44221 Dortmund, Germany — [2]Technische Physik, Physikalisches Institut, Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, D-97074 Würzburg, Germany

We report on a systematic study of the phase transitions to polariton condensation and further to cavity lasing in a GaAs-based microcavity with respect to exciton-cavity detuning and lattice temperature. Using far field and time-resolved spectroscopy we identify two different modes which are attributed to polariton condensation and cavity lasing, respectively. Thereby we can determine the parameterspace in which polariton condensation can be achieved and the corresponding variation of threshold power. For the investigated sample, we found a lower bound of −12 meV for the exciton-cavity detuning and an upper bound of 90 K for the lattice temperature.[1]

[1] J. Schmutzler et al., Applied Physics Letters 102, 081115 (2013)

HL 95.4 Thu 12:15 POT 051

Textured microcavity trapped polaritons — •Karol Winkler[1], Anne Schade[1], Julian Fischer[1], 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]School of Physics and Astronomy, University of St Andrews, St Andrews, United Kingdom

Trapping of microcavity exciton polaritons by introducing an additional lateral confinement has been shown to support condensation into the bosonic ground state of the system. These 0D polariton traps then, for example, allow the investigation of interacting polariton condensates by enabling arbitrary configurations into advanced lattice structures.

We will focus here on the trapping technique of an elongated textured microcavity. Through an etch-and-overgrowth step a three-dimensional confinement potential for photons and therefore polaritons is introduced. In devices based on a single GaInAs QW in a GaAs λ-cavity, optical and electrical injection of 0D-polaritons has been demonstrated. We will present resonant photocurrent measurements to probe density dependent energy shift of the ground state in such an electrical device.

These systems undergo a transition into weak coupling by further pumping. We will further present a textured microcavity platform that enables arbitrary lattice configurations with deep confinement while condensation in the ground state is possible.

HL 95.5 Thu 12:30 POT 051

Magnetic field properties of zero- and two-dimensional polariton-condensates — •Julian Fischer[1], Sebastian Brodbeck[1], Bo Zhang[2], Alexander Chernenko[3], Steffen Holzinger[1], Matthias Amthor[1], Vladimir D. Kulakovskii[3], Lukas Worschech[1], Mikhail Durnev[4], Hui Deng[2], Martin Kamp[1], Christian Schneider[1], Alexey V. Kavokin[4], and Sven Höfling[1,5] — [1]Technische Physik, Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Department of Physics, University of Michigan, Ann Arbor, Michigan, 48109, USA — [3]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, 142432, Russia — [4]Ioffe Physical-Technical Institute of RAS, 194021 St.-Petersburg, Russia — [5]SUPA, School of Physics and Astronomy, University of St Andrews, UK

We discuss magnetic field properties of zero- (0D) and two-dimensional (2D) polariton-condensates in GaAs microcavities. For the 2D polariton-condensate we observe a sign reversal of the Zeeman-splitting above a critical magnetic field. This experimental result is explained by a nonequilibrium spin Meissner effect. In the second part we investigate the magnetic field response of 0D microcavity structure, where the three-dimensional photonic confinement is archieved by replacing the top distributed Bragg reflector by a sub-wavelength high index contrast grating. The emission characteristics are dominated by discrete, zero-dimensional resonances. Magnetic field investigations allow us to prove the matter part of the polariton-emission above the threshold by directly measuring the polariton's diamagnetic shift.

HL 95.6 Thu 12:45 POT 051

Low dimensional GaAs/Air vertical microcavity lasers — •Jonas Gessler[1], Theresa Steinl[1], Arkadiusz Mika[1,2], Julian Fischer[1], Jan Misiewic[2], Sven Höfling[1], Christian Schneider[1], and Martin Kamp[1] — [1]Technische Physik, Universität Würzburg, Am Hubland, D-97074, Würzburg, Germany — [2]Wroclaw University of Technology, 27 Wybrzeze Wyspiańskiego St, 50-370 Wrocław, Poland

Microcavities consisting of gallium arsenide (GaAs)/ aluminum gallium arsenide (AlGaAs) distributed Bragg reflectors have been the platform for many pioneering light matter interaction studies in semiconductors. GaAs/air microcavities that can be fabricated by selective etching of layers with high Al-content have the major advantage that they show a very large index contrast. This enables smaller mode vol-

ume by decreasing the effective cavity length and to obtain the same quality factors with a notably smaller number of mirror pairs. Our cavity design is promising to reach the strong coupling regime and demonstrate polariton formation in the GaAs/ air microresonator.

We report on the fabrication of GaAs/ air distributed Bragg reflector microresonators with indium gallium arsenide quantum wells. The structures are studied via momentum resolved photoluminescence spectroscopy which allows us to investigate a pronounced optical mode quantization of the photonic dispersion. Via analytical simulations we extract the lateral physical extensions of our microcavity from the energetic distance between the discrete states. Power dependent investigations of our structures revealed clear evidence of photon lasing.

HL 96: Invited Talk Arash Rahimi-Iman

Time: Thursday 15:00–15:30 Location: POT 051

Invited Talk HL 96.1 Thu 15:00 POT 051

An Electrically Driven Polariton Laser — •Arash Rahimi-Iman — Present Address: Department of Physics and Material Sciences Center, Philipps-Universität Marburg, Renthof 5, 35032 Marburg, Germany

A new type of electrically pumped semiconductor laser has been demonstrated which promises an energy efficient laser operation. In a *polariton laser*, stimulated scattering of bosons into a common particle energy state—an effect closely related to Bose-Einstein condensation of atoms—is exploited to provide a coherent emission of light. The involved polaritons are bosonic quasiparticles which arise from strong light-matter coupling in quantum-well microcavities. Unambiguous evidence of polaritonic condensate emission under electrical pumping has been provided by magneto-optical experiments. This presented breakthrough study has been performed by a team of researchers from the University of Würzburg and their international partners from the United States, Japan, Russia, Singapore, Iceland and Germany:

[C. Schneider, A. Rahimi-Iman, N. Y. Kim, J. Fischer, I. G. Savenko, M. Amthor, L. Worschech, V. D. Kulakovskii, I. A. Shelykh, M. Kamp, S. Reitzenstein, A. Forchel, Y. Yamamoto and S. Höfling, *Nature* **497**, 348 (2013)]

HL 97: Semiconductor laser II: Microcavities and quantum-dot laser

Time: Thursday 15:30–17:15 Location: POT 051

HL 97.1 Thu 15:30 POT 051

Direct Net Gain Measurements in Organic Microcavities — •Christian Tzschaschel, Markas Sudzius, Andreas Mischok, Hartmut Fröb, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, Georg-Bähr Str. 1, 01069 Dresden

A profound knowledge of absorption and net gain coefficients of the active material is crucial for designing microcavity lasers. An extremely high degree of optical confinement in such systems modifies the spontaneous emission properties of the gain medium. Standard gain measurement techniques, such as the variable stripe length method, are thus rendered unreliable and hardly applicable.

In this work, a novel technique is presented. It allows direct measurements of both net gain and absorption coefficients of optically pumped organic microcavities. The method involves an in-depth analysis of the line shape of the cavity mode, which is then compared to transfer-matrix simulations. The use of wedge-shaped cavities provides tunable devices and allows for a detailed analysis of spectral net gain properties. The method is applied to organic microcavity structures consisting of a highly fluorescent laser dye (DCM), doped into a matrix material (Alq_3) and sandwiched between distributed Bragg reflectors. For this system, gain coefficients as high as $750\,cm^{-1}$ have been extracted at optical pumping close to the lasing threshold.

HL 97.2 Thu 15:45 POT 051

Bloch-like Photonic States in Laterally Structured Organic Microcavities — •Andreas Mischok[1], Robert Brückner[1], Alexander A. Zakhidov[2], Vadim G. Lyssenko[1], Hartmut Fröb[1], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, TU Dresden, George-Bähr Str. 1, 01069 Dresden, Germany — [2]Fraunhofer COMEDD, Maria-Reiche-Str. 2, 01109 Dresden, Germany

Organic microcavities offer broad spectral coverage and low lasing thresholds with comparably simple preparation techniques. In this work, a highly fluorescent laser dye (DCM) is doped into a matrix material (Alq3) and sandwiched between distributed Bragg reflectors, creating a high-quality cavity emitting around 590-680nm. Introducing an almost non-absorptive SiO2 layer next to the cavity, we are able to shape the photonic landscape in the cavity by micron-scale lateral structuring via photolithography. Periodic stripes in this layer create a periodic array of photonic potential wells, evoking memories of the crystal potential observed for electrons in solid state materials. This structuring creates a mode spectrum showing great similarity to Bloch states, reproducing confined modes below the confining potential and extended modes exhibiting mini-bands and mini-bandgaps above. Numerical simulations and analytical calculations provide further insight into the device as an easily accessible model for quantum mechanical effects in macroscopic systems. Lasing can be observed in a multitude of confined states - tunable by modifying the optical excitation patterns.

HL 97.3 Thu 16:00 POT 051

Jitter Reduction by Optical Feedback of Passively Mode-locked Quantum-Dot Lasers — •Marc Spiegelberg[1], Dejan Arsenijević[1], Moritz Kleinert[2], and Dieter Bimberg[1] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Berlin, Germany — [2]Fraunhofer Heinrich Hertz Institut, Berlin, Germany

Monolithically integrated two-section quantum-dot mode-locked lasers (MLL) providing optical pulse trains at several tens of Gigahertz are ideal candidates for applications in optical communication systems, e.g. as an optical clock or as a transmitter. Low jitter of the pulse comb is at least as crucial as repetition rates of or beyond 40GHz. The integrated jitter of passively MLLs is of the order of a few picoseconds. For hybrid mode-locking, a standard technique to reduce the jitter, an external electrical signal source is necessary, which is costly. Optical self-feedback (OFB), where a part of the MLL light is injected back into the device, is used here as a simple and effective way to reduce the jitter and to tune the repetition frequency of the MLL at the same time. For the first time, five different regimes of OFB are identified, depending on the OFB parameters: overall fiber length, feedback strength and the relative delay between emitted and injected pulses. But only one, the resonant regime, yield a jitter reduction of 94.2% down to 219fs. In this regime the repetition frequency of the MLL shows a linear dependence on the delay and can be tuned within 6.5MHz.

HL 97.4 Thu 16:15 POT 051

Timing jitter reduction in a mode-locked laser subject to optical feedback — •Lina Jaurigue[1], Christian Otto[1,2], Eckehard Schöll[1], and Kathy Lüdge[1] — [1]Institut f. Theo. Physik, Sekr. EW 7-1, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Potsdam Institute for Climate Impact Research, Telegrafenberg A26, 14412 Potsdam, Germany

Passively mode-locked (ML) lasers have a relatively large timing jitter due to the absence of an external reference clock. We investigate the effect of optical feedback (FB) on the timing stability of a passively ML laser. To model the ML laser we use a set of three coupled delay differential equations (DDE) describing a ring cavity, consisting of a gain section and a saturable absorber section. Optical FB is modeled by coupling the ring cavity to an external cavity. In the absence of FB the free running laser produces ultra-short pulses which have an internal cavity round trip time of $T_{ISI,0}$. When FB is added there is a

second important time scale, the external cavity round-trip time τ. FB is resonant when $pT_{ISI,0} = q\tau$, where p and q are integers. Through resonant FB the timing jitter of the ML laser can be reduced and it has been shown that longer external cavities lead to a greater reduction in the timing jitter. This is, however, not always the case. For example, with non-zero α-factors (linewidth enhancement factors) resonant FB can give rise to destabilized pulse streams. For non-resonant FB the timing jitter is dramatically increased.

HL 97.5 Thu 16:30 POT 051

Excited state lasing and ground state quenching in quantum dot lasers: An analytical approach — •Andre Röhm, Benjamin Lingnau, Eckehard Schöll, and Kathy Lüdge — Institut f. Theo. Physik, Sekr. EW 7-1, Technische Universität Berlin, Hardenbergstr. 36, 10623Berlin, Germany

We theoretically investigate semiconductor quantum dot (QD) lasers and their transition from ground state (GS) lasing to two-state lasing as well as the physical mechanisms behind GS quenching. The QD laser device is described by a rate-equation approach based on the semiconductor-Bloch equations, and the electric field dynamics by Maxwell's equations. We compare our numerical simulations with an analytical approach. Based on that we are able to predict regions of GS as well as excited state (ES) lasing as a function of the different energy gaps between GS and ES for electrons and holes. Different ground state quenching mechanisms are studied in the framework of this analytical approach. Key parameters and their impact on the two-state lasing properties of the QD laser are discussed, which allows to predict the different lasing regimes for a wide range of possible QD sets. Furthermore, the influence of doping is investigated.

The GS quenching can be mainly attributed to a charge carrier asymmetry in the quantum dots which increases with pump current. This critical electron to hole ratio can be influenced by temperature, gain and GS-ES energy separation.

HL 97.6 Thu 16:45 POT 051

1.55 μm InAs/InP(100) Based Quantum Dot Lasers for High-Speed Optical Communication — Vitalii Ivanov[1], •Vitalii Sichkovskyi[1], Florian Schnabel[1], Anna Rippien[1], David Gready[2], Gadi Eisenstein[2], and Johann Peter Reithmaier[1] — [1]Institute of Nanostructure Technologies and Analytics, CINSaT, University of Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel, Germany — [2]2Department of Electrical Engineering, Technion, Haifa 32000, Israel

Self-organized InAs/InP quantum dot systems are promising candidates for telecommunication applications at 1.55 μm. Here we report on the latest development of high-speed directly modulated 1.55 μm lasers utilizing recently developed high-density round-shaped InAs quantum dots (QDs) as active material. The laser structures were specially optimized for high-speed operation using a unique spatially resolved model. In particular, the waveguide thickness is significantly reduced down to 100 nm on each side of the active region in order to minimize the carrier transport time. Static and dynamic properties of ridge waveguide lasers with ridge widths of 2 μm and relatively short cavity lengths of 275 μm to 350 μm were investigated. Due to the high modal gain of 70 cm-1 for lasers consisting of 6 QDs layers in the active region, 275 μm long devices are lasing at ground state up to 50 °C. Such lasers exhibit new record values in direct digital modulation of 22 GBit/s with a clear open eye.

HL 97.7 Thu 17:00 POT 051

InAs/InP based quantum dots laser with high gain at 1.55 μm emission wavelength — •Saddam Banyoudeh[1], Johann Peter Reithmaier[1], Christian Gilfert[1], Vitalii Ivanov[1], Vitalii Sichkovskyi[1], David Gready[2], and Gadi Eisenstein[2] — [1]Technische Physik, Institute of Nanostructure Technologies and Analytics, Universität Kassel, 34132 Kassel, Germany — [2]Technion - Israel Institute of Technology, Haifa 32000, Israel

The Self-organized InAs/InP(100) quantum dot (QD) systems are promising canidates for the future telecommunication applications at 1.55 μm. Here we report on the recent advances in the performance of 1.55 μm QD laser, which allow to digital modulation at 22GBit/s with a 3 dB on/off ratio .The strong impact of different parameters on the dynamic proparties of directed modulated laser related to the QD material itself and the the laser design were investigated. The grown laser structure by molecular beam epitaxy consists of 100 nm waveguide layers composed of In0.528Al0.238Ga0.234As in which the InAs QD layers QD laser embedded. The cladding is formed by a 300 nm In0.523Al0.477As layer, 200 nm InP buffer layer and the InPsubstrate on the n-side while 300 nm thick In0.523Al0.477As and 1.7 μm InP layers are deposited for the p-cladding, re-spectively. A highly p-doped 200 nm thick In.532Ga.468Aslayer serves as p-contact. As active region a stacked QD are used, which emit around 1.55 μm with a high internal modal gain of 10 cm-1 per active layer.

HL 98: Graphene: Spintronics, transistors, and sensors (with DY/MA/O/TT)

Time: Thursday 15:00–18:00 Location: POT 081

HL 98.1 Thu 15:00 POT 081

Graphene's RF Potential: How harmful is the Zero Bandgap? — Kyle D. Holland[1], Navid Paydavosi[1], Neophytos Neophytou[2], •Diego Kienle[3], and Mani Vaidyanathan[1] — [1]Department of Electical and Computer Engineering, University of Alberta — [2]Institute for Microelectronics, Technical University of Vienna — [3]Institute of Theoretical Physics I, University of Bayreuth

With the aid of self-consistent quantum-mechanical simulations and simple expressions for the radio-frequency (RF) metrics, we examine the impact of a lack of a bandgap on limiting the RF potential of graphene transistors. Considering various RF figures of merit, we show that the lack of a bandgap leads to all RF metrics being optimal when the bias point is chosen such that the drain Fermi level aligns with the Dirac point at the midpoint of the channel. We further quantify the precise extent to which the lack of a bandgap limits the transistor's cutoff frequencies, an issue that has been flagged as requiring crucial attention to make graphene transistors competitive. For an 18-nm channel length, we show that the extrinsic unity-current-gain frequency could be improved by 300 GHz and the unity-power-gain frequency could be doubled if a bandgap could be introduced to reduce the output conductance to zero. [1] K. D. Holland, N. Paydavosi, N. Neophytou, D. Kienle, and M. Vaidyanathan, IEEE Trans. Nanotechnol. 12, 566 (2013).

HL 98.2 Thu 15:15 POT 081

Atomic layer deposited aluminum oxide on epitaxial graphene without surface activation — •Peter Wehrfritz[1], Florian Speck[2], Felix Fromm[1], Stefan Malzer[3], and Thomas Seyller[1] — [1]TU Chemnitz, Institut für Physik, Chemnitz, Deutschland — [2]FAU Erlangen-Nürnberg, Department Physik, Erlangen, Deutschland — [3]FAU Erlangen-Nürnberg, Angewandte Physik, Erlangen, Deutschland

Graphene with its high charge carrier mobility is a promising material for analog RF field effect transistors. The preparation of the required insulating layer is still challenging. Atomic layer deposition (ALD) has been extensively studied in the context of alternative dielectrics for silicon-based field effect transistors owing to its capabilities to produce high-quality, homogeneous oxide layers. However, nucleation of ALD growth is strongly suppressed on inert graphene surfaces.

In this contribution we present an approach to obtain conformal aluminum oxide (Al_2O_3) on epitaxial monolayer graphene on silicon carbide (SiC). We demonstrate that closed layers of Al_2O_3 can be deposited on the so called buffer layer. This buffer layer covered by ALD-Al_2O_3 can then be decoupled from the SiC substrate by means of hydrogen intercalation yielding quasi-freestanding monolayer graphene with an insulating dielectric on top. We investigated the quality of the graphene layer and ALD-Al_2O_3 using X-ray photoelectron spectroscopy (XPS), Raman spectroscopy, AFM, and Hall effect measurements.

HL 98.3 Thu 15:30 POT 081

Spin-dependent negative differential resistance in composite graphene superlattices — •Christopher Gaul[1,2], Javier Munárriz[2], Andrey V Malyshev[2], Pedro A Orellana[3], Cord A Müller[4], and Francisco Domínguez-Adame[2] — [1]Max-Planck-Institut für Physik Komplexer Systeme, Dresden — [2]Universidad

Complutense de Madrid, Spain — [3]Universidad Técnica Federico Santa María, Casilla 110 V, Valparaíso, Chile — [4]Fachbereich Physik, Universität Konstanz

We propose and study a compound system of a graphene nanoribbon and a set of ferromagnetic insulator strips deposited on top of it. The periodic array of ferromagnetic strips induces a proximity exchange splitting of the electronic states in graphene, resulting in the appearance of a superlattice with a spin-dependent energy spectrum. We find clear signatures of spin-dependent negative differential resistance. The electric current through the device can be highly polarized and both the current and its polarization manifest non-monotonic dependence on the bias voltage. The device operates therefore as an Esaki spin diode, which opens possibilities to design new spintronic circuits.

Phys. Rev. B 88, 155423 (2013)

HL 98.4 Thu 15:45 POT 081

Exchange coupling between localized defect states in graphene nanoflakes — •Matthias Droth and Guido Burkard — University of Konstanz, Germany

Graphene nanoflakes are interesting because electrons are naturally confined in these quasi zero-dimensional structures, thus eluding the need for a bandgap. Defects inside the graphene lattice lead to localized states and the spins of two such localized states may be used for spintronics. We perform a tight-binding description on the entire system and, by virtue of a Schrieffer-Wolff-transformation on the bonding and antibonding states, we extract the coupling strength between the localized states. The coupling strength allows us to estimate the exchange coupling, which governs the dynamics of singlet-triplet spintronics.

HL 98.5 Thu 16:00 POT 081

Novel fabrication method of lateral spin valve devices based on graphene on hexagonal boron nitride — Marc Drögeler[1], Frank Volmer[1], •Maik Wolter[1], Bernat Terrés[1], Kenji Watanabe[3], Takashi Taniguchi[3], Gernot Güntherodt[1], Christoph Stampfer[1,2], and Bernd Beschoten[1] — [1]2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany, EU — [2]Peter Grünberg Institute (PGI-8/9), Forschungszentrum Jülich, 52425 Jülich, Germany, EU — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan

Despite tremendous efforts in improving graphene-based spin transport devices the measured spin lifetimes are still orders of magnitude less than theoretically predicted. Contact-induced spin dephasing has recently been identified as the bottleneck for spin transport through Co/MgO spin injection and detection electrodes. It can, however, significantly be suppressed for devices with large contact resistance area products [1]. Simultaneously, a strong reduction of the charge carrier mobility is usually observed. We present a new method to fabricate graphene-based non-local spin valves on hexagonal boron nitride yielding spin lifetimes above 3 ns, spin diffusion length above 10 μm and large charge carrier mobilities above 30.000 cm^2/Vs.

[1] F. Volmer *et al.*, Phys. Rev. B **88**, 161405(R) (2013).

This work has been supported by DFG through FOR 912 and by EU through Graphene Flagship.

HL 98.6 Thu 16:15 POT 081

Suppression of contact-induced spin dephasing in graphene/Co/MgO$_x$ spin-valve devices by successive oxygen treatments — Frank Volmer, •Christopher Franzen, Marc Drögeler, Eva Maynicke, Nils von den Driesch, Maren Laura Boschen, Gernot Güntherodt, and Bernd Beschoten — 2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany

By successive oxygen treatments of graphene non-local spin-valve devices we achieve a gradual increase of the contact resistance area products R_cA of the Co/MgO$_x$ spin injection and detection electrodes and a transition from linear to non-linear characteristics in the corresponding dV/dI-curves. With this manipulation of the contacts both spin lifetime and amplitude of the spin signal can significantly be increased by a factor of seven in the same device. This demonstrates that contact-induced spin dephasing is the bottleneck for spin transport in graphene devices with small R_cA values [1]. With increasing R_cA we furthermore observe the appearance of a second charge neutrality point (CNP) in gate dependent resistance measurements. Simultaneously we observe a decrease of the gate voltage separation between the two CNPs. The strong enhancement of the spin transport properties as well as the charge transport will be explained by the same gradual suppression of a Co/graphene interaction by improving the oxide barrier.

Work was supported by DFG/FOR 912 and EU/Graphene Flagship.

[1] F. Volmer *et al.* Phys. Rev. B **88**, 161405 (2013).

Coffee break (15 min.)

HL 98.7 Thu 16:45 POT 081

Development of an amperometric H2O2 sensor based on graphene — •Masoumeh Sisakhti[1], Alexander Zöpfl[2], Jonathan Eroms[1], Thomas Hirsch[2], and Christoph Strunk[1] — [1]Institut für Experimentelle und Angewandte Physik,Universität Regensburg — [2]Institut für analytische Chemie,Universität Regensburg

The precise detection of Hydrogen peroxide (H2O2) has been a widely researched topic and the focus of a vast amount of attention, owing to its vital role in biological systems, as well as its utility in food, pharmaceutical and biochemical industries.

The objective of this work is to investigate a novel nonenzymatic, amperometric sensor for reliable determination of H2O2 based on graphene.

We produced graphene sensors based on three types of graphene: exfoliated graphene, CVD grown graphene and reduced graphene oxide and carried out cyclic voltammetry and amperometric experiments using a CH Instrument electrochemical analyzer. We demonstrate that all three graphene materials show excellent sensitivity to the catalytic reduction of H2O2 and are able to detect H2O2 concentrations down to 0.1 mM. rGO as well as graphene prepared by CVD are promising candidates for sensor applications since they are able to detect hydrogen peroxide with high sensitivity at moderate electrode potentials. Both materials are superior in the signal-to-noise ratio compared to exfoliated graphene. A further conjugation of enzymes to the defects within the carbon nano material as well as the assembly of 2D-layered composite materials will be perspective to biosensor applications.

HL 98.8 Thu 17:00 POT 081

Controlled chemical modification of graphene for applications in biosensing — •Marco R. Bobinger, Max Seifert, Anna Cattani-Scholz, and Jose A. Garrido — Walter Schottky Institut, Technische Universität München, Germany

Given its exceptional chemical and mechanical stability as well as its unique electronic properties, graphene is an extremely promising platform for biosensors. In order to use graphene in the biological environment and to improve sensing specificity and device performance, chemical functionalization schemes are needed to allow stable grafting of organic and bioorganic molecules onto graphene. In particular for applications in bioelectronics, the influence of the chemical functionalization of graphene on the generation of defects, strain, and doping has to be balanced with the desired modulation of the electronic properties of the produced graphene-organic hybrid material. In this work the effect of the controlled chemical modification of large area CVD-grown graphene via ozone treatment is investigated. This process creates sp3-like defects, related to covalently bound surface groups, e.g. OH-. Such ozone-treated surfaces are characterized by Raman- and X-ray photoelectron spectroscopy in order to investigate the degree of surface modification and the chemical composition of the surface terminations. The generated anchor groups are further used as binding sites for the modification of graphene with organic molecules.

HL 98.9 Thu 17:15 POT 081

Functionalization of Graphene for Bioelectronic Applications — •Alina Lyuleeva[1], Lucas Hess[1], Frank Deubel[2], and Jose Antonio Garrido[1] — [1]Walter Schottky Institut, TU München, 85748 Garching — [2]Wacker Chemie AG, 81379 München, Germany

With its fascinating structural, chemical and electronic properties, graphene outperforms many materials and is expected to pare the way for a vast range of applications such as transparent electrodes, energy storage devices, high-frequency electronics, or biosensors. The performance of the devices for these various applications can be enhanced with the help of surface functionalization, allowing a versatile modification of the properties of this material. Here, we report on the covalent and thus robust functionalization of CVD graphene with enzymes for the development of novel devices for bioelectronic applications. Graphene solution-gated field-effect transistors (SGFETs) are functionalized using a controlled grafting of polymethacrylate (PMA) brushes. We will show how this material platform can be used for further functionalization with the enzyme acetylcholinesterase (AChE).

The enzymes' activity can be monitored with the modified-graphene transistor allowing both the measurement of the concentration of the neurotransmitter acetylcholine as well as the inhibition of the enzyme by neurotoxins such as nerve agents or pesticides. Our study demonstrates the potential of graphene-based functionalized transistors for biosensing and bioelectronic application.

HL 98.10 Thu 17:30 POT 081

Coupling of electrogenic cells to graphene devices — Michael Sejer Wismer, Felix Rolf, Damia Viana, •Martin Lottner, Lucas Hess, and Jose A. Garrido — Walter Schottky Institut - Technische Universität München, Am Coulombwall 4, 85748 Garching

In this contribution, we will demonstrate the electrical coupling between electrogenic cells and graphene-based solution-gated field effect transistors (SGFETs). To this end, HEK293 and HL1 cells were cultured on 8x8 arrays of graphene SGFETs with feature sizes of 10 mu x 20 mu. Graphene was grown by chemical vapour deposition (CVD) on copper foil and transferred to sapphire substrates, on which field effect transistors were fabricated using standard semiconductor technology. The devices show a typical maximum transconductance of >100 muS at 0.1 V drain-source voltage. This value is stable over months of storage. HEK293 cells were used to analyse the electrical coupling between cells and transistors. A model considering the distribution of ions within the cell transistor cleft and ion sensitivity of the graphene SGFETs fits the measured signals very well. Additionally, nano-transistors were defined by e-beam lithography, which allowed feature sizes down to 50 nm. With these nanoscale devices a signal-to-noise ratio of 2.5 could be obtained within single recordings of HL1 activity. Analysis of the measured ionic currents allowed to draw conclusions about local inhomogeneities of ion channel concentration within the membrane. Further, experiments for the stimulation of PC12 cells using arrays of graphene SGFET and graphene-based microelectrode arrays (MEAs) are under preparation.

HL 98.11 Thu 17:45 POT 081

Graphene solution-gated field effect transistors on flexible substrates — •Andrea Bonaccini Calia, Benno M. Blaschke, Lucas H. Hess, Max Seifert, and Jose A. Garrido — Walter Schottky Institut, Technische Universität München, Germany

Graphene based solution-gated field effect transistors (SGFETs) hold great promise for biosensors and bioelectronic applications. Due to its unique combination of electronic, mechanical, and chemical properties, such as high charge carrier mobility, flexibility and good biocompatibility, graphene has been shown to be an excellent material for sensing in electrolyte environments. Sensors based on graphene SGFETs have already been realized on rigid substrates for various analytes, as well as for the detection of cell signals. However, this technology hold some severe problems for biomedical and in vivo applications. One of the major problems is the rigidity of the substrate itself, which does not allow a proper mechanical matching to the biological tissue, resulting in the formation of scar tissue. Therefore, flexible devices are currently considered as a major step towards the development of more biocompatible implants. In this work, an array of graphene SGFETs is fabricated on a flexible polymer substrate. We present a detailed electrical characterization of the flexible graphene SGFETs in electrolyte and compare their performance to graphene SGFETs on rigid substrates. In addition, we analyze the effect of changes in the electrolyte's pH and ionic strength on the transistor performance and present a model to explain the obtained results. Furthermore, the low-frequency noise performance of graphene devices on flexible substrates is discussed.

HL 99: Electronic structure theory

Time: Thursday 15:00–17:00 Location: POT 151

HL 99.1 Thu 15:00 POT 151

Time-dependent density functional theory of magneto-optical response of periodic insulators — •Irina V. Lebedeva[1], Ilya V. Tokatly[1,2], and Angel Rubio[1,3,4] — [1]Nano-bio Spectroscopy Group, Universidad del Pais Vasco, San Sebastian, Spain — [2]IKERBASQUE, Bilbao, Spain — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [4]ETSF

Though the linear response theory has been successfully used for molecular systems for a long time, the extension of this theory to solids is not straightforward since the position operator is ill defined in extended periodic systems. The theoretical description of homogeneous static magnetic field in periodic systems is particularly challenging as the corresponding vector potential breaks the translational invariance of the Hamiltonian. We present a unified approach to calculation of all-order response to arbitrary electromagnetic fields both for periodic and molecular systems within the formalism of non-equilibrium Green functions. The approach is applied to derive the expression for the magneto-optical response of insulating solids in the approximation of non-interacting electrons. The formula obtained is completely identical to the expression for molecular systems if the proper position and orbital magnetization operators are chosen. The terms corresponding to changes in the optical response due to the orbital magnetization of Bloch states and due to the modified density of Bloch states in the magnetic field are identified. A computational scheme based on the density matrix-perturbation theory is developed for practical calculations of the magneto-optical response.

HL 99.2 Thu 15:15 POT 151

Predictive *GW* calculations with pseudopotentials and plane-waves — •Jiri Klimes and Georg Kresse — Faculty of Physics, University of Vienna, Sensengasse 8/12, A-1090 Wien, Austria

The *GW* approximation is the standard approach to obtain quasiparticle (QP) energies in solid state physics. Despite its wide use, the agreement between values obtained by different implementations is often unsatisfactory, even for the simplest case of G_0W_0@LDA. This is often attributed to the use of pseudopotentials or to the limited size of local basis sets in all-electron codes. Moreover, little attention is usually paid to obtain results that are converged with respect to the size of the basis sets for orbitals and for the response function. Here we derive an analytic formula for the contribution of unoccupied states with high kinetic energies to the QP corrections. This clearly shows the necessity to converge with the number and basis set size for unoccupied states as well as with the basis set size for the response function. It also points to a problem in the current projector-augmented-wave (PAW) *GW* calculations that originates from the incompleteness of the on-site basis set of partial waves. We show that this issue can be avoided by using norm-conserving PAW partial-waves in the *GW* calculations. Our results are then in a very good agreement with the values obtained using all-electron FLAPW+lo method, even for the problematic case of ZnO [1].

[1] C. Friedrich, M. C. Müller, and S. Blügel, PRB **83**, 081101(R) (2011); **84**, 039906 (2011).

HL 99.3 Thu 15:30 POT 151

Eigenvalues from Density Functional Theory with exact exchange – chances and limitations — •Tobias Schmidt and Stephan Kümmel — University of Bayreuth, Germany

Density Functional Theory (DFT) has become one of the most widely used methods for electronic structure calculations, e.g., for predicting molecular geometries and binding energies. Also DFT eigenvalues are often used for physical predictions, e.g., for band structure studies. However, while functionals such as the Generalized Gradient Approximations can predict electronic binding reasonably, their limitations in band structure prediction are well known. On the other hand it has been reported that exact Kohn-Sham exchange (EXX) yields reasonable band structures, but its binding energy predictions are poor.

We here report a detailed investigation of so called Local Hybrid Functionals (LHFs), which strive to combine full, non-local Fock-exchange with a non-local, compatible correlation functional. We demonstrate that this functional class allows for an improved description of binding properties and an enhanced interpretability of the eigenvalues. However, we also point out that all presently available functionals that incorporate EXX lead to a fundamental imbalance between their accuracy for eigenvalues and for binding energies.

To shed light on this issue we analyze the local multiplicative potential from LHFs, finding that it does not reach the correct form in the limit $|\mathbf{r}| \to \infty$. The potential is affected by the occurrence of nodal planes in the highest occupied KS orbital, and counterintuitively approaches different limits in different directions of space.

HL 99.4 Thu 15:45 POT 151

Energy Curvature of Solids with Fractional Charge in DFT — •Vojtech Vlcek[1], Helen Eisenberg[2], Gerd Steinle-Neumann[1], Leeor Kronik[3], and Roi Baer[2] — [1]Universitat Bayreuth, Germany — [2]Hebrew University, Jerusalem, Israel — [3]Weizmann Institute of Science, Rehovoth, Israel

DFT often does not perform well in terms of prediction of electron removal and addition energies. In exact DFT, the total energy of the system E versus number of electrons N upon addition/removal of a fraction of an electron is a series of linear segments between integer N. At these points the exchange-correlation potential can jump discontinuously by a derivative discontinuity (DD), which contributes to the change of the derivative of E and thus to the fundamental band gap. Without employing ensemble-DFT, commonly used approximations, however, do not satisfy the straight line condition and lack DD. In finite systems, this error is manifested by a curvature of the energy which has been studied extensively over the past decade.

The concept of energy curvature in infinite systems is still under debate. Competing concepts have emerged: 1) curvature was shown to approach zero in the infinite system size limit; 2) the energy per unit cell was shown to have curvature if the electron addition/removal per unit cell is considered. Here we analyze the missing DD by introducing a new measure for the curvature in an infinite periodic system. This allows us to compute the curvature in the thermodynamic limit when only an infinitesimal amount of electronic charge is removed or added to the system.

HL 99.5 Thu 16:00 POT 151

First-principles study of excitonic effects in Raman intensities — •Yannick Gillet, Matteo Giantomassi, and Xavier Gonze — Université catholique de Louvain, Louvain-la-Neuve (Belgium)

A resonance phenomenon appears in the Raman intensity when the exciting light has frequency close to electronic transitions. The theoretical prediction of the frequency-dependent Raman response of crystalline systems has received little attention.

Indeed, many Raman calculations are nowadays done in the static limit (vanishing light frequency), using Density-Functional Theory and Density-Functional Perturbation Theory, thus neglecting excitonic effects. In this work [1], a finite difference method is used to obtain the frequency-dependent Raman intensity of silicon within the Many-Body Perturbation Theory (excitonic effects are included by solving the Bethe-Salpeter equation). Since the convergence with the sampling of the Brillouin Zone is extremely slow, a double-grid technique needs to be used.

Two main conclusions can be drawn from our analysis. First, the double-grid technique permits to obtain well converged results without requiring huge memory and time requirements. Then, excitonic effects are of crucial importance in the resonance part of the Raman spectrum. The inclusion of these excitonic effects in the computations improves the agreement with the experimental data [2] with respect to analogous results obtained within the independent-particle approach.

[1] Y. Gillet, M. Giantomassi, X. Gonze, Phys. Rev. B 88, 094305 (2013). [2] A. Compaan and H. J. Trodahl, Phys. Rev. B 29, 793 (1984).

HL 99.6 Thu 16:15 POT 151

Zero-point motion effect on the bandgap of diamond: validation of codes — •Samuel Poncé[1], Gabriel Antonius[2], Paul Boulanger[3], Elena Cannuccia[4], Andrea Marini[5], Michel Côté[2], and Xavier Gonze[1] — [1]UCL, 1348 LLN, Belgium — [2]UMontréal, C.P. 6128, Montréal, Canada — [3]Institut Néel, BP 166, 38042 Grenoble, France — [4]ILL, BP 156 38042 Grenoble, France — [5]CNR, CP 10, Mont. Stazione, Italy

Verification and validation of codes, as well as new theoretical methods, are of utmost importance if one wants to provide reliable results.

In this work we present a rigorous and careful study of all the quantities that enters into the calculation of the zero-point motion renormalization of the direct band gap of diamond due to electron-phonon coupling. This study has been done within the Allen-Heine-Cardona (AHC) formalism as implemented into Abinit and Yambo on top of Quantum Espresso. In this work we aim at quantifying the agreement between the codes for the different quantities of interest. This study shows that one can get less than $10^{-5} Ha/at$ differences on the total energy, 0.07 cm^{-1} on the phonon frequencies, 0.5% on the electron-phonon matrix elements and less than 4 meV on the zero-point motion renormalization.

At the LDA level, the converged direct bandgap renormalization in diamond due to electron-phonon coupling in the AHC formalism is -409 meV (reduction of the bandgap)[1].

[1] S. Poncé *et al.*, arXiv:1309.0729 [cond-mat.mtrl-sci] and submitted for publication in Comput. Mat. Science (2013).

HL 99.7 Thu 16:30 POT 151

Wavefunction localisation and acceptor ionisation in $Ga_{1-x}Mn_xAs$, an electronic structure perspective — •Jerome Jackson and Gabriel Bester — Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany.

The Mn acceptor level in GaMnAs, although it has a binding energy well beyond that of a simple effective-mass impurity, is nevertheless weakly localized and has considerable valence band character. We discuss critically the ability of density functional theory methods to correctly reproduce the acceptor level localization, in direct contrast to clear experimental evidence (photoluminescence and tunneling experiments) for discrete Mn acceptor levels in the dilute limit. Using a non-selfconsistent wavefunction based approach, relying upon the essentially shortranged nature of the Mn defect potential, we are able to study the localization behavior of the acceptor wavefunction and apply corrections (in agreement with previous tight binding results) which improve upon the density functional description. We identify the principle problem with such calculations as being a poor description of the important $sp-d$ coupling, distinct from the problem of the deep Mn d state position. By calculating the screened Coulomb integrals between the defect states and the host bands and using a configuration-interaction method we are able to explicitly model the acceptor level ionization, illustrating the fundamentally many-body nature of such processes.

HL 99.8 Thu 16:45 POT 151

Origin of electronic subgap states in amorphous semiconductor oxides on the example of In-Ga-Zn-O (IGZO) — Wolfgang Körner, •Daniel Urban, and Christian Elsässer — Fraunhofer IWM, Freiburg, Germany

A density-functional-theory study of amorphous In-Ga-Zn-O (IGZO) with focus on the use as transparent conducting oxide is presented [1]. We studied stoichiometric and oxygen-poor amorphous IGZO samples concerning their electronic properties and compared the results to those for crystalline IGZO. Subgap states in the electronic density of states of amorphous IGZO due to imperfections are calculated by means of the LDA and with a self-interaction-correction (SIC). In our study we relate the electronic subgap states, which were observed recently by Nomura et al. [2] to structural features of the amorphous samples. According to our analysis the valence band tail, caused by the disordered O 2p orbitals, is superimposed by deep defect states above the valence band which can be assigned to undercoordinated O atoms. Our interpretation is further supported by the observation that additional H suppresses these states by creating O-H bonds. This hydrogen doping improves the transparency and is consistent with experimental findings [2]. The deep levels below the conduction band arise mainly from miscoordinated metal atoms, mostly In–Zn pairs. By addition of O, i.e., by oxygen annealing, the frequency of such defect levels can be reduced.

[1] W. Körner, D. F. Urban and C. Elsässer, J. Appl. Phys. 114, 163704 (2013). [2] K. Nomura et al., J. Appl.Phys. 109, 073726 (2011).

HL 100: Metamorphic structures: Bringing together incompatible materials II (Focus session with DF)

Continuation of the morning session 'Metamorphic structures: Bringing together incompatible materials I'

Organizers: Ferdinand Scholz, Universität Ulm, and Andreas Hangleiter, TU Braunschweig.

Time: Thursday 15:00–16:30 Location: POT 251

Topical Talk HL 100.1 Thu 15:00 POT 251

Integration of cubic III/V semiconductors on silicon (001) — •Kerstin Volz — Philipps-Universität Marburg, Fachbereich Physik & Wissenschaftliches Zentrum für Materialwissenschaften

GaP layers on Si(001) can serve as pseudo-substrates for a variety of novel optoelectronic devices, like integrated lasers, solar cells and n-channel layers. The quality of the GaP nucleation layer is a crucial parameter for the performance of such a device. This presentation will summarize our current understanding of III/V heteroepitaxy on Si substrates and give several examples of successful integration of multinary III/V semiconductors on GaP/Si(001) virtual substrates.

HL 100.2 Thu 15:30 POT 251

Optical and structural characterization of an InGaN SQW embedded between quaternary InAlGaN barriers of varying In-concentration — •Christopher Karbaum[1], Frank Bertram[1], Marcus Müller[1], Peter Veit[1], Jürgen Christen[1], Jürgen Bläsing[1], Alois Krost[1], Martin Feneberg[1], Rüdiger Goldhahn[1], Jan Wagner[2], Michael Jetter[2], and Peter Michler[2] — [1]Institute of Experimental Physics, OvGUniversity Magdeburg, Germany — [2]IHFG, University Stuttgart, Germany

The change of the optical and structural properties of an InGaN SQW within InAlGaN barriers have been investigated using time resolved SEM-CL and STEM-CL spectroscopy at liquid helium temperature, PL, and HRXRD. The set of samples was grown on an optimized 1 μm thick GaN:Si buffer ontop of a c-oriented sapphire substrate. Subsequently, an InGaN SQW was embedded between InAlGaN barrier layers. The In gas flow during the pulsed MOVPE growth of these barriers was varied from 3 sccm up to 50 sccm. PL-spectra are dominated by the bound exciton emission of GaN (355 nm), a DAP at about 380 nm, the broad emission band from the InGaN SQW between 450 nm and 500 nm and the quaternary InAlGaN barrier emission. The fundamental idea behind the variation of the In-flux during growth is to achieve polarization matched conditions to decrease the QCSE of the InGaN SQW emission. For higher In-fluxes the InGaN emission undergoes a blueshift (150 meV) accompanied by a decrease of initial lifetime from 18 ns down to 5 ns. The temperature dependence of the luminescence and the recombination kinetics will be discussed.

HL 100.3 Thu 15:45 POT 251

Characterization of strained GaN on nanometer scale by IR near field microscopy — •Fabian Gaussmann[1], Stefanie Bensmann[1], Jochen Wüppen[1], and Thomas Taubner[1,2] — [1]Fraunhofer-Institut für Lasertechnik ILT, Aachen — [2]1. Physikalisches Institut 1A, RWTH Aachen Universität

Near-field microscopy combines the high spatial resolution of an atomic force microscopy with the depth of information that comes with spectroscopical analysis techniques. By using laser light in the mid IR range this technique is amongst others sensitive to the structure of polar materials like SiC or GaN. Regardless of the wavelength of the input laser light, the spatial resolution of these analyses is typical only a few tens of nanometer. This talk is focused on the characterization of strained gallium nitride systems. For near field analyses of GaN, laser light in the spectral range of 12 μm to 16 μm is required. This range, combined with a sufficient power density, is first covered by a novel developed tunable broadband laser system at the Fraunhofer ILT. While the two dimensional visualization of local stress fields using monochromatic laser systems is a common technique for near field analyses, we will present a method to transfer this capability to broadband laser systems. By recording single near field spectra, the optical properties and subsequent information for example about the strain, doping concentration or electron mobility can be achieved. Applied to cross-sections of layered systems, this technique gives a unique insight to the relaxation of crystal strain along the layer structure.

HL 100.4 Thu 16:00 POT 251

Measurement of strain in the InGaN/GaN heterogeneous nanostructures — •Tomaš Stankevič[1], Simas Mickevičius[1], Mikkel Schou Nielsen[1], Robert Feidenhans'l[1], Olga Kryliouk[2], Rafal Ciechonski[2], Giuliano Vescovi[2], Zhaoxia Bi[3], and Anders Mikkelsen[3] — [1]University of Copenhagen, Niels Bohr Institute, Copenhagen, Denmark — [2]GLO AB, Lund, Sweden — [3]Lund University, Nanometer Structure Consortium, Lund, Sweden

Growth and electrical properties of the core-shell nanostructures are often infulenced by the lattice mismatch induced strain. In contrast to planar films nanostructures contain multiple facets that act as independent substrates for the shell growth. In this study we present experimental results obtained by X-ray diffraction showing that the InGaN shells grown on the GaN cores are strained along each of the facets independently. Reciprocal space maps (RSMs) reveal multiple Bragg peaks corresponding to different parts of the shell strained along individual facet planes. Strained lattice constants were found from the peak positions. Vegard's law and Hooke's law for an anisotropic medium were applied in order to find the composition and strain in the InGaN shell. Simple atomistic kinematic simulations of the RSMs showed good agreement with the experimental data. We conclude that 8 nm the InGaN shells of up to 27% indium composition were nearly fully strained bixially along each of the $10\bar{1}0$ facets of the nanowires and the $10\bar{1}1$ facets of the nanopyramids.

HL 100.5 Thu 16:15 POT 251

Direct correlation of optical and structural properties of InGaN/GaN core-shell microrods by STEM-Cathodoluminescence — •Benjamin Max[1], Marcus Müller[1], Gordon Schmidt[1], Anja Dempewolf[1], Thomas Hempel[1], Peter Veit[1], Frank Bertram[1], Jürgen Christen[1], Martin Mandl[2], Tilman Schimpke[2], and Martin Strassburg[2] — [1]Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Germany — [2]OSRAM Opto Semiconductors GmbH, Regensburg, Germany

We present a direct nano-scale correlation of the optical properties with the crystalline real structure of InGaN/GaN core-shell microrods using highly spatially resolved cathodoluminescence spectroscopy (CL). The characterized three microrod samples were grown by MOVPE on c-plane GaN/sapphire template via selective area growth using a SiO_2 mask: a GaN microrod reference structure without shell, a sample with InGaN single quantum well (SQW), and finally a complete core-shell LED structure were investigated. In all samples the GaN NBE emission originates exclusively from the compressively strained GaN template with an emission line at 356 nm. Spatially resolved CL mappings of the undoped sample and the LED structure exhibit luminescence from the InGaN SQW on the non-polar facet at about 400 nm. In contrast, on the semi-polar facet at the tip of the microrod the InGaN SQW luminescence is shifted to longer wavelengths. Additionally, the final core-shell LED structure shows DAP recombination at 380 nm, superimposing the InGaN SQW emission at the non-polar facets.

HL 101: Theoretical advances in interacting topological phases (organized by TT)

Topological insulators have attracted considerable attention recently. Today, the theoretical and experimental understanding of such systems has become comparably well. The continued high interest in this topic is caused by exciting proposals and concepts for new exotic physics based on the interplay of the non-trivial band topology and strong electron-electron interactions. Fractional Chern insulators, topological Mott insulators, topological Kondo insulators, and spin liquids are just a few examples. Some of these phases have already been claimed to be found in experiments.

The aim of this focus session is to give an overview of the most recent advances in this exciting and rapidly evolving field presented by leading experts in the field.

Organizer: Stephan Rachel (TU Dresden)

Time: Thursday 15:00–18:25 Location: HSZ 03

Invited Talk HL 101.1 Thu 15:00 HSZ 03

Fractional Topological Insulators — •Andrei Bernevig — Princeton University

Topological insulators are remarkable materials whose insulating "boring" bulk nonetheless gives rise to perfectly metallic edge or surface states not disturbed by disorder. In this talk, I will relay new phenomena beyond the recently discovered topological insulators with time-reversal symmetry. I will show that topological insulators exist with any point group symmetry, and, upon adding interactions, can transform in much more interesting systems. I will show that fractionally filling a band of a one-body topological insulator and then subjecting its electrons to repulsive interaction can create new states of matter non-existent in the continuum, whose quasiparticles exhibit non-abelian braiding. I will then show that a new description of these states in terms of matrix product forms can greatly enhance our capability to calculate their many-body properties.

Invited Talk HL 101.2 Thu 15:30 HSZ 03

Non-Fermi Liquid, Quantum Critical, and Topological States in Iridates — •Leon Balents — Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA, USA

The combination of band topology and strong correlations is an intriguing and largely open area for theory and experiment. I will discuss a theory of a "parent state" for both topological and quantum critical descendants. This state is suggested to describe one of the prototypical materials families in this area: the pyrochlore iridates.

Parts of this work were done in collaboration with Yong-Baek Kim, Eun-Gook Moon, Lucile Savary, and Cenke Xu

Topical Talk HL 101.3 Thu 16:00 HSZ 03

Collective Spin-Orbit Physics in $j = 1/2$ Mott Insulators — •Simon Trebst — Universität zu Köln

The greatly enhanced spin-orbit coupling in 5d transition metal oxides can lead to a novel class of Mott insulators in which the local moment is a $j = 1/2$ spin-orbit entangled momentum. The rich physics arising in these novel Mott insulators has been extensively probed in the context of the quasi two-dimensional compounds Sr_2IrO_4 (square lattice) with regard to superconducting instabilities and Na_2IrO_3 (honeycomb lattice) in context of possible spin liquid behavior. Here we report on our endeavor to understand the collective states of such spin-orbit entangled j=1/2 momenta when considering other lattice geometries, in particular the triangular lattice motivated by the recent synthesis of $Ba_3IrTi_2O_9$ and the three-dimensional hyperoctagon lattice in the context of β-Li_2IrO_3. For the triangular system we find that weak anisotropic Kitaev-like interactions stabilize a Z_2-vortex phase. For the hyperoctagon lattice (the premedial lattice of the hyperkagome lattice) we find that strong Kitaev-like couplings give rise to a gapless quantum spin liquid with a Majorana Fermi surface – a highly unusual spin liquid state, which is intimately connected to and protected by the lattice symmetries.

15 min. break.

Topical Talk HL 101.4 Thu 16:45 HSZ 03

Topological Kondo Insulators: An Example of Correlated Quantum Spin Hall States — •Fakher Assaad — Universität Würzburg

In the very same way as the heavy fermion paramagnetic state at $T = 0$ is adiabatically linked to a gas of free electrons, the topological Kondo insulator can be deformed to a quantum spin Hall insulator without going through a quantum phase transition. The interest however lies in the fact the quasi-particles forming this coherence state are dynamically created by correlation effects, and may be viewed as the Kondo screening clouds of the magnetic impurities. The minimal model to capture this piece of physics consists of odd parity localized f-states hybridizing with an even parity conduction band alongside strong spin-orbit coupling and time reversal symmetry. In this talk we will consider such a minimal model, and concentrate on the temperature dependence of various quantities from the mixed valence to local moment regimes [1-2] The quantities we consider include topological invariants as well as the single particle spectral function on slab topologies. We show that there is a single low energy scale, the coherence scale, below which one observes the emergence of the topological state.

This work has been carried out in collaboration with J. Werner.

[1] J. Werner and F. F. Assaad, Phys. Rev. B 88, 035113 (2013).
[2] J. Werner and F. F. Assaad, arXiv:1311.3668.

Topical Talk HL 101.5 Thu 17:15 HSZ 03

Fractional Chern Insulators in Strongly Correlated Multiorbital Systems — •Maria Daghofer, Stefanos Kourtis, Jörn W. F. Venderbos, and Jeroen van den Brink — IFW Dresden, Dresden, Germany

Interaction between itinerant carriers and localized spins on frustrated lattices can stabilize phases that are in many respects similar to a Landau level, with a non-coplanar spin background taking the role of the magnetic field. If the bands are nearly flat, longer-range Coulomb repulsion can then induce states that are like lattice-analogs of fractional Quantum-Hall (FQH) states, but do not require an external magnetic field. I will discuss a t_{2g}-orbital system on a triangular lattice that supports a spin-chiral magnetic ordering pattern with precisely the required topologically non-trivial and flat bands[1]. Exact-diagonalization methods reveal signatures of a FQH-like ground state. Moreover, we also find states that go beyond the physics of Landau levels: They show a combination of conventional (charge) and topological order and are related to the frustration of the underlying triangular lattice [2].

[1] J. W. F. Venderbos et al., PRL **108**, 126405 (2012)
[2] S. Kourtis and M. Daghofer, arXiv:1305.6948

HL 101.6 Thu 17:45 HSZ 03

Non-Abelian quasiparticles in strongly interacting helical liquids — •Thomas Schmidt, Christoph Orth, and Rakesh Tiwari — Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

The interplay of strong Coulomb interactions with Rashba spin-orbit coupling can lead to the opening of a gap in the edge spectrum of a two-dimensional topological insulator, even if the system Hamiltonian is time-reversal invariant. We investigate the properties of such a strongly interacting helical system in proximity to an s-wave superconductor. We show that the interface between a region gapped out by the proximity effect and a region gapped out by strong interactions can host non-Abelian bound states, and determine their exchange statistics.

HL 101.7 Thu 18:05 HSZ 03

From fractionally charged solitons to Majorana bound states in a one-dimensional interacting model — •Frank Pollmann[1], Doru Sticlet[1,2], Luis Seabra[1,3], and Jerome Cayssol[1,2] — [1]Max-Planck-Institute for the Physics of Complex Systems, Dresden, Ger-

many — [2]CNRS and University Bordeaux, Talence, France — [3]Technion, Haifa, Israel

We investigate the one-dimensional Creutz model in the presence of induced superconductivity and Hubbard type interactions. We show that zero-energy Majorana edge modes develop in the presence of superconducting pairing for a certain range of parameters. Additionally, the system hosts regular electronic zero-energy modes in a trivial superconducting phase. We study the effect of interactions using a combination of density matrix renormalization group (DRMG) methods and mean field theory. It is shown how local repulsive interactions expand the parameter range for which a topological Majorana phase is stabilized. In contrast, we find that interactions remove the zero-energy modes found in the trivial superconducting phase.

HL 102: Sustainable photovoltaics with earth-abundant materials II (organized by DS)

Time: Thursday 15:00–17:30 Location: CHE 91

HL 102.1 Thu 15:00 CHE 91

Electroless deposition of porous zinc oxide films on sheets of aluminium — •Stephanie Künze and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany

Metal foils, wires or metalized polymer fibres are of interest as substrate electrodes for porous wide band-gap semiconductors in dye-sensitized solar cells (DSC) if protected against corrosion by a passivating oxide layer. Here, aluminium sheets were used to deposit porous zinc oxide for DSC. For the deposition of ZnO, the natural insulating Al_2O_3 layer on Al was removed by chemical etching in hydrochloric acid (HCl). A subsequent treatment in alkaline zinc hydroxide (zincate stain) was used to grow Zn in order to protect the metal and to provide a reactive surface for the deposition of ZnO. Porous ZnO films were then prepared by electroless deposition without any electrical connections on such pre-treated Al substrates from aqueous $ZnCl_2$ saturated with O_2. The xanthene dye $EosinY$ was used to form pores in the growing crystalline ZnO. The film thickness of porous ZnO and the coverage of the metal surface increase with the deposition time and with the amount of Zn from the pre-treatment. These results were contrasted with the results from electrochemical depositions at an applied potential under otherwise identical conditions. For comparison purposes, depositions of porous zinc oxide on etched sheets of Zn were analyzed to provide a virtually unlimited supply of Zn. Al and Zn unlike other elements often used in photovoltaics offer the chance of large-scale applications since both are abundant on earth.

HL 102.2 Thu 15:15 CHE 91

Copper oxide for photovoltaic applications — Alexander Wagner, Nikolai Ehrhardt, Mathieu Stahl, Andreas Fahl, Johannes Ledig, Lorenzo Caccamo, Andreas Waag, and •Andrey Bakin — Institute of Semiconductor Technology, Technische Universität Braunschweig, Hans-Sommer-Strasse 66, 38106 Braunschweig, Germany

Oxides and related materials are extremely promising materials for sustainable photovoltaics providing abundance and nontoxicity. For an all-oxide solar cell p-type Cu2O is a promising absorber material with a high absorption coefficient and 2.1 eV band gap. Theoretically predicted efficiencies of Cu2O based solar cells are up to 20% but till now the devices on the base of copper oxide show significantly lower efficiencies. Further fundamental investigations are needed in order to understand in depth the physics behind the devices on the base of these materials and to improve the efficiency of the cells. Influence of different buffer layers on the performance of an all oxide solar cell is discussed. Controllably grown Cu2O layers are also prerequisites for fabrication of high efficiency solar cells and vapor phase epitaxial growth of Cu2O is presented.

HL 102.3 Thu 15:30 CHE 91

The effect of hydrogen in RF-sputtered copper oxide thin films — •Philipp Hering, Benedikt Kramm, Julian Benz, Peter Klar, and Bruno Meyer — 1. phys. Inst., JLU Giessen, Deutschland

Cuprous oxide (Cu2O), despite its band gap of 2.17 eV, is a promising material for photovoltaic applications, due to its high absorption coefficient, non-toxicity and the abundance of its composing elements. While recently more attention has been paid to heterojunctions, highest efficiencies were reached by employing copper sheets, which were oxidized and annealed at high temperatures. For technological applicability, a thin film deposition process with mass production capabilities, which provides decent film properties at low temperatures, has to be established. Such thin films however suffer from low carrier mobilities and lifetimes, due to their polycrystalline nature. It has been reported that post treatments with hydrogen can passivate grain boundaries. Copper oxide thin films were deposited from a metallic copper target via reactive radio frequency magnetron sputtering, utilizing gaseous argon and oxygen under the addition of hydrogen. The films were characterized and the influence of hydrogen was investigated via X-ray diffraction, X-ray photoelectron spectroscopy, Raman spectroscopy, photoluminescence and Hall effect.

HL 102.4 Thu 15:45 CHE 91

Improved Anchoring of Indoline Dyes for the Sensitization of ZnO — Felix Fiehler[1], •Jane Falgenhauer[1], Melanie Rudolph[1], Christoph Richter[1], Hidetoshi Miura[2], and Derck Schlettwein[1] — [1]Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. — [2]Chemicrea Inc, Iwaki, Fukushima, Japan.

D149 is a well-established indoline dye for the sensitization of ZnO. Although high efficiencies can be obtained, the dye partly desorbs from the ZnO surface in contact with the redox electrolytes in dye-sensitized solar cells. Similar indoline dyes with a second carboxylic binding group at the molecule to attach to the ZnO surface showed higher stability [1]. In this work, sandwich-cells were built with electrodeposited ZnO on conductive glass as the working electrode which was sensitized with D149 or D149-derivatives DN91, DN216 and DN285 having two binding groups of different length of a hydrocarbon spacer. Current-voltage curves and dynamic measurements like electrical impedance spectroscopy at AM1.5 illumination and intensity-modulated photovoltage/photocurrent spectroscopy (IMVS/IMPS) were performed. The observed shift of effective band positions, the recombination resistance and the observed lifetime of the excited state were found to be comparable for the different sensitizers. DN216, however, showed higher photocurrent densities than the D149 reference and the cell characteristics were more reproducible. Implications for the future development of dye-sensitized solar cells based on solution-processed ZnO will be discussed. [1] J. Falgenhauer, C. Richter, H. Miura, D. Schlettwein *Chem.Phys.Chem.*, 13, 2893-2897 (2012).

HL 102.5 Thu 16:00 CHE 91

Silver nanowire networks for ITO replacement — •Julian Reindl and Lukas Schmidt-Mende — Department of Physics, University of Konstanz, Germany

Indium-tin oxide (ITO) is the state-of-the-art material for transparent electrodes in optoelectronic devices such as solar cells. However, Indium is a very scarce material and the increasing demand for transparent conductors drives the need for alternative materials.

Here we present networks of silver nanowires which are embedded in a matrix of the doped polymer PEDOT:PSS. This system enables a good conductivity through the metallic pathways, supported by the polymer. The latter also provides a good light transmission in the visible range.

HL 102.6 Thu 16:15 CHE 91

Study of the Crystalline Fraction Dependent Microstructure Characteristics of $\mu c - SiOx : H$ for Micromorph Solar Cells — •Max Klingsporn[1], Simon Kirner[2], Ioan Costina[1], and Daniel Abou-Ras[3] — [1]IHP, im Technologiepark 25, Frankfurt (Oder), Germany — [2]PVcomB, Schwarzschildstr. 3, 12489 Berlin, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Since some years $\mu c - SiOx : H$ attracted attention as a wide band gap material for the use in silicon based thin film solar cells. With material parameters tunable over wide ranges it qualifies for several applications. One of the most popular today is the use as an intermediate reflector layer in tandem solar cells. In the present work a SiOx sample series with a fixed elemental composition and a crystalline fraction (Fc) varied between 10 and 60 % was studied by X-ray photo-

electron spectroscopy and scanning transmission electron microscopy combined with electron energy loss spectroscopy. The analysis reveals a transition from an amorphous phase of silicon suboxides to a two-phase system of silicon nanofilaments embedded in a SiO_2 matrix. A consistent correlation between Fc and electrical properties is found.

Keywords: $\mu c - SiOx : H$, STEM, EELS, Plasmon Imaging, XPS, ESCA, Raman, IRL, Micromorph, Solar Cells, Silicon Filaments

HL 102.7 Thu 16:30 CHE 91

High Vapour Pressure Selenization and Grain Growth Mechanisms of Sulfide-CZTS Precursors — •Justus Just[1], Steffen Kretzschmar[1], Stephan van Duren[1], Roland Mainz[1], Claudia Coughlan[2], Kevin Ryan[2], and Thomas Unold[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie — [2]University of Limerick, Irland

We report about the fundamental growth mechanisms and properties of CZTS,Se absorber layers, produced by selenization of various different precursors at high selenium partial pressures deposited in vacuum as well as in non-vacuum processes. We will compare the selenization and growth mechanisms of precursors consisting of PVD-deposited CZTS at low temperature, CZTS nanoparticles and wurzite CZTS nanorods. Samples are characterized by scanning electron microscopy, depth resolved elemental analysis (energy dispersive X-ray fluorescence) and X-ray diffraction. In order to estimate the electronic quality of the selenized material, photoluminescence measurements are carried out additionally. While the selenization is similar depending on the temperature and selenium partial pressure for different types of precursors, the grain growth mechanisms are found to be substantially different, as the grain growth is depending on nucleation and interdiffusion of cations.

HL 102.8 Thu 16:45 CHE 91

Growth and characterization of polycrystalline $Cu_2ZnSnSe_4$ layers with a preferential grain orientation — •Christoph Krämmer[1], Johannes Sachs[1], Mario Lang[1], Chao Gao[1], Sabine Schuster[1], Michael Powalla[2], Heinz Kalt[1], 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 (ZSW), 70565 Stuttgart, Germany

The absence of the technologically relevant metals indium and gallium makes the kesterite $Cu_2ZnSnSe_4$ (CZTSe) material system a promising alternative to the established $Cu(In,Ga)Se_2$. Hiqh-quality CZTSe layers on GaAs would be highly desirable for the study of basic material properties such as the band structure. We use selenization of a Sn/Cu/ZnSe(001) structure on GaAs(001) substrate in order to fabricate polycrystalline CZTSe layers with preferential grain orientation. In this contribution we present a detailed investigation of those layers by means of X-ray diffraction and Raman spectroscopy. These measurements prove that a highly preferential grain orientation in all three dimensions is indeed obtained in the formed CZTSe film.

HL 102.9 Thu 17:00 CHE 91

Raman investigation of $Cu_2ZnSnSe_4$ layers with and without preferential grain orientation — •Mario Lang[1], Christoph Krämmer[1], Johannes Sachs[1], Chao Gao[1], Sabine Schuster[1], Michael Powalla[2], Heinz Kalt[1], 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 (ZSW), 70565 Stuttgart, Germany

$Cu_2ZnSnSe_4$ (CZTSe) is attracting more and more attention as an alternative to the well-established $Cu(In,Ga)Se_2$ material system for thin-film photovoltaics due to its composition of earth-abundant elements. Raman spectroscopy is a powerful technique to detect secondary phases in the thin-film absorber layers. Futhermore, using polarization-dependent measurements it is possible to gain information on the crystal orientation when performed on samples with a preferential grain orientation. We present a comparative study of polycrystalline absorber layers with and without a preferential grain orientation. The results are analyzed using theoretical modeling of the Raman line intensities.

HL 102.10 Thu 17:15 CHE 91

Radiative recombination in Cu2ZnGeSe4 single crystals — •Sergiu Levcenko[1], Maxim Guc[2], Steffen Kretzschmar[1], Ernest Arushanov[2], and Thomas Unold[1] — [1]Helmholtz Zentrum Berlin für Materialien und Energie, 14109 Berlin,Germany — [2]Institute of Applied Physics, Academy of Sciences of Moldova, MD 2028 Chisinau, Moldova

Cu2ZnGeSe4 (CZGSe) is considered as a promising absorber material for thin film solar cells, owing to its high absorption coefficient and its optimum band gap for the sunlight spectrum. While structure and optical properties of CZGSe are studied, little is known about its electronic structure. To reveal intrinsic defect properties of this semiconductor we carried out photoluminescence spectroscopy on the CZGSe single crystals grown by chemical vapour transport. At low temperature two defect related transitions at about 1.2 and 1.3eV were observed. These transitions are systematically investigated by means of temperature and excitation dependent measurements and the defect recombination model has been proposed.

HL 103: Graphene: Adsorption, intercalation, doping (organized by O)

Time: Thursday 16:00–18:45 Location: WIL C107

HL 103.1 Thu 16:00 WIL C107

Covalent binding of single iron phtalocyanine molecules to graphene on Ir(111) — •Simon J. Altenburg[1], Shiri R. Burema[2], Bin Wang[3], Richard Berndt[1], and Marie-Laure Bocquet[2,4] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Université de Lyon, Laboratoire de Chimie, Ecole Normale Supérieure de Lyon, CNRS, F69007 Lyon, France — [3]Department of Physics & Astronomy, Vanderbilt University, Nashville, TN 37235 — [4]Department of Civil and Environmental Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139

Single iron phtalocyanine (FePc) molecules on graphene on Ir(111) are studied by low temperature scanning tunneling microscopy. The molecules are either unperturbed and weakly coupled to the substrate or bound to graphene by a lobe in a specific region of the moiré unit cell. Concomittant density functional calculations reveal that the binding between the FePc lobe and graphene is the result of a new kind of cyclization reaction. This reaction is activated in certain regions of the moiré unit cell by the presence of the iridium substrate.

HL 103.2 Thu 16:15 WIL C107

Adsorption of Pentacene on Epitaxial Graphene and BN — •Alexei Nefedov[1], Wenua Zhang[1,2], Hikmet Sezen[1], Alexandr Fedorov[3], Nikolay Verbitskiy[4], Alexander Grüneis[3,4], and Christof Woell[1] — [1]Institute of Funcional Interfaces, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany — [2]NSRL, Hefei, China — [3]IFW, Dresden, Germany — [4]University of Vienna, Vienna, Austria

Smooth interfaces are a prerequisite for future high-performance and low-cost organic electronic devices based on small conjugated molecules. Since all important charge transport processes are confined to the first several monolayers, the quality of the first layer plays a key role on device performance. Pentacene stands out as a model molecule among organic semiconductors due to its ability to form well-ordered films showing a high field effect mobility. Moreover, the morphology of the first layer of a thin Pn film is known to be strongly influenced by the substrate termination, which further decisively affects the interfacial charge transport properties. Thus, information on the molecular orientation of pentacene in a case of (sub)monolayer coverages can provide a key information on improvement of device performance. In this study the adsorption of pentacene on a single layer of graphene or boron nitride (BN) has been investigated by means of XPS and NEXAFS spectroscopy. The experiments were performed on the HE-SGM beamline at BESSY II in Berlin. It was found that pentacene molecules demonstrate a dependence of their orientation and electronic structure on the coverage.

HL 103.3 Thu 16:30 WIL C107

Wetting properties of parahexaphenyl on exfoliated graphene — •Markus Kratzer[1], Stefan Klima[1], Borislav Vasić[1], Aleksandar Matković[2], Marijana Milićević[2], Rados Gajić[2], and Christian Teichert[1] — [1]Institute of Physics, Montanuniversität Leoben,Franz Josef Straße 18, 8700 Leoben, Austria — [2]Institute of Physics, University of Belgrade, Pregrevica 118 P.O. Box 68, 11080 Belgrade, Serbia

Graphene (Gr) bears potential to serve as transparent and flexible electrode material in organic electronics. Therefore, understanding of the growth of organic thin films on it is essential. Here, we investigated the growth morphology of films formed by the rodlike para-hexaphenyl (6P) molecule on Gr as a model system. As substrates exfoliated graphene transferred onto a silicon oxide support were used. Submonolayer amounts of 6P were deposited by means of hot-wall epitaxy between 333 K and 393K. The evolving film morphologies, investigated by atomic-force microscopy (AFM), exhibited a strong dependence on temperature and number of supporting Gr layers. At 333 K, needle like structures - which are known to be composed of flat lying molecules [1]- and islands composed of upright standing molecules coexist on the Gr. For the higher temperatures solely needles, forming networks, are found. The needles forming at 363 K exhibit an increasing dewetting with increasing number of Gr layers which is attributed to Gr layer dependent changes in surface energy, diffusion properties and preferential adsorption sites.

[1] C. Teichert et al. Appl. Phys. A 82 (2006) 665.

HL 103.4 Thu 16:45 WIL C107

H-adsorption and H_2-splitting on graphene/SiC(0001) — •Gabriele Sclauzero and Alfredo Pasquarello — École Polytechnique Fédérale de Lausanne (EPFL), Lausanne (Switzerland)

High-quality graphene grown epitaxially on SiC(0001) can be regarded as a convenient template for the realization of graphene-based electronics. However, the presence of a carbon "buffer" layer buried at the interface between the SiC surface and the epitaxial graphene is detrimental to the electronic transport properties of graphene. Hydrogen intercalation at high temperatures can be used to convert the buffer layer into a quasi-free standing graphene lying directly above a H-saturated SiC(0001) surface, which provides a much more effective decoupling from the substrate.

Here, the processes of H-adsorption and H_2-splitting at the graphene/SiC(0001) interface is addressed through first-principles atomistic simulations based on realistic interface models, including the experimentally observed $6\sqrt{(3)}\times 6\sqrt{(3)}R30°$ reconstruction. Our main finding is a great enhancement of the chemical reactivity of the carbon buffer layer with respect to pristine graphene, as a result of the partial sp^2 to sp^3 rehybridization of the C atoms in the buffer. H-binding energies on threefold-coordinated C atoms of the buffer are three-to-four times larger than on graphene and H_2-splitting becomes an exothermic process, with activation barriers that can be up to four times smaller than on graphene. On favorable sites, energy barriers can become as low as 1 eV and are in agreement with the observation of atomic-H intercalation also when H_2 is used as hydrogen source.

HL 103.5 Thu 17:00 WIL C107

Deuterium adsorption on (and desorption from) SiC(0001)-(3x3), (R3xR3)R30°, (6R3x6R3)R30° and quasi-free-standing graphene obtained by hydrogen intercalation — •Bocquet F.C.[1], Bisson R.[2], Themlin J.-M.[3], Layet J.-M.[2], and Angot T.[2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich - 52425 Jülich, Germany — [2]Aix-Marseille Université, PIIM, CNRS, UMR 7345, 13013 Marseille, France — [3]Aix-Marseille Université, IM2NP, 13397, Marseille, France and CNRS, UMR 7334, 13397, Marseille - Toulon, France

I present a comparative High-Resolution Electron Energy-Loss Spectroscopy (HREELS) study on the interaction of atomic hydrogen and deuterium with various reconstructions of SiC(0001). We show that deuterium passivation of the (3x3) is only reversible when exposed to atomic deuterium at a surface temperature of 700 K since tri- and dideuterides, necessary precursors for silicon etching, are not stable at this temperature. On the other hand, we show that the deuteration of the (R3xR3)R30° is always reversible because precursors to silicon etching are scarce on the surface [1]. Further, the comparison of the deuterium binding in the intercalation layer of quasi-free-standing graphene with the deuterated (R3xR3)R30° surface provides some indication on the bonding structure at the substrate intercalation layer [1,2].

[1] F.C. Bocquet et al. J. Phys. D: Appl. Phys. (2014) in press
[2] F.C. Bocquet et al. Phys. Rev. B. 85 (2012) 201401

HL 103.6 Thu 17:15 WIL C107

Charge doping induced phase transitions in hydrogenated and fluorinated graphene — •Tim Wehling[1,2], Bernhard Grundkötter-Stock[2], Bálint Aradi[2], Thomas Niehaus[3], and Thomas Frauenheim[2] — [1]Institute for Theoretical Physics, Universität Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]Bremen Center for Computational Material Science, Universität Bremen, Am Fallturm 1, 28359 Bremen, Germany — [3]Department of Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

We show that charge doping can induce transitions between three distinct adsorbate phases in hydrogenated and fluorinated graphene. By combining ab initio, approximate density functional theory and tight binding calculations we identify a transition from islands of C_8H_2 and C_8F_2 to random adsorbate distributions around a doping level of ± 0.05 e/C-atom. Furthermore, in situations with random adsorbate coverage, charge doping is shown to trigger an ordering transition where the sublattice symmetry is spontaneously broken when the doping level exceeds the adsorbate concentration. Rehybridization and lattice distortion energies make graphene which is covalently functionalized from one side only most susceptible to these two kinds of phase transitions. The energy gains associated with the clustering and ordering transitions exceed room temperature thermal energies.

HL 103.7 Thu 17:30 WIL C107

Graphene Oxide Formation by Adsorption and Photolysis of NO_2 and SO_2 on Graphene/Ir(111) — •Stefan Böttcher, Hendrik Vita, and Karsten Horn — Fritz-Haber Institute of the Max-Planck Society, Faradayweg 4-6, 14195 Berlin, Germany

Graphene oxide is a widely discussed precursor for the technological application of graphene-based systems; for example, its controlled reduction into graphene may lead to a tunable band gap. We report on the formation of oxidized graphene layers on Ir(111) by adsorption and photodissociation of NO_2 and SO_2 at low temperatures. Both adsorbates induce atomic oxygen on the surface when irradiated with intense UV light, leading to an oxidation of the graphene layer. The method presented here is expected to be less intrusive compared for example to oxygen bombardment methods. We also believe the photon induced oxidation to be more selective compared to other physical or wet chemical methods. A band gap opening at room temperature is observed, showing that the graphene oxide phase is also stable above 100 K. High quality graphene can be recovered after annealing, judged by the reappearance of its core and valence level spectral features. Apart from the selective formation of the epoxidic phase, the reaction can also be driven towards a metastable oxide phase from NO_2 using low photon flux. SO_2 on the other hand produces fragments upon dissociation, which have a strong influence on the hybridization state of the graphene backbone.

HL 103.8 Thu 17:45 WIL C107

Tuning the van der Waals Interaction of Graphene with Molecules by Doping — •Felix Huttmann[1], Antonio Javier Martinez-Galera[1], Nicolae Atodiresei[2], Vasile Caciuc[2], Stefan Blügel[2], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [2]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich, 52428 Jülich, Germany

Strong n-doping of graphene on its epitaxial substrate can be introduced via intercalation of highly electropositive elements such as Cs and Eu, and has recently been shown to lead to reduced binding energy for electropositive, ionic adsorbates [1].

Here, we explore tuning of graphene's van der Waals (vdW) interaction with adsorbates via doping. Employing an all in-situ surface science approach, we find by scanning tunneling microscopy and thermal desorption spectroscopy a significantly higher binding energy on n-doped as opposed to undoped graphene for the vdW-bonded molecules benzene and naphthalene. This is just opposite to the case of electropositive, ionic adsorbates. Based on the model character of these simple pi-conjugated molecules [2], we propose that the strength of the van der Waals interaction is modified by doping. The experimental results are compared to density functional calculations, including van der Waals interactions.

References:

[1] S. Schumacher et al., Nano Lett. 13, 5013 (2013)
[2] S. D. Chakarova-Käck et al., Phys. Rev. Lett. 96, 146107 (2006)

HL 103.9 Thu 18:00 WIL C107

Li intercalation at the graphene/Cu interface: An electronic structure view of synchrotron-based spectroscopy — •Liang Zhang[1,2], Jinghua Guo[2], and Junfa Zhu[1] — [1]National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, 230029, China — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA, 94720, USA

The synthesis of graphene on metal surfaces (such as Ni, Pd, Ru or Cu) by chemical vapor deposition (CVD) is one of the most promising, inexpensive and readily accessible methods to prepare single-layer graphene, which is a prerequisite for the fabrication of graphene-based electronic devices. In particular, graphene grown on Cu foils over large areas has allowed access to high quality of this material.

In this presentation, we report our recent studies on the electronic structure of graphene/Cu and Li-intercalated graphene/Cu by synchrotron-based spectroscopy. The results indicate a high degree of alignment and a slight corrugation/rippling of the graphene layer on Cu. The deposition of Li atoms on graphene surface under ultrahigh vacuum condition at room temperature results in a charge transfer from the adsorbed Li atoms to graphene. After annealing the as-deposited Li/graphene/Cu sample at 300 °C for 10 min, the Li atoms intercalate into the interface of graphene/Cu. These interfacial Li atoms show a strong passivation from oxidation environment due to the protection of graphene layer.

HL 103.10 Thu 18:15 WIL C107

Progressive nitrogen-doping of graphene on SiC(0001) — •Mykola Telychko, Pingo Mutombo, Martin Ondráček, Prokop Hapala, Jan Berger, Pavel Jelinek, and Martin Švec — Institute of Physics ASCR, Cukrovarnická 10, Praha, Czech republic

Doping of epitaxial graphene on SiC substrates was achieved by direct nitrogen ion implantation and stabilization at temperatures above 1300K. Scanning tunneling microscopy reveals very well-defined single substitutional defects on single and bilayer graphene. Repeated nitrogen implantation and stabilization leads to formation of double defects, which comprise of two nitrogen defects in a second-nearest-neighbour (meta) configuration. DFT calculations and scanning tunneling microscopy simulations are used to evaluate the electronic properties and to explain varying contrast of these defects in the atomically-resolved images, depending on the probe type. A mechanism of defect formation is proposed.

HL 103.11 Thu 18:30 WIL C107

Electronic and magnetic properties of cobalt interaction with graphene on Ir(111) — Hendrik Vita, Stefan Böttcher, and •Karsten Horn — Fritz-Haber-Institut of the Max-Planck-Society, Faradayweg 4-6, 14195 Berlin, Germany

The interaction of graphene with transition metal surfaces has attracted much interest because these are ideal templates for the growth of high quality films. Ferromagnetic substrates such as Ni(111) and Co(0001) are interesting since graphene grown on these surfaces can act as a spin filter. We have earlier found that the proximity of graphene to the ferromagnetic Ni(111) substrate induces a sizeable magnetic moment in the carbon π -states as determined from carbon K edge XMCD. Here we study the influence of thin layers of ferromagnetic Co sandwiched between Ir(111) and graphene with consequences for the magnetic properties expected. We find that the cobalt films show ferromagnetic behavior even for very low thicknesses. In order to study the behavior of magnetic heterostructures utilizing graphene as an interlayer we examine sandwich systems consisting of a thin layer of cobalt on top graphene/Ni(111). Using element-specific XMCD and hysteresis measurements it is possible to gain insight into the magnetic coupling across this magnetic heterostructure.

HL 104: Organic electronics and photovoltaics II (organized by DS)

Time: Thursday 17:45–19:45 Location: CHE 91

HL 104.1 Thu 17:45 CHE 91

The role of residual additives on the stability of polymer blend materials for organic photovoltaic applications. — •Aurélien Tournebize[1,2], Agnès Rivaton[2], Heiko Peisert[1], and Thomas Chassé[1] — [1]Institute of Physical and Theoretical Chemistry, Tübingen, Germany — [2]Institut de Chimie de Clermont-Ferrand, France

Processing additives for improved the morphology of the bulk heterojunction (BHJ) materials used in organic solar cells (OSCs) is now very popular. Thus, by optimizing the donor and acceptor nano domains, the efficiency of OSCs devices could be significantly increased. [1] The impact of those additives on the performances has been widely explored recently but nothing in terms of stability. And yet, a part of the additives stays trapped in the thin film [2] and could participate in the complex photodegradation of the polymer blend materials.

In the present work, we have investigated the impact of residual additives on the polymer blend photostability. By using essentially spectroscopic technics, we have observed an acceleration of the polymer blend photodegradation in presence of additives. In this context, the use of new additives providing a better morphology and by the way a better stability was also explored.

[1] J.K. Lee, W.L. Ma, C.J. Brabec, J. Yuen, J.S. Moon, J.Y. Kim, K. Lee, G.C. Bazan, and A.J. Heeger JACS. 2008, 130, 3619-3623 [2] L. Ye, Y. Jing, X. Guo, H. Sun, S. Zhang, M. Zhang, L. Huo, and J. Hou J. Phys. Chem. C 2013, 117, 14920-14928

HL 104.2 Thu 18:00 CHE 91

Electronic States and Electrochemical Properties of Polymeric Phthalocyanine Sheets — •Clemens Geis and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany

Phthalocyanines are forming organic semiconducting thin films applicable in field-effect transistors, organic solar cells and as heterogeneous chemical catalysts. They consist of a planar organic aromatic ligand around a central metal atom like *Cu*, *Fe* or *Co*. In a chemical vapour deposition reaction (CVD) phthalocyanines with polymerized ligands were synthesized by reactions of bifunctional 1,2,4,5-tetracyanobenzene with thin metal films. By these means a high concentration of the catalytically active metal-sites on the substrate is established, they are electronically coupled and a molecular network is formed by such sheet polymers. Photoelectron spectroscopy was used to characterize the electronic states of the metals and ligands. Metal ions in the complexes as well as neutral metal clusters were detected in the films. Optical transmission spectroscopy was used to discuss the uniformity of the electronic excitation energy and its dependence on preparation conditions. The films were electrochemically reduced and oxidized to further study their accessible electronic states, study consequences for their optical absorbance and to test the polymeric phthalocyanines as electrocatalysts for water oxidation to oxygen and reduction to hydrogen, reactions of highest interest for the chemical storage of electrical energy from fluctuating renewable sources.

HL 104.3 Thu 18:15 CHE 91

Asymmetry of mixing length scales and kinetics of phase-separation in co-evaporated donor-acceptor organic thin film blends — •Rupak Banerjee, Christopher Lorch, Alexander Gerlach, Jiří Novák, Christian Frank, Johannes Dieterle, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

Small molecular organic semiconductors have found widespread usage in organic photovoltaics (OPV) due to their attractive optical, structural and electronic properties [1]. One of the many ways to tune the efficiency of an OPV is by mixing donor (D) and acceptor (A) materials [1] since the efficiency depends on the interplay of the diffusion lengths of the excitons generated by the absorption of light and the structural length scales of the D:A mixture. Controlling the structural length scales in D:A mixtures is thus of paramount importance [2]. We discuss *in situ* and real-time x-ray scattering studies on the structure of mixed D:A films as a function of mixing ratio which reveal the kinetics and thickness dependence of phase separation and in particular the asymmetry between top and bottom interfaces [3]. We further discuss the influence of interrupted growth on the phase-separation kinetics of such systems.

[1] W. Brütting and C. Adachi, Physics of Organic Semiconductors, Wiley-VCH, Weinheim (2012).
[2] A. Opitz *et al.*, IEEE J. Sel. Top. Quant. **16**, 1707 (2010).
[3] R. Banerjee, J. Novák, C. Frank, C. Lorch, A. Hinderhofer, A. Gerlach, and F. Schreiber, Phys. Rev. Lett. **110**, 185506 (2013).

HL 104.4 Thu 18:30 CHE 91

UPS studies on different air-stable molecular n-dopants — •Martin Schwarze[1], Max L. Tietze[1], Paul Pahner[1], Ben Naab[2], Zhenan Bao[2], Björn Lüssen[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. A defined doping level allows for the control of the Fermi level position and the conductivity of transport layers. In comparison to molecular p-doping of organic semiconductors, n-doping has 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, an air stable cationic DMBI and DMBI dimer with the air sensitive W2(hpp)4. Doping efficiency, Fermi-level shift, air stability, and conductivity at different doping concentrations are investigated by ultraviolet photoelectron spectroscopy (UPS) and electrical measurements.

HL 104.5 Thu 18:45 CHE 91

Fracture and corrosion protection for thin-film encapsulation - Fine-tuning the electrical calcium corrosion test for water vapor permeation measurements — •Frederik Nehm, Hannes Klumbies, Lars Müller-Meskamp, and Karl Leo — Institut für Angewandte Photophysik, TU Dresden, Dresden, Deutschland

In recent years, the demand for ultra-high moisture barriers has strongly increased due to the ongoing development of organic electronics. Thus, the ability to measure water vapor transmission rates (WVTRs) below $10^{-5}\ \frac{g(H_2O)}{m^2 d}$ - less than a monolayer in 10 days - is crucial for barrier development. The electrical calcium corrosion test - monitoring the decreasing conductivity of a thin calcium film turning into calcium hydroxide - is a sensitive, cost-efficient method to measure such low WVTRs. However, poor design can cause a high background rate or test breakdown. We show that calcium corrosion causes barrier breaking by both expansion and hydrogen emission. As a countermeasure, we introduce organic (C_{60}) buffer layers for decoupling on both sides of the calcium film. Further investigations show elevated calcium corrosion at the calcium-electrode-interface which can be prevented by a proper choice of the electrode material. Finally, the massive corrosion of barrier thin films is shown to be prevented by glueing a polymer foil onto the barrier under testing. With these precautions, we show atomic layer deposited alumina barriers measured in thin film encapsulation structure close to an actual device architecture. At 30°C, 90% rh, WVTRs of below $5 \cdot 10^{-5}\ \frac{g(H_2O)}{m^2 d}$ were obtained.

HL 104.6 Thu 19:00 CHE 91

Commensurability as the determining factor for molecular tilt and multilayer growth: In-situ and real-time growth study of the nanographene HBC on SiO_2 and HOPG — •Paul Beyer[1], Tobias Breuer[2], Saliou Ndiaye[2], Anton Zykov[1], Andreas Viertel[1], Manuel Gensler[1], Jürgen P. Rabe[1], Stefan Hecht[1], Gregor Witte[2], and Stefan Kowarik[1] — [1]HU Berlin, 12489 Berlin — [2]Philipps-Universität Marburg, 35032 Marburg

We investigate the influence of symmetries and the substrate-molecule commensurability on the structure and growth kinetics of the nanographene hexa-*peri*-hexabenzocoronene (HBC). We study organic molecular beam deposited ultrathin HBC films on SiO_2, pristine and sputtered HOPG because of the similar surface energies, singling out the influence of the lattice-matching between HBC and graphite. Using real-time and *in situ* x-ray growth oscillations we find the first ad-layer to grow lying down on both substrates. On pristine HOPG we find a superstructure of hexagonally arranged, recumbent molecules in a new polymorph using GIXD, XRR and NEXAFS. The loss of commensurability in the sputtered HOPG leads to mainly upright molecules. Equally, we find a transition to upright molecules on amorphous SiO_2 surfaces. On SiO_2 micro-crystallites in the bulk structure that completely cover the substrate are found, while the strong ordering on HOPG leads to island growth of the new polymorph as observed by AFM. Our results demonstrate that the (lack of) symmetry- and lattice-matching critically determines the molecular orientation and occurrence of surface induced polymorphs.

HL 104.7 Thu 19:15 CHE 91

Spray coating process for highly conductive silver nanowire networks as transparent top electrode for small molecule organic photovoltaics — •Franz Selzer[1], Nelli Weiss[2], David Kneppe[1], Ludwig Bormann[1], Christoph Sachse[1], Nikolai Gaponik[2], Lars Müller-Meskamp[1], Alexander Eychmüller[2], and Karl Leo[1] — [1]IAPP, TU Dresden — [2]Phy. Chem., TU Dresden

Organic photovoltaics are a promising technology for fabrication in high throughput R2R-coating machines. Therefore, flexible and highly conducting transparent electrodes on temperature sensible polymer films are required. Percolative networks made of silver nanowires (AgNWs) are a flexible alternative, showing an opto-electrical performance comparable to ITO. Usually, they are deposited from solution, followed by post-annealing (200°C). The solvents involved in the deposition limit the versatility of this type of electrode and do not allow the direct deposition as top contact onto evaporated small molecule devices. Here, we present a novel spray-coated AgNW mesh, showing excellent opto-electrical performance although processed below 80°C. We investigate different types of wire functionalization and the consequences on typical network parameters of AgNWs. By comparing all investigated materials for different parameters like varying concentration and by scanning electron microscopy, the basics of the sheet resistance reduction mechanism are extracted and AgNW electrodes (<50Ohm/sq@>80%) are processed at 30°C. Finally, the successful implementation as transparent top electrode for high-performance organic p-i-n type solar cells is demonstrated.

HL 104.8 Thu 19:30 CHE 91

Tuning the energy levels of carbon nanotubes by functionalization — •Gerhard Lackner[1], Wei Xia[2], Vladimir Shvartsman[1], Martin Muhler[2], and Doru C. Lupascu[1] — [1]Institute for Materials Science, University of Duisburg-Essen, 45141 Essen, Germany — [2]Laboratory of Industrial Chemistry, Ruhr-University Bochum, 44801 Bochum, Germany

Carbon nanotubes (CNT) are a promising material for electrical applications due to their extraordinary properties. Nevertheless, a defined tuning of the energy levels of this material has not been reported so far. We show a possible route to set the energy levels of CNT by functionalization. The energy levels before and after the functionalization are analysed by Kelvin Probe measurements. Additionally, the functionalized and non-functionalized CNT are applied in organic solar cells and a comparative study about the solar cell performances is given.

HL 105: Poster: Topological insulators (with MA/O)

Time: Thursday 17:00–20:00 Location: P1

HL 105.1 Thu 17:00 P1

Theoretical description of scanning gate microscopy on quantum Hall point contacts — •Martin Treffkorn and Bernd Rosenow — Institut für theoretische Physik, Universität Leipzig, Germany

In the integer quantum Hall regime, the concept of edge states allows to describe dissipationless, one-dimensional transport along the boundary of a sample. Recent experimental progress in the application of low-temperature scan-gate microscopy has allowed to image the spatial structure of edge states with high resolution [1]. To this end, a negatively charged scanning tip approaches a quantum point contact (QPC), such that changes in the spatial edge structure can be measured in the differential resistance of the QPC. The resistance only change when the tip induced change in electron density prevents an edge channel from passing through the point contact, since electrons may only travel along the quasi one dimensional channels at the edge. From the differential change of resistance versus the tip position one obtains a picture of the edge channels that are present in the system. We use a recursive Greens function algorithm to calculate the conductance of a QPC in the presence of a scanning tip. In our calculations we consider the existence of alternating compressible and incompressible strips across the system, paying particular attention to the influence of Coulomb interactions on the edge structure.

[1] N. Pascher, C. Rössler, T. Ihn, K. Ensslin, C. Reichl, and W. Wegscheider, arXiv:1309.4918 (2013).

HL 105.2 Thu 17:00 P1

Dirac and Weyl semimetal states in Na_3Bi from first principles — •Patrick Buhl, Stefan Blügel, and Yuriy Mokrousov — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Recently, the three-dimensional Dirac semimetal state was theoretically predicted to exist [1] and experimentally observed [2] in bulk Na_3Bi. Using first principles methods in combination with the Wannier functions technique [3], we construct and analyze the topological phase diagram of Na_3Bi as a function of spin-orbit strength and external exchange field. In particular we aim at realization of the Weyl semimetal phase in this material. The topological properties are characterized in terms of what computed from ab initio Chern and spin Chern numbers of the Berry curvature flux around the points of band degeneracy. Additionally, we consider finite slabs of Na_3Bi and focus on the electronic structure of the surface states in correlation to the bulk topological phase diagram. Financial support by the HGF-YIG Programme VH-NG-513 is gratefully acknowledged.

[1] Z. Wang *et al.*, Phys. Rev. B **85**, 195320 (2012)
[2] Z.K. Liu *et al.*, arXiv:1310.0391 (2013)
[3] www.flapw.de

HL 105.3 Thu 17:00 P1

Dielectric Function of the Topological Surface States of Bi_2Se_3 — •Markus Heinemann, Christian Franz, and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University, 35392 Giessen, Germany

We investigate the material system Bi_2Se_3 which recently has been discovered to belong to the new class of topological insulators (TI). In this TI, robust surface states located in the insulating band gap of the bulk are protected by time-reversal symmetry and consist of a single Dirac cone at the Γ-point [1]. We use density functional theory to investigate the electronic structure and dielectric function of Bi_2Se_3 by first principles. In our calculations we study the bulk material and the Se terminated surface of Bi_2Se_3 which we simulate by a slab model and examine the effect of the slab thickness, i.e. the number of atomic layers. The essential effect of spin-orbit-coupling for the topological state and thus on the electronic and dielectric properties is presented by comparing calculations with and without this feature.

[1] H. Zhang, C.-X. Liu, X.-L. Qi, X. Dai, Z. Fang, and S.-C. Zhang, Nature Phys. 5, 438 (2009)

HL 105.4 Thu 17:00 P1

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

Topological insulators (TIs) are a new state of quantum matter which insulates in the bulk and conducts on the surface. The study of bulk TIs has been hindered by high conductivity inside the bulk, arising from crystalline defects. Such problems can be tackled through compositional engineering or the synthesis of TI nanomaterials. We combined both approaches in a systematic study of various growth parameters to achieve uniform, high purity nanowires with high substrate coverage.

The highlight of this study is the development of a new growth route for nanowires, based on a TiO_2 catalyst rather than the conventional Au. Comparative studies demonstrate that Au significantly contaminates the nanowires, whereas TiO_2 stays well separated. Details of the Au and TiO_2-catalysed growth mechanism were investigated. For Au it was found that the growth mechanism is vapour-liquid-solid. For TiO_2 nanoparticles, in contrast, the growth mechanism can be described in the vapour-solid scheme.

Nanowires of the doped compound $(Bi_{0.78}Sb_{0.22})_2Se_3$ were studied using synchrotron radiation. It was discovered that the material mainly adopts an orthorhombic phase known from Sb_2Se_3. The Raman spectrum is reported and matched with the structural information for the first time. Further, a method to control the length and diameter of Bi_2Se_3 nanowires through laser-cutting was developed.

HL 105.5 Thu 17:00 P1

Strained HgTe shell on CdTe nanowires grown by Au catalyst MBE — •Maximilian Kessel, Rebekka Pfeuffer, Claus Schumacher, Hartmut Buhmann, and Laurens W. Molenkamp — Experimental Physics 3, University of Würzburg, Germany

The topological insulator properties of 2D and strained 3D HgTe layers have attracted strong attention over the past years. One interesting question that rose was how the TI state evolves in quasi-one dimensional geometry. Here, we present the first realization of a strained HgTe shell on CdTe nanowires.

Doped GaAs wafers are used as substrates for the nanowire growth in a multi-chamber ultra-high vacuum system. The CdTe growth is seeded by liquid Au/Ga eutectic droplets. For straight, uniform and smooth shaped CdTe wires, a special growth start is performed and the substrate temperature is hold within narrow limits. The wires have a diameter of 30 to 100 nm and grow along the [111]B direction up to a length of 3 μm. The ensemble of CdTe wires is used as substrate for HgTe molecular beam epitaxy. Shell and core of the nanowires are characterized by electron and X-ray diffraction. The radial heterostructures show strained crystalline structure. Transport characterization measurements on separated radial HgTe/CdTe heterostructures are done at low temperature.

HL 105.6 Thu 17:00 P1

Weak anti-localization in HgTe quantum wire arrays — •Johannes Ziegler[1], Sabine Weishäupl[1], Christopher Ames[2], Christoph Brüne[2], Harmut Buhmann[2], Laurens W. Molenkamp[2], and Dieter Weiss[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]Physikalisches Institut (EP III), Universität Würzburg, Germany

We present our progress in fabricating quasi-1D quantum wire arrays in inverted HgTe quantum wells, being a 2D topological insulator. These quasi-1D quantum wire arrays were fabricated with widths between 120 nm and 250 nm. Our experiments focus on phase-coherent effects, like weak anti-localization and weak-localization, in both wire arrays and 15 and 40 μm wide Hall-bars. From these measurements we extract the phase-coherence length l_ϕ and the spin-relaxation length l_{SO}.

Our work is motivated by a proposal for all-electrical detection of the relative spin-orbit interaction strength α / β [1,2], where α is the Rashba and β the Dresselhaus spin-orbit parameter. A key requirement for this method is the transition from weak anti-localization (WAL) to weak localization (WL) through 1D confinement. The analysis of these characteristic lengths allows us to check when the suppression of WAL occurs.

[1] M. Scheid *et al.*, Phys. Rev. L **101**, 266401 (2008).
[1] M. Scheid *et al.*, Semicond. Sci. Technol. **24**, 064005 (2009).

HL 105.7 Thu 17:00 P1

Magnetotransport and ac conductivity in 2D and 3D topological insulators — •Christian Michel and Ewelina M. Hankiewicz — Institute for Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany

We study theoretically Landau level structure and optical selection rules in 2D and 3D TIs. Our focus is to find the features which are specific to the Dirac physics. We show that the optical selection rules are different for the particle-hole symmetric Dirac model in comparison with the particle-hole asymmetric models. We explain the influence of dimensionality on the characteristic features of optical selection rules.

We acknowledge grant HA 5893/4-1 within SPP 1666.

HL 105.8 Thu 17:00 P1

Ferromagnetic contacts on topological insulators: Lithographic realization on strained 3-dimensional HgTe — •Kalle Bendias, Erwann Bocquillon, Simon Hartinger, Christoph Brüne, Hartmut Buhmann, and Laurens Molenkamp — EP3, Physikalisches Institut, Universität Würzburg, Am Hubland, D-97074 Würzburg

Topological insulators are a new class of material with insulating bulk and conducting Dirac-like surface states. These states are associated with spin-momentum locking, which is supposed to lead to numerous applications in spintronics [1].

Here we report on lithographic ways to realize the concept of spin injection and detection into the Dirac-like surface states of the 3-dimensional topological insulator HgTe. We discuss fabrication challenges such as unstrained deposition of ferromagnetic material and the realization of a diffusion barrier on the high temperature-sensitive HgTe material system.

[1]C. Brüne, et. al, Phys. Rev. Lett. 106, 126803 (2011)

HL 105.9 Thu 17:00 P1

Transport properties of the high mobility topological insulator HgTe — •Jonas Wiedenmann[1], Cornelius Thienel[1], Christopher Ames[1], Christopher Brüne[1], Steffen Wiedmann[2], Hartmut Buhmann[1], and Laurens Molenkamp[1] — [1]Universität Würzburg, Würzburg, Deutschland — [2]Radboud Universität Nijmegen, Nijmegen, Holland

It has been demonstrated recently, that the semimetal HgTe opens a band gap of approximately 20 meV when grown strained on a CdTe substrate and thus becomes a three dimensional topological insulator (3D TI)[1].

We show that it is possible to increase the mobility of the surface states by an order of magnitude, if HgTe is sandwiched between epitaxial layers of HgCdTe. The topological insulator is investigated in transport measurements at low temperatures and magnetic fields up to 30 T. Through the enhanced surface mobilites we are able to observe a Dirac specific quantum hall effect. The experimental data suggest, that it has to be discussed within a two surface model for Dirac fermions.

[1] C. Brüne et al., Phys. Rev. Lett. 106, 126803 (2011)

HL 105.10 Thu 17:00 P1

Heteroepitaxial Li_2IrO_3 Thin Films Grown by Pulsed Laser Deposition — •Marcus Jenderka, Heiko Frenzel, Rüdiger Schmidt-Grund, Marius Grundmann, and Michael Lorenz — Institut für Experimentelle Physik II, Universität Leipzig, Linnéstraße 5, D-04103 Leipzig. Germany

The layered perovskite oxides A_2IrO_3 (A = Na, Li) have been studied in recent years in terms of a physical realization of spin-liquid [1] and topological insulator [2] phases, desired within certain quantum computation proposals. We report on the pulsed laser deposition of heteroepitaxial Li_2IrO_3 films on ZrO_2:Y(001) single crystalline substrates. As in Na_2IrO_3 [3], X-ray diffraction confirms a preferential (001) out-of-plane crystalline orientation with a defined in-plane epitaxial relationship. Resistivity between 35 and 300 K is dominated by a three-dimensional variable range hopping mechanism. Infrared optical transmission from 0 to 1.85 eV, measured by Fourier transform infrared spectroscopy (FTIR), reveals a small optical gap $E_{\mathrm{go}} \approx 300$ meV together with a splitting of the $5d$-t_{2g} manifold caused by the interplay of spin-orbit coupling and electronic correlations. By means of infrared spectroscopic ellipsometry, the dielectric function (DF) is presented in the spectral range between 0.03 and 3.50 eV. The calculated absorption coefficient confirms the value for E_{go}.

[1] J. Chaloupka *et al.*, Physical Review Letters **105**, 027204 (2010).
[2] H.-S. Kim *et al.*, Physical Review B **87**, 165117 (2013).
[3] M. Jenderka *et al.*, Physical Review B **88**, 045111 (2013).

HL 105.11 Thu 17:00 P1

Epitaxial growth of $LaNiO_3$ and $LaAlO_3$ thin films and multilayers by PLD — •Haoming Wei, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig, Germany

As predicted by recent theoretical study, the superlattices (SLs) consisting of paramagnetic metal $LaNiO_3$ (LNO) and band insulator $LaAlO_3$ (LAO) may exhibit exotic topological phases[1]. We have grown LNO, LAO films and LNO/LAO heterostructures by plused laser deposition (PLD). All the films show good out-of-plane and in-plane crystalline orientation and definite epitaxial relationship. The lattice constant and strain of LNO films could be controlled by adjusting growth conditions. The LNO films have an excellent metallic conductivity and the resistivity is related to strain. The low resistivity is about $300\mu\Omega\cdot$cm at 300 K, which is low enough for use as an electrode material. The LAO films obtained by interval PLD exhibit terraced surface even when grown at a low temperature. The height of the terraces is about 0.4 nm in accord with the calculated result from XRD pattern. Further, LNO/LAO multilayer structures were fabricated. Atomic force microscopy (AFM) together with reflection high-energy electron diffraction (RHEED) images show that the multilayers have a smooth surface with the root mean square roughness about 3.2 nm.

[1] K. Y. Yang, et al. Physical Review B 84, 201104(R) (2011).

HL 105.12 Thu 17:00 P1

Combined XMCD and STS study of transition metal adatoms adsorbed on the surface of prototypical 3D topological insulators — •Jonas Warmuth[1], Martin Vondráček[2], Matteo Michiardi[3], Lucas Barreto[3], Cinthia Piamonteze[4], Andreas Eich[1], Alexander Khajetoorians[1], Jian-Li Mi[3], Bo Brummerstedt Iversen[3], Philip Hofmann[3], Jens Wiebe[1], and Roland Wiesendanger[1] — [1]Institute of Applied Physics, Uni Hamburg, Germany — [2]Institute of Physics ASCR, Prague, Czech Republic — [3]iNano, Aarhus University, Denmark — [4]Laboratory of Condensed Matter Physics, PSI, Switzerland

The spin of Dirac electrons in topological surface states is rigidly locked to the direction of their momentum leading, e.g., to prohibited backscattering. Their interaction with magnetic impurities is currently a matter of debate, because it can destroy this effect, heavily depending on the magnetic properties of the impurities. Using x-ray magnetic circular dichroism techniques we investigated 3d transition metal adatoms adsorbed on the surface of different prototypical 3D topological insulators. We compare our results to crystal field multiplet calculations [1] of the 3d states. For some of the adatom species, we find a considerable magnetic anisotropy, which depends crucially on the coupling of their 3d states to the substrate electrons. Furthermore, we investigate the interaction of the adatoms and the Dirac electrons by Fourier-transform scanning tunneling spectroscopy [2], which reveals shifts of the linear dispersion due to surface doping effects.

[1] J. Honolka et al., PRL 108, 256811 (2012)

HL 106: Poster: Spintronics (with MA/O)

Time: Thursday 17:00–20:00 Location: P1

HL 106.1 Thu 17:00 P1

Electrical detection of spin Hall effect in semiconductors — •Markus Ehlert[1], Cheng Song[1,2], Mariusz Ciorga[1], Thomas Hupfauer[1], Martin Utz[1], Dieter Schuh[1], Dominique Bougeard[1], and Dieter Weiss[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, Germany — [2]Key Laboratory of Advanced Materials, School of Material Science & Engineering, Tsinghua University, Beijing, China

We present different geometries which allow for the all-electrical detection of either direct spin Hall effect (DSHE) or inverse spin Hall effect (ISHE) in semiconductor microstructures. We describe our experimental methods and compare results to previous experiments and theory. In our DSHE experiments a spin-unpolarized charge current flows through a *n*-GaAs channel and induces, due to DSHE, a transverse spin current. Hence, spins accumulate at the boundaries of the channel and are detected by spin-sensitive Esaki diodes [1]. For ISHE experiments in *p*-GaAs we used spin-injecting contacts to generate a spin current, which, via ISHE, should lead to a measurable charge imbalance in a Hall bar geometry. Another ISHE device consists of the so-called H-bar geometry, where an electric current is driven in one leg of an H-shaped structure. This generates, due to DSHE, a transverse spin current, which flows along the connection between both legs of the "H". By means of ISHE a charge imbalance is then induced in the second leg of the "H" [2].

[1] M. Ehlert *et al.*, Phys. Rev. B **86**, 205204 (2012).
[2] M. Ehlert *et al.*, Phys. Status Solidi B (2013) (acc.).

HL 106.2 Thu 17:00 P1

Spin blockade effects in a GaMnAs double quantum dot system — Stefan Geissler[1], •Sebastian Pfaller[2], Andrea Donarini[2], Milena Grifoni[2], and Dieter Weiss[1] — [1]Institute for Exp. and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

Spin polarized transport measurements of a double quantum dot defined in a GaMnAs nano constriction are presented. In the experimental setup, the polarization of the leads as well as of the quantum dot system can be controlled by an external magnetic field. In presence of a magnetic field, differential conductance measurements show a gap opening in the charge stability diagrams, that can be explained by spin blockade effects. Transport calculations of metallic quantum double dots coupled to spin polarized leads show excellent agreement with experimental data.

HL 106.3 Thu 17:00 P1

Exciton dynamics in transition metal dichalcogenides — •Igor Libman, Hendrik Kuhn, Jan G. Lonnemann, Julia Wiegand, Michael Oestreich, and Jens Hübner — Institute for Solid State Physics, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany

Among the newly emerging two-dimensional transition metal dichalcogenides molybdenum disulfide (MoS_2) has attracted an increasing attention as promising material for transport, optical and spintronic applications [1]. A contrasting key feature to the ubiquitous mono- and bilayer graphene is the easily accessible direct optical band gap of single layer MoS_2 [2]. Furthermore, the two-component nature breaks the inversion symmetry [3] and leads jointly with spin-orbit interaction to a copious number of spin-optoelectronic effects. Here, we present a scheme for the investigation of the complex dynamics of A and B excitons and their excited states (A' and B') in single layer MoS_2 [4] by ultrafast two-color time-resolved laser spectroscopy with focus on distinct impact of the electron-phonon interaction [5] onto the spectral shape of the s- and p-equivalent excitons states.

[1] Q. H. Wang *et al.*, Nature Nanotech. **7**, 11 (2012).
[2] Andrea Splendiani *et al.*, Nano Lett., **10**, 1271 (2010).
[3] G. Sallen *et al.*, Phys. Rev. B, **86**, 081301(R) (2012).
[4] Diana Y. *et al.*, Phys. Rev. Lett, **111**, 216805 (2013).
[5] A. Marini, Phys. Rev. Lett. **101**, 106405 (2008).

HL 106.4 Thu 17:00 P1

Spin dynamics in quantum wells under surface acoustic waves — •Johannes Wanner[1], Cosimo Gorini[2], Peter Schwab[1], and Ulrich Eckern[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Service de Physique de l'Etat Condensé, CEA-Saclay, 91191 Gif sur Yvette, France

Various recent experiments have shown the flexibility of surface acoustic waves (SAW) as a mean for transporting charge and spin in quantum wells [1]. In particular, SAW have proven highly effective for the coherent transport of spin-polarized wave packets, suggesting their potential in spintronics applications. Motivated by these experimental observations we have theoretically studied the spin and charge dynamics in a quantum well under surface acoustic waves. Based on previous work by some of us [2], we show that the dynamics acquires a simple and transparent form in a reference frame co-moving with the SAW. The observed values for spin relaxation and precession length can thus be explained.

[1] H. Sanada et. al., Phys. Rev. Lett. **106**, 216602 (2011); O. Couto et. al., Phys. Rev. B **78**, 153305 (2008)
[2] P. Schwab et al., Phys. Rev. B **74**, 155316 (2006)

HL 106.5 Thu 17:00 P1

Electron spin control in Manganese doped GaAs/AlAs nanostructures — •Markus Kuhnert[1], Ilya A. Akimov[1], Vladimir L. Korenev[2], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]2A.F. Ioffe Physical-Technical Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia

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/AlAs quantum wells, which might offer long lived spin coherence as well as spin manipulation mediated by the magnetic Manganese ions. We use pump-probe Kerr effect measurement techniques and time resolved photoluminescence measurements to investigate properties such as spin coherence and spin lifetime of the Mn doped nanostructures. The temperatures at the time of measurement range from 2K to 8K. Further studies are done on optically induced EPR of the Mn ions by applying a microwave modulation to the excitation laser beam. Exchange interaction between the Manganese ions and electrons in the quantum well might function as a channel for spin manipulation or conservation.

HL 106.6 Thu 17:00 P1

Coherence Properties of Nitrogen Vacancy Centers in Nano Diamond — •Bernd Sontheimer, Niko Nikolay, Max Strauss, Andreas W. Schell, Janik Wolters, and Oliver Benson — Humbold Universität zu Berlin, Institut für Physik AG Nano-Optik, Newtonstr. 15, 12489 Berlin

The nitrogen vacancy (NV) center in diamond is a stable single photon emitter, combining optical transitions with a long-lived electronic spin with excellent coherence properties [1]. NV centers in nano diamonds are of special interest due to their integrability in photonic hybrid devices [2]. In our research we examine the coherence properties of nano diamonds based on optically detected magnetic resonance (ODMR) [3]. In particular the influence of surface treatments on the T_2 time is examined via spin-echo experiments [4]. Also a change of spectral diffusion is determined using correlation interferometry.

[1] G. Balasubramanian, et al., Ultralong spin coherence time in isotopically engineered diamond. Nat. Mater. 8, 383 (2009).
[2] J. Wolters, et al., Enhancement of the zero phonon line emission from a single nitrogen vacancy center in a nanodiamond via coupling to a photonic crystal cavity. Appl. Phys. Lett. 97, 141108 (2010).
[3] J. Wolters, et al., Measurement of the Ultrafast Spectral Diffusion of the Optical Transition of Nitrogen Vacancy Centers in Nano-Size Diamond Using Correlation Interferometry. Phys. Rev. Lett. 110, 027401 (2013).
[4] F. Jelezko, et al., Observation of Coherent Oscillations in a Single Electron Spin. Phys. Rev. Lett. 92, 076401 (2004).

HL 106.7 Thu 17:00 P1

Magnetic susceptibility of 2 dimensional electron gases with Rashba spin-orbit coupling — •Christiane Scholl, Tobias Hartenstein, and Hans Christian Schneider — TU Kaiserslautern

The transverse spin-spin correlation, or dynamical magnetic susceptibility, is an important quantity both from the experimental and theoretcial point of view. It determines light-scattering and spin noise spectra, as well as the dispersions of elementary excitations of the magnetic type, such as magnons or magneto-magnons. Here, we consider a two-dimensional electron gas including Rashba spin-orbit coupling and Coulomb interaction. We use a decoupling scheme to derive the equations of motion for the relevant Green functions. Approximating the full Coulomb matrix element by a local interaction U, a closed expression for the dynamic transverse magnetic susceptibility results, which we analyze numerically. We find a complex interplay of internal effective Rashba fields with the external magnetic field. Further, the elementary "magnetic" excitations arise from resonances of the magnetic suscpetibility that are very different from plasmon resonances [1,2] with Rashba spin-orbit coupling or magneto-magnon [3] resonances.

[1] M. Pletyukhov, V. Gritsev, Phys. Rev. B 74, 045307 (2006).
[2] S. M. Badalyan, A. Matos-Abiague, G. Vignale, and J. Fabian, Phys. Rev. B 79, 205305 (2009.)
[3] D. M. Edwards, J. Phys. C. 2, 84 (1969).

HL 107: Poster: Emerging oxide semiconductors / Oxides other than ZnO and its relatives

Time: Thursday 17:00–20:00 Location: P1

HL 107.1 Thu 17:00 P1

Structural properties of $Cu_2O_{1-x}S_x$ alloys from first principles — •Raphael Knecht, Marcel Giar, Markus Heinemann, and Christian Heiliger — I. Physikalisches Institut, Justus-Liebig-University, D-35392 Giessen, Germany

We present *ab initio* investigations of the structural parameter in $Cu_2O_{1-x}S_x$ alloys by a substitutional supercell approach. To simulate a random arrangement of sulfur and oxygen in the anion lattice several different arrangements (configurations) for the same sulfur concentration are considered. The different sulfur concentrations are simulated in a 3x3x3 supercell and for each configuration the equilibrium lattice parameter is determined by calculating the hydrostatic pressure for different lattice parameters. We compute the lattice parameters in a concentration range from pure Cu_2O up to $Cu_2O_{0.61}S_{0.39}$ and compare our results with experimental data in the same concentration range.

HL 107.2 Thu 17:00 P1

Growth of Cuprous Oxide by Plasma-Assisted Molecular Beam Epitaxy — •Max Kracht, Jörg Schörmann, Martin Eickhoff, and Philip Klement — I.Physikalisches Institut JLU-Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Deutschland

The research on cuprous oxide (Cu_2O) is a topic with growing interest, since this intrinsic p-type material with a direct optical band gap of 2.17 eV consists of abundant elements only and has suitable properties for photovoltaic applications. Up to now the growth of high quality single crystalline thin films is quite challenging. Here we report on the growth of Cu_2O thin films by plasma assisted molecular beam epitaxy (PAMBE) on MgO and sapphire. High resolution X-ray diffraction (HRXRD) shows epitaxial crystal growth on both substrates. On MgO two different orientations occur with the (100) and (110) planes parallel to the MgO(100) substrate surface, which can be influenced by the copper to oxygen ratio. On sapphire substrates the utilization of a MgO buffer leads to the formation of (111)-oriented crystallites. Electrical and optical properties were determined by Hall-effect and photoluminescence measurements.

HL 107.3 Thu 17:00 P1

TEM investigation of structural changes in epitaxial $(In,Sn)_2O_3$ and $(Sn,In)O_2$ films — •Stephan Scholz[1], Anna Mogilatenko[1,2], Holm Kirmse[1], Oliver Bierwagen[3,4], Mark E. White[4], Min-Ying Tsai[4], Martin Schmidbauer[5], James S. Speck[4], and Saskia F. Fischer[1] — [1]Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, 12489 Berlin, Germany — [3]Paul-Drude-Institut für Festkörperelektronik, 10117 Berlin, Germany — [4]University of California, Santa Barbara, CA 93106, USA — [5]Leibniz-Institut für Kristallzüchtung, 12489 Berlin, Germany

Transparent conducting oxides in In_2O_3-SnO_2 pseudo-binary system are used in many optoelectronic applications, e.g. solar cells, flatscreens and touchscreens. In single-crystalline In_2O_3 and SnO_2 films, the conductivity extrema with regard to the In:Sn ratio are accompanied by crystal structure degradation [1][2]. Thus, analysis of growth-induced defects and possible structural changes in thin oxide films is important for understanding the electrical properties of these materials.

We have applied transmission electron microscopy to characterize structural changes and compositional homogeneity in epitaxial $(In,Sn)_2O_3$ as well as $(Sn,In)O_2$ films grown by plasma-assisted molecular beam epitaxy. The obtained information contributes to the understanding of the mechanisms that lead to conductivity saturation in indium-tin-oxides. [1] O. Bierwagen and J. Speck, Phys. Status Solidi A. doi:10.1002/pssa.201330224 (2013). [2] M. White, O. Bierwagen, M. Tsai, and J. Speck, APEX **3**, 051101 (2010)

HL 107.4 Thu 17:00 P1

Towards realization of bipolar devices based on In2O3: Epitaxy of Be doped InAs on In2O3 — •Fariba Hatami[1], Ted Masselink[1], Martin Schmidbauer[2], Patrick Vogt[3], and Oliver Bierwagen[3] — [1]Inst. für Physik, Humboldt-Universität zu Berlin, Berlin, Germany — [2]Leibniz-Inst. für Kristalzüchtung, Berlin, Germany — [3]Paul-Drude-Inst. für Festkörperelektronik, Berlin, Germany

In2O3 is an important transparent semiconducting oxide and has a great potential for applications in transparent microelectronics, optoelectronics, and short wavelength photonics. In2O3 exists only as n-type material. Even nominally undoped material is n type. This characteristic limits the application of In2O3 to the unipolar devices. A hybrid structure based on p-doped III-V semiconductors and In2O3 opens the possibility of realization of bipolar devices. This work presents the gas-source molecular-beam epitaxy growth of Be doped InAs on In2O3(111). In2O3 films with high crystalline quality were grown by PA-MBE on Y-stabilized ZrO2(111) wafers. The InAs layers were grown at different growth conditions and temperatures. According to the x-ray analysis InAs in all samples has zinc-blende structure and with increasing growth temperature the InAs film grows epitaxially and it changes from polycrystalline to monocrystalline.

HL 107.5 Thu 17:00 P1

First principles investigation of influence of point defects on the magnetic properties of zinc ferrite — •Waheed A. Adeagbo[1], Sanjeev K. Nayak[1], Martin Hoffmann[1,2], Arthur Ernst[2,3], and Wolfram Hergert[1] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, Halle, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany — [3]Wilhelm-Ostwald-Institut für Physikalishe und Theoretishe Chemie, Universität Leipzig, Leipzig, Germany

We investigate the role of point defects (vacancies and impurities) in inducing local ferromagnetic order in $ZnFe_2O_4$, which is otherwise an antiferromagnetic system. Our studies are performed by the first-principles density functional theory using the VASP package with GGA and GGA+U. Lattice defects such as anion (V_O) and cation (V_{Fe}, V_{Zn}) vacancies and vacancy complexes (V_{Fe-O}, V_{Zn-O}), substitution of Mg at the tetrahedral Zn site and the interstitial Fe at the empty tetrahedral site are some of the defects under our consideration. In a recent experimental work, by characterization of nanoparticles and thin films of $ZnFe_2O_4$ samples from XMCD measurements [1], it is deduced that V_O is responsible for enhancement of local ferromagnetic ordering. In a similar line, the influence of other defects on the magnetic properties of both normal and inverse spinel are of interest. The stability of the defects at different experimental growth conditions are estimated by analysis of the defect formation energies at various chemical potentials of the constituting elements in our calculations.
[1] C. E. Rodríguez Torres *et al.*, Phys. Rev. Lett. (2013) (submitted).

HL 107.6 Thu 17:00 P1

TEM and FIB-based EBIC investigations to study photovoltaic properties of a complex oxide pn-heterojunction — •Patrick Peretzki[1], Pablo Marín Perera[1], Benedikt Ifland[2], Daniel Mierwaldt[2], Philipp Saring[1], Christian Jooss[2], and

Michael Seibt[1] — [1]IV. Physikalisches Institut, Georg-August-Universität Göttingen, Germany — [2]Institut für Materialphysik, Georg-August-Universität Göttingen, Germany

The perovskite-structured p-doped manganite $Pr_{1-x}Ca_xMnO_3$ (PCMO) combined with n-doped $SrTi_{1-y}Nb_yO_3$ (STNO) is presently explored as a model system for manganite-based pn-heterojunctions. It is expected that the rapid thermalization of low-energy photoexcitated charge carriers can be quenched by making use of hot-polaron type correlated states with long lifetimes and/or long diffusion lengths, opening the possibility of converting a broad range of the solar spectrum. In this work, PCMO/STNO interfaces are investigated by Electron Beam Induced Current (EBIC) cross-section measurements by combining SEM-based EBIC with Focused Ion Beam preparation in dual beam instruments. As SEM-based EBIC is resolution-limited because of the probe size and the broad carrier generation volume, TEM lamellae are prepared from the material, which reduces the generation volume to a minimum and results in precise EBIC images of the PCMO/STNO interface. We thank the DFG for funding the research through CRC1073.

HL 107.7 Thu 17:00 P1

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

The phase diagram of $Zr_{1-x}Ce_xO_2$ has been investigated with Raman spectroscopy [1] but is still yet not fully understood. We perform DFT supercell calculations of $Zr_{1-x}Ce_xO_2$ for the different phases with different cerium concentrations. For each concentration we calculate supercells with different configurations. We present concentration dependent lattice constants, bandgaps and Raman spectra. All quantities are obtained by thermodynamic and statistic weighting.
[1] Yashima et al. J.Am. Ceram. Soc. 77 1067 (1994)

HL 107.8 Thu 17:00 P1

Ab-initio investigation of intermediate 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. Both are of great interest for applications as diverse as optoelectronics and electrochemistry. Electronically, the two oxides are quite different: 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. SnO_2 has been investigated in some depth both experimentally and theoretically, but SnO is less well-examined. Moreover, SnO disproportionates into Sn and SnO_2 at elevated temperatures, forming intermediate oxides of varying stoichiometry in the process. The preferred stoichiometries and crystal structures of these metastable phases are still unknown. In the present work, we use density functional theory (DFT) to determine and compare possible crystal structures as well as their stabilities relative to SnO and SnO_2 in order to suggest whether one of these structures might be grown experimentally. We also present calculations for the electronic structure of these intermediate oxides.

HL 107.9 Thu 17:00 P1

Growth and characterization of cuprous oxide thin films by chemical vapor deposition — Johannes Bieber, •Elisabeth A. Zolnowski, Gunther Haas, Yinmei Lu, Benedikt Kramm, Martin Becker, and Bruno K. Meyer — I. Physics Institute, Justus-Liebig-University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, DE-Germany

In the future all the forms of fossil energy will have to be replaced, due to the fact that these resources are limited. Solar cells have already been an important part of renewable energies, but to enlarge the competitiveness, they should be cheaper and more efficient than the present ones. A possible material which could comply with these requirements is cuprous oxide. It is a sustainable, cheap and nontoxic optoelectronic p-type semiconductor with a direct band gap of about 2.1 eV. It has been predicted that Cu_2O is promising for solar cell applications, with a theoretical energy conversion efficiency of 20%. Therefore we tried to optimize the growth of cuprous oxide thin films by chemical vapor deposition (CVD) and investigated their crystalline, electrical and optical properties under different growth conditions, respectively.

HL 107.10 Thu 17:00 P1

Optical spectroscopy of doped Cu_2O thin films — •Julian Benz[1], Philipp Hering[1], Torsten Henning[1], Uwe Kaiser[2], Wolfram Heimbrodt[2], Bruno K. Meyer[1], and Peter J. Klar[1] — [1]I. Physikalisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, 35392 Gießen — [2]Department of Physics and Material Sciences Center, Philipps-University of Marburg, Renthof 5, 35032 Marburg, Germany

Although the semicondutcing nature of cuprous oxide (Cu_2O) is already known since the early 20th century, little research was done besides studies of its excitonic properties. Recently the interest in Cu_2O, as a sustainable material, revived due to its potential use in photovoltaics. Here we report on the influence of doping on the optical properties of Cu_2O. We investigated series of RF sputtered thin films of Cu_2O doped with nitrogen and hydrogen, respectively. The photoluminesence (PL) of the samples was measured in a temperature range from 4 K to 300 K. The spectra will be interpreted with respect to the electrical properties. Furthermore the lifetime of the defect related luminescence was studied by means of time resolved PL spectroscopy. The results obtained are compared with those of a mechanical polished, natural Cu_2O single crystal.

HL 107.11 Thu 17:00 P1

High-quality SnO_2 thin films grown by chemical vapor deposition — •Yinmei Lu, Martin Becker, Benedikt Kramm, Johannes Bieber, Jie Jiang, Angelika Polity, and Bruno Meyer — 1. Physics Institute, Justus-Liebig-University Giessen, Germany

SnO_2 films with thicknesses of 10 - 1800 nm were deposited on c-sapphire, r-sapphire and quartz glass substrates with or without a SnO_2 buffer layer via chemical vapor deposition (CVD), using SnI_2 powder and oxygen gas as source materials, and at substrate temperatures ranging from 300 to 800 °C. The crystal structure and morphology of the films were studied by X-ray diffraction (XRD) and scanning electron microscopy (SEM), respectively, which reveal a high crystallinity of films with a smooth and homogeneous surface. For the ultra-thin films grown on c sapphire, the XRD rocking curve of SnO_2 (200) diffraction showed a small full width at half maximum (FWHM) of 0.02° (72 arcsec), indicating an almost perfect epitaxial growth of SnO_2 on c-sapphire. Optical properties of the films with different thicknesses were compared via transmittance measurements, which reveal thickness-dependence of the band gaps of the films. Both secondary ion mass spectrometry (SIMS) and X-ray photoelectron spectroscopy (XPS) were used to examine the composition and element states of the films. Electrical the properties of the films grown under different oxygen flows were investigated with Hall effect measurements. At room temperature, the Hall mobility, carrier density, and resistivity are in the ranges of (2.31 - 41.39) cm^2/Vs, (0.902 - 41.4)$\cdot 10^{18}$ cm^{-3} and (6.09 $\cdot$ 10^{-3} - 2.99) Ωcm, respectively.

HL 107.12 Thu 17:00 P1

Nitrogen doping in SnO_2 thin films grown by chemical vapor deposition — •Jie Jiang, Yinmei Lu, Johannes Bieber, and Bruno Meyer — 1. Physics Institute, Justus-Liebig-University, Giessen, Germany

As a direct band gap semiconductor, tin oxide (SnO_2) is a promising candidate for constructing next generation ultraviolet light emitting diodes (LEDs) and photodetectors, due to its large band gap of 3.6 eV, high exciton binding energy of 130 meV, and high carrier mobility of about 250 cm^2/Vs at room temperature. An essential step to fabricate SnO_2-based optoelectronic devices is to obtain high quality p-type SnO_2 films. Nitrogen is theoretically predicted to be an excellent p-type dopant in SnO_2 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 SnO_2. For this reason, we deposit the N-doped SnO_2 thin films on c-sapphire and r-sapphire substrates via chemical vapor deposition (CVD), using SnI_2 powder and NO_2 (or NH_3) gas as source materials. The crystal structure, morphology, electrical properties and optical properties of the films were measured and investigated by X-ray diffraction (XRD), scanning electron microscopy (SEM), Hall effect measurements and transmittance measurements, respectively.

HL 107.13 Thu 17:00 P1

three dimensional character of the near-E_F band of cleaved In_2O_3(111) single crystals — •valentina scherer[1], christoph janowitz[1], zbigniew galazka[2], and recardo manzke[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung,

Max-Born-Straße 2, 12489 Berlin, Germany

The near-E_F band of the in situ cleaved (111) surface of high quality n-type In_2O_3 single crystals obtained from the melt was investigated by high-resolution ARPES along major symmetry lines of the Brillouin zone. Several criteria to pin down Fermi level crossings and Fermi momenta were applied. To good approximation the near-E_F band is of three-dimensional character in momentum space and simply monitors the dispersion of the bottom of the conduction band bent below the Fermi energy. The results are explained without explicit reference to two-dimensional models by the assumption of a degenerate semiconductor due to high n-type doping ($n = 1.3 \times 10^{18} cm^{-3}$).

HL 107.14 Thu 17:00 P1

Electronic and optical properties of Ga_2O_3 — •Jürgen Furthmüller and Friedhelm Bechstedt — IFTO, FSU Jena, Max-Wien-Platz 1, D-07743 Jena, Germany

We present *first-principles* calculations of the electronic structure and optical properties of the monoclinic β-Ga_2O_3 phase which is the only stable polymorph under ambient conditions. In addition, we also study the metastable rhombohedral α-Ga_2O_3 (corundum-type) structure and compare the properties of the two polymorphs. Quasi-particle band structures on G_0W_0 level and excitonic spectra on BSE level are presented. It is demonstrated that these two polymorphs of Ga_2O_3 differ mainly in their optical anisotropies. Isotropically averaged optical properties and in particular densities of states look quite similar. This can also be shown for more complicated polymorphs on DFT level (where a treatment on GW and BSE level is imposible).

HL 107.15 Thu 17:00 P1

A spectroscopic comparison of AOS thin films and TCO single crystals — •Jörg Haeberle[1], Diana Gaspar[2], Pedro Barquinha[2], Stephan Machulik[3], Christoph Janowitz[3], Zbigniew Galazka[4], and Dieter Schmeisser[1] — [1]Angewandte Physik/Sensorik, Brandenburgische TU Cottbus-Senftenberg,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]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstraße 15, 12489 Berlin, Germany — [4]Leibnitz-Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Germany

Amorphous oxide semiconductors (AOS) and transparent conductive oxides (TCO) are today one of most attractive fields of research in many industrial products, like e.g. high definition, low cost, transparent, and flexible displays. We got the unique possibility to measure a-GIZO and a-SnOx thin films and compare their electronic properties with those of In2O3, Ga2O3, ZnO, and SnO2 single crystals. We use resPES to study the electronic properties. We report on the core levels, the VB PES data, partial Integrated Yield (pIY) and the XAS absorption data. From these we are able to derive the elemental ratio, the pDOS as well as the band scheme. At the O1s resonance we observe multiple Auger processes from which we deduce that a band of localized defect states is located between the Fermi energy and the CBM. The resonant profiles taken at the corresponding metal edges indicate that metal states are involved in the DOS.

HL 107.16 Thu 17:00 P1

3ω thermal conductivity measurements of $\beta - Ga_2O_3$ bulk crystal — •Martin Handwerg, Christine Bülow, Rüdiger Mitdank, and Saskia F. Fischer — Neue Materialien, Institut f. Physik, Humboldt-Universität zu Berlin, D-10099 Berlin

Ga_2O_3 belongs to the group of transparent conducting oxides with scarce information about thermal and electric properties. Here, the thermal conductivity λ of a $\beta - Ga_2O_3$ bulk-crystal is determined by using the 3ω-method. Therefore, a lineheater in 4 point geometry is placed above the crystal. An AC-heating current causes an increase of the temperature followed by an increasing heater resistance. The rising temperature generates an AC-signal with three times the frequency of the input current. This 3ω-voltage depends on the input frequency, which is related to the thermal penetration depth. In a common measurement setup a thermal penetration depth up to 1 mm below the heater can be reached. The thermal conductivity is calcuated by the slope of $U_{3\omega}(\ln f)$ and the heater parameters [1].

As a result of the $U_{3\omega}$ measurements of an 1 mm thick Ga_2O_3 [100] crystal the thermal conductivity was determined for a temperature interval between 4.2 K and 300 K. The temperature-dependent behaviour of the thermal conductivity fits with the theoretic explanations for insulators. Comparing the $U_{3\omega}$-method for thermal conductivity measurments at room temperature with optical methods there are consistent results with $\lambda = 13.6\,\mathrm{Wm^{-1}K^{-1}}$.

[1] D. Cahill *et al*, Physical Review B **35** (1987)

HL 107.17 Thu 17:00 P1

Structural and electrical investigations of Si-doped $(In_xGa_{1-x})_2O_3$ thin films — •Anna Werner, Stefan Müller, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Semiconductor Physics Group, Institut für Experimentelle Physik II, Leipzig, Germany

For the realization of solar-blind photodetectors the semiconductor β-Ga_2O_3 is due to the large band gap E_g of 4.9 eV especially suitable. Alloying β-Ga_2O_3 with indium allows to decrease E_g significantly and allows to control E_g and makes wavelength-selective photo detectors feasible. In this contribution we present structural and electrical properties of $(In_xGa_{1-x})_2O_3$ thin films grown by pulsed laser deposition on c-plane saphire substrate in dependence of the alloy composition. For our investigations we used a wafer having a continuous composition spread. The In content varies between $x = 0.008 - 0.69$. Additionally the wafer is doped with 0.1% silicon to improve the electric conductivity. The lateral composition gradient was realized by ablating a segmented PLD target [1]. The thin film has monoclinic crystal structure and is (-201) oriented. The incorporation of In increases the spacing between (-201) planes. Transmission measurements exhibit a decrease of E_g with increasing In content. We investigated the properties of Schottky contacts fabricated in front-front geometry on a stripe of the wafer containing the complete range of In compositions. For that we used reactively sputtered PdO_x Schottky contacts and determined their characteristic parameters in dependence on the In content.

[1] H. von Wenckstern *et al.*, CrystEngComm. **15**, 10020 (2013)

HL 107.18 Thu 17:00 P1

Electrical characterization of Si-doped β-Ga_2O_3 thin films grown by pulsed laser deposition — •David Diering, Florian Schmidt, Stefan Müller, Daniel Splith, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Abteilung Halbleiterphysik, Linnéstraße 5, 04103 Leipzig

Its large band gap of 4.9 eV makes β-gallium oxide (Ga_2O_3) an auspicious candidate for high power electronics and transparent optoelectronic devices. In order to investigate the electrical properties of β-Ga_2O_3 thin films we have applied current-voltage (I-V) characterization and space-charge spectroscopic methods (C-V, AS, TAS, DLTS) to Schottky contacts (SCs). The thin films have been grown by pulsed laser deposition at approx. 650 °C and an oxygen partial pressure of 10^{-3} mbar. Using Ga_2O_3 targets with 0.1 wt% and 1 wt% SiO_2 the thin films have been fabricated on c-plane sapphire substrates and (00.1) ZnO/ZnO:Ga templates. The SCs have been formed by DC sputtering of Cu. The temperature dependent measurements have been conducted in the temperature range from 10 K to 330 K. First TAS measurements indicate a defect state with a thermal activation energy of $E_t = 216$ meV with an apparent capture cross-section $\sigma_a = 7 \times 10^{-17}\,\mathrm{cm^2}$.

HL 107.19 Thu 17:00 P1

Raman scattering in $(In,Ga)_2O_3$ thin films — •Christian Kranert, Christian Dähne, Jörg Lenzner, Holger von Wenckstern, Rüdiger Schmidt-Grund, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Semiconductor Physics Group, Leipzig, Germany

Raman scattering in the $(In,Ga)_2O_3$ material system greatly benefits from excitation with ultraviolet (UV) laser light. For pure β-Ga_2O_3 and Ga-rich alloys with the same crystal structure, the increased scattering cross section due to the high photon energy enhances the feasibility of Raman measurements carried out on thin films with thicknesses down to 100 nm or even less. In case of pure In_2O_3, resonant excitation near the band gap enables the observation of most Raman active modes, which have not yet been reported.

In this contribution, we make use of the above mentioned advantages of UV excitation to characterize the $(In,Ga)_2O_3$ material system by Raman scattering. We present the dependence of the energy of several phonon modes on the indium concentration in the Ga-rich β-phase. The obtained results allow a precise determination of the composition based on the Raman spectrum. We further give the energy and symmetry of previously not observed phonon modes in bixbyite-type In_2O_3. These show a distinct sensitivity to the growth parameters. Conse-

quently, UV Raman scattering appears to be a promising method for the characterization of such films.

HL 107.20 Thu 17:00 P1

NIR-VUV dielectric function of $(In,Ga)_2O_3$ thin film with lateral composition spread — •Hannes Krauss, Tammo Böntgen, Holger von Wenckstern, Jörg Lenzner, Rüdiger Schmidt-Grund, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Leipzig, Germany

We present the dielectric function spectra of $(In,Ga)_2O_3$ in the full composition range obtained by means of spectroscopic ellipsometry. By model analysis of the experimental data using parametric model dielectric function approaches 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. A clear red shift of the transition energies with increasing In content is found.

The $(In,Ga)_2O_3$ thin film with compositional spread was deposited on 2" *a*-plane sapphire substrates by means of pulsed laser deposition. A two-fold segmented target was used where one half was pure Ga_2O_3 and the other In_2O_3. Target and substrate were then rotated synchronously to facilitate a continues gradient of the Ga/In ratio on the substrate [1].

[1] H. von Wenckstern *et al.*, CrystEngComm **15**, 10020 (2013).

HL 107.21 Thu 17:00 P1

Properties of MIS-diodes based on Si-doped β-Ga_2O_3 — •Anna Reinhardt, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Semiconductor Physics Group

In the field of high-power electronics gallium oxide (Ga_2O_3) has a tremendous potential for future power device applications due to its large bandgap of 4.9 eV and its theoretically high breakdown field of about 8×10^8 V/m. For the development of Ga_2O_3-based power devices such as metal-insulator-semiconductor field-effect transistors (MISFET) the realization of MIS-diodes is essential.

We present our results on MIS-diodes deposited on silicon doped β-Ga_2O_3 thin films fabricated using pulsed-laser deposition. The electrical properties of the MIS-diodes were varied via the dielectric thickness and the oxygen partial pressure during contact deposition. Current-voltage measurements (IV) reveal leakage current densities of down to 10^{-9} Acm^{-2}. In order to determine the dielectric constant of the insulator we performed quasi-static capacitance-voltage measurements. Furthermore, the possible origin of conduction through the insulator is investigated by means of temperature-dependent IV-measurements.

HL 108: Poster: Ultra-fast phenomena / Optical properties / Semiconductor laser / Devices and device concepts

Time: Thursday 17:00–20:00 Location: P1

HL 108.1 Thu 17:00 P1

Laserinduced heating of nanocrystalline graphene monitored by Ultrafast Electron Diffraction — Silvio Morgenstern[1], Christian Gerbig[1], •Xaver Holzapfel[1], Christan Sarpe[1], Arne Senftleben[1], Matthias Wollenhaupt[2], and Thomas Baumert[1] — [1]University of Kassel, Institute of Physics and Center of Interdisciplinary Nanostructure Science and Technology (CINSaT), D-34132 Kassel, Germany — [2]University of Oldenburg, Institute of Physics, D-26111 Oldenburg, Germany

Ultrafast Electron Diffraction (UED) has lately become one of the most promising techniques to directly provide insights into fundamental dynamics in solids at the microscopic level and on the pico- to subpicosecond timescale [1,2].

In this contribution we present our UED-setup to reach a high spatial and temporal resolution below 200 fs [3]. Additionally we present first results of time-resolved diffraction experiments on nanocrystalline graphene [4] and discuss the possibility of time-resolved observations of out-of-plane dynamics in such materials [5]. Finally we compare our results to results from CVD-graphene [6].

[1] A. H. Zewail, J. Phys. Chem. 98, 2782-2796 (1994)
[2] B. Siwick & D. Miller, Science 302, (5649), 1382-1385 (2003)
[3] C. T. Hebeisen, Opt. Letters Vol. 31, No. 23, 3571 (2006)
[4] A. Truchanin, ACS Nano Vol. 5, No. 5, 3896 (2011)
[5] J. C. Meyer, Nature 446, 60-63 (2007)
[6] M. Schäfer, New J. Phys. 13, 063030 (2011)

HL 108.2 Thu 17:00 P1

Resolution studies on a compact femtosecond transmission electron diffractometer and phonon decay in single crystalline graphite — Christian Gerbig[1], Silvio Morgenstern[1], •Marlene Adrian[1], Christian Sarpe[1], Arne Senftleben[1], Matthias Wollenhaupt[2], and Thomas Baumert[1] — [1]University of Kassel, Institute of Physics (CINSaT), D-34132 Kassel, Germany — [2]University of Oldenburg, Institute of Physics, D-26111 Oldenburg, Germany

Time-resolved diffraction, using x-ray or electron probes, has become a promising technique to directly provide insights into dynamics at the molecular level with ultrafast precision [1]. We study dynamical processes in single crystalline graphite by means of ultrafast electron diffraction in order to expand the understanding of phonon generation and decay mechanisms being essential for future carbon based electronic devices [2]. Our highly compact DC electron diffractometer is fully characterized by experiments and N-body simulations. At balanced conditions a temporal resolution of 200 fs along with high-definition diffraction is achieved for dynamical studies on graphite single crystals in a maintainable measurement time [3]. We further present generation and decay processes of incoherent as well as coherent phonons in graphite as a function of film thickness down to few-layer graphene.

[1] M. Chergui and A. H. Zewail, Chem. Phys. Chem. 10, 28 (2009).
[2] T. Kampfrath et al., Phys. Rev. Lett. 95, 187403 (2005).
[3] C. Gerbig et al., submitted (2013).

HL 108.3 Thu 17:00 P1

Towards Nonlinear Phononics, probing acoustic phonon wave packets with X-ray and visible light — •Andre Bojahr[1], Matthias Gohlke[2], Marc Herzog[3], Daniel Schick[1], Peter Gaal[4], and Matias Bargheer[1,4] — [1]Institut für Physik und Astronomie, Universität Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam/Golm, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [4]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Wilhelm-Conrad-Röntgen Campus, Albert-Einstein-Str. 15, 12489 Berlin, Germany

We use ultrashort visible and hard X-ray pulses as a real-time probe of the occupation of phonon modes constituting large amplitude phonon wave packets. These time-domain Brillouin scattering experiments permit the time-resolved observation of the phonon dynamics including phonon damping and nonlinear interaction. High strain fields lead to nonlinear phenomena like sum and difference-frequency mixing, which depend strictly on the shape of the excited phonon wave packet. Via multiple pumping of an epitaxially grown metal transducer film on a SrTiO3 substrate we generate spectrally narrow phonon wave packets. The nonlinear evolution such a wave packet can be understood by difference and sum-frequency mixing of its spectral components, explaining the amplitude dependent damping of phonon wave packets. Our measurements are supported by calculations of a nonlinear masses and springs model, which describes the experiments quantitatively.

HL 108.4 Thu 17:00 P1

Incoherent Phonon Heating Model derived from the system Hamiltonian — •Messan Afande, Eeuwe S. Zijlstra, and Martin E. Garcia — Theoretische Physik, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

The purpose of the current work is the derivation of the equation of motion of atoms in solid state materials with emphasis on incoherent phonon heating. The modeling is based upon the application of the Ehrenfest theorem by considering the overall system Hamiltonian, in particular, including electron-phonon interactions. In the following, it is planned to integrate the derived model into an ab initio Molecular Dynamics simulation code for studying lattice vibrations in solid state

materials after femtosecond-laser excitation.

HL 108.5 Thu 17:00 P1

Formation and hybridization of Bloch and plasma oscillations — •Klaus Morawetz — Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics (IIP), Avenida Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — Max-Planck- Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Using a conserving relaxation-time approximation an analytic formula is derived which describes the time dependence of the dielectric function in a plasma created by a short intense laser pulse with an additional external electric field bias. This formula reproduces universal features of the formation of collective modes seen in experimental data of femtosecond spectroscopy (Phys. Rev. B 72 (2005) 233203). Due to the electric field Bloch oscillations in a semiconductor are created which form a hybridization with plasma oscillations. This short-time expansion of lower-order quantum perturbation theory can be used to describe the dynamics of strongly correlated classical systems (Phys. Rev. E 66 (2002) 022103).

HL 108.6 Thu 17:00 P1

Terahertz two-photon quantum well infrared photodetectors — •Carsten Franke[1,2], Harald Schneider[1], and Martin Walther[3] — [1]Helmholtz-Zentrum Dresden-Rossendorf — [2]TU Dresden — [3]Fraunhofer IAF Freiburg

Two-photon quantum well infrared photodetectors (QWIPs) are nonlinear detectors for the investigation of ultrashort pulses in the mid-infrared and THz-regime. In these devices the photocurrent shows a quadratical dependence on the intensity of the incoming radiation which is useful in autocorrelation experiments.

We are currently investigating two-photon QWIPs based on the GaAs/AlGaAs material system with an aluminum content lower than 5% in the barrier, which leads to intersubband absorption energies below 25 meV.

Here we present results of interferometric autocorrelation experiments performed with the free-electron laser FELBE at photon energies of 15 to 25 meV.

HL 108.7 Thu 17:00 P1

Optical characterization of CuI films — •Katharina Rudisch, Friedrich-Leonhard Schein, Gabriele Benndorf, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Fakultät für Physik und Geowissenschaften, Institut für Experimentelle Physik II, Linnéstraße 5, 04103 Leipzig

CuI is a transparent semiconductor with a wide band gap of 3.1eV. It features intrinsic p-conductivity and a large exciton binding energy that make it attractive for future semiconductor applications [1].

We have produced CuI thin films by exposing sputtered copper thin films on glass substrates to iodine vapour until CuI was formed. From X-ray diffraction measurements of the CuI film a cubic zincblende crystal structure could be confirmed. For a characterization of optical properties of CuI, photoluminescence and transmission measurements were performed from 2K to room temperature. Low temperature emission spectra exhibit transitons of free and bound excitons and donor acceptor pair recombinations with phonon coupled transitions. In transmission spectra a splitting of the light and heavy hole excitonic transitions is observed at low temperatures and discussed in terms of crystal structure.

[1] M. Grundmann, F.-L. Schein, M. Lorenz, T. Böntgen, J. Lenzner und H. von Wenckstern, phys. stat. sol. (a) 210(9), 1671-1703 (2013)

HL 108.8 Thu 17:00 P1

Parametric scattering in a multimode polariton system — •Rüdiger Schmidt-Grund[1], Christof P. Dietrich[1], Tom Michalsky[1], Robert Johne[2], Paul Eastham[3], Helena Franke[1], Chris Sturm[1], Martin Lange[1], and Marius Grundmann[1] — [1]Universität Leipzig, Institut für Experimentelle Physik II, Leipzig, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [3]Trinity College Dublin, Dublin, Ireland

We present the observation of parametric scattering of whispering gallery mode exciton-polaritons in a ZnO micro-wire resonator at low temperature. In this geometry, in contrast to a planar microcavity, many polariton modes exist, and furthermore the ground state is energetically well separated from the exciton energy. In this complex many-mode system, we observe the formation of a polariton Bose-Einstein condensate with some special features. First, it is resonantly fed by the radiative decay of defect bound excitons and secondly it appears in polariton branches energetically close to this defect bound exciton state. By increasing the excitation power, the occupation of this initial state becomes very high and a parametric scattering process sets in. Thereby, a relaxation of the condensed polaritons into states with lower energy and higher momentum occurs. The experimental findings are in good agreement with theoretical simulations taking into account polariton-polariton scattering in a multi-mode system.

HL 108.9 Thu 17:00 P1

Time-resolved photo-ellipsometry studies of exciton-polaritons in a planar ZnO-based microcavity — •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 are composite quasi-particles which arise from strong coupling between excitons and photons. They inherit exciton spin as well as light polarization which both are expressed by means of the pseudospin of a polariton ensemble. The pseudospin is subject to various effective magnetic fields whereof one in particular can be related to population imbalances of polariton states with different pseudospin orientation.

We present investigations of the exciton-polariton pseudospin in a planar microcavity. The influence of the occupation of the lower polariton branch on the evolution of the eigenmode polarization is studied using pulsed laser excitation combined with time-resolved ellipsometry. Ellipsometry probes the density of states (DOS) while the combination with photoluminescence allows to deduce the dependence of the DOS on the states' occupation. Furthermore, despite non-resonant excitation, the polarization of the laser can influence the occupation as well. The consequences are examined.

The planar microcavity consists of a $\lambda/2$ layer of ZnO with a slight thickness gradient. The splitting between the TE- and TM-polarized eigenmodes has values of up to 20meV for 37° emission angle while the detuning between exciton and cavity photon energy is negative.

HL 108.10 Thu 17:00 P1

Influence of metal layers on the optical properties of Bragg reflectors — •Merle Cornelius[1], SK. Shaid-Ur Rahman[1], Tim Schönfeld[2], Thorsten Klein[2], Carsten Kruse[2], Detlef Hommel[2], Jürgen Gutowski[1], and Katrin Sebald[1] — [1]Institute of Solid State Physics, Semiconductor Optics, University of Bremen, P.O. Box 330440, 28334 Bremen, Germany — [2]Institute of Solid State Physics, Semiconductor Epitaxy, University of Bremen, P.O. Box 330440, 28334 Bremen, Germany

Polaritons being generated in a planar microcavity structure by strong light-matter interaction can be controlled and manipulated through an additional lateral confinement applied. This can result in an increase of their relaxation probability being highly advantageous for polariton lasers. Such a confinement can be achieved by a metal grating on top of the upper distributed Bragg reflector (DBR) of the planar microcavity since in this case, Tamm plasmons, being photon modes localized at the interface, can be optically generated. Their excitation results in a change of the cavity photon energy and thus in a lateral polariton confinement. In this contribution we report on the influence of metal layers with different thicknesses on the optical properties of DBRs grown by MBE and consisting of ZnMgSSe as high-index material and a superlattice consisting of MgS/ZnCdSe as low-index material. The metal layers, being gold or silver stripes with thicknesses between 40 nm to 60 nm, were generated by lithography. By performing reflectivity measurements changes of the spectral position of the DBR oscillations as well as of the center of the stopband are analyzed.

HL 108.11 Thu 17:00 P1

Design and fabrication of acoustic devices in ZnO/SiO2 planar microcavities — •Jakov Buller[1], Odilon D. D. Couto Jr.[2], Edgar A. Cerda-Méndez[1], Sander Rauwerdink[1], Abbes Tahraoui[1], and Paulo V. Santos[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]Universidade Estadual de Campinas, Campinas, Brazil

Optical resonances in semiconductor microcavities (MC) have been exploited to enhance the light emission from single emitters, while surface acoustic waves (SAWs) have been used to modulate the band gap of semiconductor nanostructures. In this work, we investigate the acousto-optical effects in planar ZnO/SiO2 MCs rf-sputtered on sapphire. The sample design is based on numerical calculations which

show that: (i) the refractive index contrast of ZnO and SiO2 leads to high optical confinement; (ii) the piezoelectricity of ZnO enables the electric generations of SAWs for modulation of the MC resonance.

The fabricated two types of MCs consisting of a $\lambda/2$ active region spacer sandwiched by $\lambda/4$ ZnO/SiO2 distributed Bragg mirrors (DBRs). In the first one, the $\lambda/2$ spacer consists of an electron beam resist (HSQ). SEM measurements demonstrate successful resist planarisation, leading to homogeneous cavity spacers. In the second type, the upper DBR is mechanically glued on the lower one, thus forming air-gap MCs. Reflectivity measurements in MCs demonstrate quality (Q) factors of up to 2000, which are in reasonable agreement with transfer-matrix calculations. The process allows the insertion of light emitters into the MC active region and their manipulation by SAWs.

HL 108.12 Thu 17:00 P1

Time-resolved spectroscopy of defect luminescence in aluminium nitride — •Tristan Koppe, Oliver Beck, Hans Christian Hofsäss, and Ulrich Vetter — II. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

We report on defect luminescence studies in HPHT synthesized or epitaxial grown aluminium nitride. The samples are excited with a femtosecond laser system at various UV-wavelengths and the luminescence is collected with a Streak Camera in the wavelength range of 200-800 nm at different time scales with a temporal resolution up to 20 ps. A special focus is drawn on the temperature dependence of intensity and lifetime in a range between 12 K and room temperature.

HL 108.13 Thu 17:00 P1

The importance of an absolutely calibrated confocal photoluminescence setup — •Hendrik Sträter, Rudolf Brüggemann, Niklas Nilius, and Gottfried H. Bauer — Carl von Ossietzky Universität Oldenburg, Institut für Physik, D-26111 Oldenburg

Photoluminescence (PL) measurements provide a contact-less method to determinate the opto-electronic properties of a semiconductor and its potential as solar cell absorber material. From the recorded PL-spectrum it is possible to extract the integrated PL yield, splitting of quasi-Fermilevels (QFL), optical threshold, Urbach energy, and subgap absorption. Especially the QFL-splitting is an important quantity, since it can be interpreted as the maximum open circuit voltage (V_{oc}), which can be achieved with a finally fabricated solar cell. Laterally resolved PL measurements are a powerful tool to determine fluctuations of the opto-electronic properties and correlations between the opto-electronic properties. Up to now it is often assumed that a spectrally calibrated PL setup is sufficient for determination of the variation of the QFL-splitting. This contribution shows that this is not always the case and that fluctuations of the QFL-splitting and all quantities correlated to it heavily depend on the absolute calibration function of the PL setup. A mathematical framework is presented which proves that even small deviations from the ideal calibration function can lead to arbitrary wrong results. Simulated and experimental PL results give an idea of the outcome of a wrong calibrated PL setup and a possible solution to the problem is presented.

HL 108.14 Thu 17:00 P1

Controlled lasing from active optomechanical resonators — •Thomas Czerniuk[1], Christian Brüggemann[1], Jan Tepper[1], Sebastian Brodbeck[2], Christian Schneider[2], Martin Kamp[2], Sven Höfling[2], Boris Glavin[3], Dimitri Yakovlev[1,4], Andrey Akimov[4], and Manfred Bayer[1] — [1]Experimentelle Physik 2a, TU Dortmund, Dortmund, Germany — [2]Technische Physik, Universität Würzburg, Würzburg, Germany — [3]V. E. Lashkaryov Institute of Semiconductor Physics, Kiev, Ukraine — [4]A. F. Ioffe Physical-Technical Institute, Russian Academy of Sciences, St. Petersburg, Russia

We report an effective emission intensity modulation of a microcavity laser (VCSEL) with frequencies of up to 40 GHz at room temperature. We investigate a planar microcavity laser, whose active medium are GaAs quantum wells while the DBRs are built out of alternating layers of AlAs/GaAlAs. Due to the acoustic impedance mismatch of these material system, the DBRs possess not only optical, but also acoustic resonances. In a laser with such an optomechanical resonator, the interaction between the three excitations -photons, phonons and excitons- is drastically enhanced, providing control of the emission intensity: by injecting a broadband strain pulse into the cavity, the long living resonant phonon modes are excited. For different delays between strain pulse injection and pulsed optical excitation of the VCSEL, the emission intensity is monitored. The result shows prominent oscillations with frequencies corresponding to the acoustic resonances of the optomechanical device.

HL 108.15 Thu 17:00 P1

Toward high-power passively mode-locked VECSELs in the red spectral range — •Grizelda Kersteen, Roman Bek, 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

Research during the past decade focusing on semiconductor saturable absorber mirrors (SESAMs) and vertical external-cavity surface-emitting lasers (VECSELs) has been extremely thorough in optimizing pulse duration and output power in the infrared region. However, in 2013 our group could realize the first mode-locked VECSEL in the red spectral range emitting sub-250 fs pulses with a repetition rate of 836 MHz at around 664 nm. Due to the plane diamond heatspreader bonded onto the gain structure, side pulses appear reducing the peak power.

In this contribution, we present different approaches for improvements of this first setup. To suppress the Fabry-Pérot etalon induced side pulses, we use an anti-reflection coated wedged diamond instead. The effect of an increased repetition rate on the mode locking operation is investigated by reducing the cavity length. Furthermore, we investigate different gain and absorber structures containing quantum dots instead of quantum wells inside. These provide more flexibility concerning both the gain and the absorber properties such as temperature behavior and saturation fluence.

HL 108.16 Thu 17:00 P1

Harmonically self-mode-locked vertical-external-cavity surface-emitting laser — •Mahmoud Gaafar[1], Christoph Möller[1], Matthias Wichmann[1], Bernd Heinen[1], Bernardette Kunert[2], Arash Rahimi-Iman[1], Wolfgang Stolz[1], and Martin Koch[1] — [1]Material Sciences Center and Department of Physics, Philipps-Universität Marburg, Marburg D-35032, Germany — [2]NAsP III/V GmbH, Am Knechtacker 19, Marburg D-35041, Germany

We present a sesam-free harmonically mode-locked vertical-external-cavity surface-emitting laser. Mode-locking is initiated by introducing a slit near to the high reflective end mirror of our Z-shaped laser cavity. Beside single pulse operation we observed second as well as third harmonic mode-locking for higher pump powers. Our system features pulse durations penetrating the femtosecond regime at a wavelength of 1014 nm.

HL 108.17 Thu 17:00 P1

Non-heating losses and thermal resistance of VECSELs — •Dalia Al Nakdali[1], Mohammad Khaled Shakfa[1], Bernd Heinen[1], Bernardette Kunert[2], Wolfgang Stolz[1], Stephan W. Koch[1], Jörg Hader[3], Jerome V. Moloney[3], Arash Rahimi-Iman[1], and Martin Koch[1] — [1]Faculty of Physics and Material Sciences Center, Philipps-University of Marburg, Renthof 5, 35032 Marburg, Germany — [2]NAsP-III/V GmbH., Am Knechtacker 19, 35041 Marburg, Germany — [3]College of Optical Sciences, University of Arizona, Tucson, Arizona 85721, USA

Optically-pumped vertical-external-cavity surface-emitting lasers (VECSELs) have recently received much attention due to their potential for application in scientific and industrial fields. Particularly, they are promising for continuous-wave (cw) high power operation. However, only a considerable improvement of the thermal management allows us to obtain cw VECSEL output-powers in excess of 100 W. Besides heating losses, non-heating power losses need to be analyzed for a deeper understanding of power-limiting factors in a VECSEL and for the improvement of its performance. In our present work, a standard V-cavity VECSEL configuration is employed. Input-output characteristics are recorded for different plane out-coupling mirrors and for varying heat sink temperatures. Here, we take into account optical-scattering losses to improve a theoretical model from which we extract the VECSEL-chips thermal resistance as well as its scattering coefficient from experimental input-output characteristics.

HL 108.18 Thu 17:00 P1

Microintegrated Laser Systems at 767 nm and 780 nm — •Kai Lampmann[1,2], Max Schiemangk[1,2], Erdenetsetseg Luvsandamdin[1], Andreas Wicht[1], Achim Peters[1,2], Götz Erbert[1], Günther Tränkle[1], and The LASUS Team[1,2,3,4] — [1]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztech-

nik, Berlin — [2]Institut für Physik, HU Berlin — [3]Institut für Quantenoptik, LU Hannover — [4]Institut für Laserphysik, U Hamburg

We present hybrid integrated laser modules in the near infrared at wavelengths of 767 nm and 780 nm suitable for atom optic applications. For narrow linewidth emission with high optical output power in the Watt range, a master oscillator power amplifier (MOPA) concept is used. A distributed feedback semiconducter laser diode (DFB) serves as the master oscillator, which provides excellent spectral properties. The light is injected into a tapered amplifier (TA), which increases the output power while preserving the linewidth of the amplified light at the same time. The laser chips, microlenses and an optical isolator are integrated on an AlN substrate with a footprint of $10 \times 50\ mm^2$ using special positioning techniques with an accuracy better than 1 μm.

The LASUS project is supported by the German Space Agency DLR with funds provided by the Federal Ministry of Economics and Technology (BMWi) under grant numbers 50WM 1237 - 1240.

HL 108.19 Thu 17:00 P1

Continuous-wave operation of a buried-heterostructure quantum cascade laser — •Mikaela Elagin, Yuri V Flores, Sergii Kurlov, Anna Aleksandrova, Grygorii Monastyrskyi, Jan F Kischkat, Mykhaylo P Semtsiv, and W Ted Masselink — Humboldt University Berlin, Institute of Physics, Newtonstr.15, 12489 Berlin, Germany

We report the continuous wave (cw)-operation of a buried-heterostructure (BH) strain-compensated quantum cascade laser (QCL) using gas-source molecular beam epitaxy both for the growth of the active region as well as for the InP:Fe regrowth of the laser ridge sidewalls. Starting the InP:Fe regrowth directly on the sides of the laser ridge leads to a number of void defects which have a significant impact on heat extraction capabilities of devices. These defects are mostly located at the arsenide-phosphide interface between the active region and the regrown insulating material. Using a 20 nm-thin InAlAs layer between the laser ridge sidewalls and the InP:Fe insulating layers we improve the crystal quality of the interface while preserving the high electrical-resistivity of the overgrownmaterial. This optimized regrowth sequence has led to cw-operation in the 100-210 K temperature range of a 7 μm-wide BH-QCL with an emission wavelength of 5.4 μm. The measured thermal conductance in this temperature range is Gth = 1400-500 W/Kcm2, which is comparable with the state of the art BH-QCLs regrown using metal-organic vapor-phase epitaxy (MOVPE).

HL 108.20 Thu 17:00 P1

Impact of elastic- and inelastic scattering on the performance of quantum-cascade lasers — •Yuri V. Flores, Sergii S. Kurlov, Mikaela Elagin, Grygorii Monastyrskyi, Mykhaylo P. Semtsiv, and W. Ted Masselink — Department of Physics, Humboldt University Berlin, Newtonstr. 15, D-12489 Berlin, Germany

Elastic- and inelastic scattering are the principal components of the leakage current in quantum-cascade lasers. Their understanding is very important, since the leakage current has a considerable impact on the overall performance of quantum-cascade lasers. In particular, this current affects two vital characteristics: The threshold current and the quantum efficiency. A large leakage current reduces the injection efficiency into the upper laser state which implies that more electrons need to be injected into the device in order to achieve the required population inversion, increasing ultimately the threshold current and reducing the quantum efficiency.

In this contribution, we analyze the relative magnitudes of the elastic- and inelastic components of the leakage current. The inelastic part is modeled as a two-particle process involving an electron and a LO-phonon. The elastic non-radiative process considers that an electron can increase- or lose its potential energy due to the roughness of the layers' interfaces. These two components are modeled and its dependence on the lattice and electron-temperatures is analyzed.

HL 108.21 Thu 17:00 P1

Phenomenological model for simulation of mid-infrared quantum cascade lasers — •Sergii S. Kurlov, Yuri V. Flores, Mikaela Elagin, Mykhaylo P. Semtsiv, and W. Ted Masselink — Humboldt University Berlin, Institute of Physics, Newtonstrasse 15, D-12489 Berlin, Germany

A phenomenological scattering-rate model for THz quantum cascade lasers is extended for mid-infrared (MIR) quantum cascade lasers (QCLs) by accounting for the energy dependence of the intersubband scattering rate beyond the phonon energy. This energy dependence is obtained from the fit of the intersubband scattering rates based on published life-times of a number of MIR QCLs. The model is currently built under assumption of low temperature, i. e., neglecting the phonon absorption by charge carriers. Using the model and solving the rate equations with periodical boundary conditions we found a good agreement with a number of published MIR QCLs in terms of current-voltage-, power-current-, and spectral-gain-characteristics. We demonstrate the matching of the modelled results and the low-temperature experimental data for a broad-gain quantum cascade laser, where gain broadening with the current (voltage) is essential.

HL 108.22 Thu 17:00 P1

Characterization of Quantum Cascade Lasers in the Terahertz Regime — •Negar Hekmat[1,2], Hanond Nong[1], Shovon Pal[1,2], Michael Kwiatek[2], Arne Ludwig[2], Paul Dean[3], Edmund Linfield[3], Andreas D. Wieck[2], and Nathan Jukam[1] — [1]AG Terahertz-Spektroskopie und Technologie, Ruhr-Universität Bochum, Germany — [2]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Germany — [3]School of Electrical Engineering, University of Leeds, UK

Quantum cascade lasers (QCLs) are powerful radiation sources in mid- and far-infrared regions with potential applications in imaging, sensing and spectroscopy. QCLs are unipolar semiconductor devices based on intersubband transitions. The active region of the QCL is a periodic sequence of modules made of multiple quantum wells. The electrons are transported in a 'cascading' scheme where several photons are generated by a single electron. QCLs are often fabricated by Molecular Beam Epitaxy (MBE), which precisely controls the thickness of the quantum wells and barriers. Terahertz time domain spectroscopy (THz-TDS) was used to characterise a THz QCL operating at 2.26 THz. The GaAs/AlGaAs QCL was cleaved and mounted on a cryostat sample holder. The Current-Voltage characteristic of the QCL was investigated in the range of 10-70 K. The gain of THz QCL was also studied with and without radio frequency (RF) pulses. Gain clamping was observed when the RF pulse was off and the QCL was biased above threshold. However, with the RF pulse on and the QCL biased below threshold, the THz pulse amplitude through the QCL increased.

HL 108.23 Thu 17:00 P1

Sub-Monolayer-Control in Epitactic 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, Deutschland — [2]AG Terahertz-Spektroskopie und Technologie, Ruhr-Universität Bochum, Deutschland

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 on the QCL's layer structure. Therefore we want to investigate the time dependent growth rate change of the EC and apply countermeasures like aligned PID control parameters and/or an adapted shutter design.

HL 108.24 Thu 17:00 P1

Photocapacitance change in YMnO3-based MIFS in the visible light regime — •O S Choudhary[1], A Bogusz[1], L P Selvaraj[1], V John[1], D Bürger[1], I Skorupa[1], A Lawerenz[2], O G Schmidt[1,3], and H Schmidt[1] — [1]Faculty of Electrical Engineering and Information Technology, Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik GmbH, 99099 Erfurt, Germany — [3]Institute for Integrative Nanosciences, IFW Dresden, 01069 Dresden, Germany

YMnO3 is one of the few materials that exhibit ferroelectricity and antiferromagnetism. Metal-YMnO3-metal thin film structures can

be switched between a high resistance state (HRS) and a low resistance state (LRS), when a positive and negative writing bias is applied, respectively. This work investigates the effect of light-irradiation on the capacitance of YMnO3-based metal-ferroelectric-insulator-semiconductor (MFIS) structures. The DC bias for the capacitance measurements was swept from +10 to -20 V and back under different light-irradiation at a sweep rate of ca. 103 mV/s. It has been found that under dark conditions two nonvolatile capacitance minima exists at -11 and at -3.55 V, possibly when the YMnO3 is in the LRS and HRS state, respectively. If we rewrite the +10 and -20 V branch in shorter period of time then, low capacitance state (LCS) is non-volatile and pseudo volatile, respectively. Under illumination the capacitance at the two minima increases in the visible spectral range, depending on the wavelength illumination, YMnO3 thickness and YMnO3 capacitance state.

HL 108.25 Thu 17:00 P1

In-Plane-Gate transistors as gas sensors — •Benjamin Feldern, Arne Ludwig, and Andreas Wieck — Ruhr-Universität Bochum, Bochum, Deutschland

We propose In-Plane-Gate transistors [1] based on MBE grown GaAs/Al_xGa_{1-x}As heterostructures with etched trenches for the detection of gases and liquids[2] at the surface of our devices. Additionally the gases or liquids are to be irradiated with THz light for the excitation of resonant states of the molecules.

It is to be determined whether the structures are capable of analyzing the gases and liquids by their dielectric function. Different gases and liquids shall be analyzed using these structures and the THz radiation. Possible interaction with passivated surfaces shall be examined.

[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, "Fabrication of planar organic nanotransistors using low temperature thermal nanoimprint lithography for chemical sensor applications", Nanotechnology 21 075301 (2010).

HL 108.26 Thu 17:00 P1

GaAs nanowires based avalanche photo diodes — Stepan Shvarkov[1], •Wadim Quiring[2], Artur Zrenner[2], Arne Ludwig[3], Andreas Dirk Wieck[3], and Dirk Reuter[1] — [1]Optoelektronische Materialien und Bauelemente, Universität Paderborn, D-33098 Paderborn — [2]Optoelektronik und Spektroskopie an Nanostrukturen, Universität Paderborn, D-33098 Paderborn — [3]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum

Modern planar Si-based avalanche photo diodes (APD) show very high multiplication factors and low dark currents, which makes Si-based planar APDs a versatile detector for single photon detection (SPD). However, in the optical C-band (1.55 μm), these detectors cannot be used and planar APDs based on III-V semiconductors show rather high dark currents. This is a severe drawback for applications in quantum communications. APDs based on nanowires can be an approach to overcome this problem. In the current work we present GaAs nanowire APDs based on planar MBE growth. The nanowires are realized in several nanofabrication steps. First a lateral p-i-n junction is defined by implanting a nominally undoped GaAs layer on an $Al_{0.95}Ga_{0.05}As$ buffer layer with Be and Si. The length of the i-region is approximately 10 μm.By electron beam lithography and reactive ion etching nanowires are defined so that one end of the wire is lying in p- and another in n-type regions of the GaAs. The resulting devices show a clear rectifying current-voltage characteristic and allow for large reverse bias before breakdown. Under illumination a large internal amplification is observed, which is attributed to avalanche multiplication.

HL 108.27 Thu 17:00 P1

Transparent p-CuI/n-ZnO heterojunction diodes — •Friedrich-Leonhard Schein[1], Tammo Böntgen[1,2], Jörg Lenzner[1], Michael Lorenz[1], Holger von Wenckstern[1], and Marius Grundmann[1] — [1]Universität Leipzig, Fakultät für Physik und Geowissenschaften, Institut für Experimentelle Physik II, Linnéstraße 5, 04103 Leipzig, Germany — [2]present address: Laser Zentrum Hannover e.V., Hollerithallee 8, 30419 Hannover, Germany

We have investigated the wide bandgap (E_g = 3.1 eV) p-type semiconductor γ-copper(I)-iodide (CuI) [1,2] as an alternative candidate to p-type transparent semiconducting oxides like SnO [3] or $ZnCo_2O_4$ [4]. Two facile methods were used to fabricate CuI thin-films, either iodization of metallic Cu films or thermal evaporation of CuI powder. Hall-effect measurements of these transparent CuI films revealed a hole mobility of about $5-15\,cm^2/Vs$, a hole density of $(0.2-3)\times10^{19}\,cm^{-3}$ and a resistivity of $0.1-0.2\,\Omega$cm. Atomic force and scanning electron microscopy as well as X-ray diffraction and optical transmission measurements of CuI on glass substrates and on c-ZnO will be discussed.

Heterostructures consisting of p-CuI on pulsed-laser deposited n-ZnO were fabricated on a-sapphire substrates and characterized electrically. The diodes showed large rectification ratios $I_f/I_r > 10^7$ at ±2 V and ideality factors down to 1.5.

[1] F.-L. Schein *et al.*, Appl. Phys. Lett. **102**, 092109 (2013).
[2] M. Grundmann, Phys. Status Solidi A **210**, 1671 (2013).
[3] E. Fortunato *et al.*, Appl. Phys. Lett. **97**, 052105 (2010).
[4] F.-L. Schein *et al.*, IEEE Electron Device Lett. **33**, 676 (2012).

HL 108.28 Thu 17:00 P1

ZnO-based inverter as biosensors — •Agnes Holtz, Fabian Klüpfel, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Fakultät für Physik und Geowissenschaften, Abteilung Halbleiterphysik, Linnéstr. 5, 04103 Leipzig

Transparent semiconducting oxides find application as switching transistor within active-matrix displays. Another interesting field of application is the integration of such transistors within multi electrode biosensor arrays. These can be used to measure the change of membrane potential of externally stimulated nerve cells cultivated on the transparent amplifier. This would permit to synchronously study the nerve cells visually and electrically providing means to establish connections between the arrangement of cells and their "communication" behavior. The inverter amplifies the cell signals directly at the measurement electrodes. This might result in a higher signal-to-noise ratio due to the short path between electrode and amplifier. The ZnO layer was deposited by pulsed-laser deposition on a-plane sapphire substrate. We compared inverters comprising field effect transistors with different gate materials such as Au, PtO_x or $ZnCo_2O_4$. The epoxy based photo resist SU 8 was used to encapsulate the chip against the elektrolyte. The inverters were characterized electrically by IU and frequency dependent measurements at room temperature. The maximal slope we measure is 80. We use simple inverters consisting of two transistors because of the high amplification and the low space requirements. To ensure measuring at the point of highest amplification of the inverter characteristics an external amplifier circuit was developed.

HL 108.29 Thu 17:00 P1

Optical gas sensing by micro-photoluminescence on single ZnO nanowires — •Julian Jakob, Manfred Madel, Sebastian Bauer, Florian Huber, and Klaus Thonke — Institute of Quantum Matter / Semiconductor Physics Group, Ulm University

Nanostructures are very promising candidates for gas sensing applications due to their high surface to volume ratio. Adsorption of oxidative and reductive gases causes a typical band bending near the surface, which leads to a change in the thickness of the depletion layer. In micro-photoluminescence measurements this results in a change of the emission intensity when switching between different ambient gas atmospheres.

An improvement of the sensitivity could be achieved by the use of different metal catalysts evaporated onto the nanowire surface. Investigations of single nanowires enable conclusions of the effect of nanowire form and diameter, and the sensitivity relating to different gas-atmospheres.

HL 108.30 Thu 17:00 P1

Fast read and write operations in quantum dot-based memory devices — •C. Pillich[1], D. Zhou[1], A. Beckel[1], D. Bimberg[2], T. Nowozin[2], M. Geller[1], and A. Lorke[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany — [2]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Self-assembled quantum dots (QDs) are ideally suited as building blocks for memory devices. Large localization energies enable long information storage and times up to 1.6 s at room temperature have already been demonstrated.[1]

Here we use a memory structure with a layer of QDs as floating gate in a high electron mobility transistor (HEMT). The HEMT is used to prepare and read the charge information of the QDs filled with 0, 2 or up to 6 electrons each, with single charging state resolution.[2]

In comparison with conventional flash memory, high bandwidth

capability for writing and reading operations is desirable. Here we demonstrate read-out times down to 3 ns at a temperature of $T = 4$ K and the capability of writing the information by hot charge injection, which can be used to enhance the ratio between writing and storage times.

[1] A. Marent et al., Appl. Phys. Lett. **91**, 242109 (2007).
[2] B. Marquardt et al., Appl. Phys. Lett. **95**, 22113, (2009).

HL 108.31 Thu 17:00 P1

Low-density InP-based quantum dots emitting at 1.5 μm telecom wavelength range — •Matusala Yacob, Johann Peter Reithmaier, and Mohamed Benyoucef — Institute of Nanostructure Technologies and Analytics (INA), Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Germany

Self-assembled semiconductor quantum dots (QDs) can be used as building blocks of quantum information processing. For this application low density circular QDs operating in the telecom wavelength bands should be realized. The InP material system is a possible candidate to achieve this goal due to its low lattice mismatch (3.2%) to the InAs QD material. In this work, low-density InAs QDs are grown using post-growth annealing on AlGaInAs surfaces lattice matched to InP by solid-source molecular beam epitaxy. The dots are then covered with an AlGaInAs layer using a special capping procedure. Spatially separated largely sized QDs with a surface dot density of 5 dots per square μm are obtained using this technique. Optimized QD structures grown on a distributed Bragg reflector exhibit single QD emission at around 1.5 μm with a narrow excitonic linewidth below 50 μeV.

HL 109: Ultra-fast phenomena I

Time: Friday 9:30–10:45 Location: POT 006

HL 109.1 Fri 9:30 POT 006

Visualization of ultrafast currents in nanowires by imaging with femtosecond low-energy electron pulses — •Melanie Müller, Alexander Paarmann, and Ralph Ernstorfer — Fritz-Haber-Institut der MPG, Berlin, Germany

We use a nanotip as laser-triggered low-energy electron point source (LEEPS) delivering coherent ultrashort electron pulses for time-resolved projection imaging of photoexcited nanostructures. Due to their high sensitivity to weak fields, low-energy electron pulses are particularly suited for mapping transient electric fields and charge distributions in nanostructures. Specifically, charge carrier separation upon above-bandgap excitation in doped nanowires (NWs) transiently induces local variations of the vacuum level, deflecting the electrons from their original trajectories. Operating our LEEPS microscope in a pump-probe scheme, we are able to probe ultrafast photocurrents in axially doped InP NWs with several 10 nm spatial and femtosecond temporal resolution.

HL 109.2 Fri 9:45 POT 006

Ultrafast charge carrier and exciton dynamics at the SP6/ZnO(10-10) interface — •Laura Foglia[1], Mino Kris Sparenberg[2], Fritz Henneberger[2], Julia Stähler[1], and Martin Wolf[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland — [2]Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Germany

The efficiency of hybrid organic inorganic devices depends strongly on the timescale of competing electronic processes, such as interfacial charge transfer and bulk exciton decay. These typically ultrafast timescales can be accessed by pump-probe techniques, where a pump laser pulse initially excites the system and the change of electronic or optical properties is probed by a second laser pulse, as a function of time delay. We apply broadband transient transmission spectroscopy to investigate the carrier dynamics at the interface between ZnO and a spirobifluorene derivative, SP6. The system is first excited at 3.6 eV (across the SP6 HOMO-LUMO and ZnO band gap) and subsequently the transmission in the visible range (1.7-2.9 eV) is monitored. In this manner the excited state absorption is probed by changes in the polarization due to the evolution of the electronic population in both the SP6 LUMO and ZnO conduction band. First results show subpicosecond dynamics, much shorter than the exciton dynamics previously observed by time-resolved photoluminescence.

HL 109.3 Fri 10:00 POT 006

Long-Lived Electronic Coherence in the Metal-Organic-Hybrid Cobalt/Alq3 — Martin Aeschlimann[1], Tobias Brixner[2], Mirko Cinchetti[1], Norman Haag[1], Matthias Hensen[3], Bernhard Huber[2], Christian Kramer[2], Walter Pfeiffer[3], •Martin Piecuch[1], Christian Strüber[3], and Philip Thielen[1] — [1]Fachbereich Physik and Research Center OPTIMAS, Technische Universität Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern, Germany — [2]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [3]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany

The coherent electron dynamics in optically pumped (400 nm excitation) molecular states of the metalorganic complex tris(8-hydroxyquinolinato)aluminium (Alq3) deposited on cobalt is investigated by coherent two-dimensional nanoscopy [1]. Upon excitation with sequences of ultrashort pulses at 800 nm quantum beats appear in the time-resolved photoemission signal. In two-dimensional nanoscopy spectra two excited electronic states are identified with an energy spacing of about 77 meV. Their linewidth are 11 meV and 48 meV, respectively, corresponding to coherence lifetimes of about 370 fs and 87 fs. The appearance of such narrow spectral features indicates that electronic excitations in an individual adsorbate state can be surprisingly long and thus can play an important role in determining charge transfer efficiencies at the metal-hybrid interface.

[1] Aeschlimann et al. Science 333, 1723-1726, (2011)

HL 109.4 Fri 10:15 POT 006

Atomistic Modeling of Excitation Energy Transfer in a Semiconductor Nanocrystal Molecule Hybrid System — •Dirk Ziemann and Volkhard May — Institut für Physik, Newtonstr. 15, Humboldt Universität zu Berlin, D-12489 Berlin, Germany

Inorganic organic hybrid systems can show completely new properties that are not achievable by each material alone. Especially photovoltaic devices like solar cells and light emitting diodes are able to benefit from these properties. Corresponding to these devices semiconductor nanocrystals interacting with organic molecules have aroused great interest. Despite the variety of experimental investigations there is a lack of theoretical studies.

In this talk an efficient model for describing energy transfer on an atomistic level between a CdSe semiconductor nanocrystal and a molecular system consisting of Pheophorbide-a molecules is presented. Despite the modeling of nanocrystals consisting of thousands of atoms also the coupling to a supramolecular complex is shown. For the nanocrystal also surface effects are taken into account and the formation of exciton states is considered.

HL 109.5 Fri 10:30 POT 006

Passively carrier-envelope phase stabilised few-cycle laser pulses in the near-infrared — •Jörg Robin, Jan Vogelsang, Kristina Strahlendorff, Petra Gross, and Christoph Lienau — Institut für Physik, Carl von Ossietzky Universität, Carl-von-Ossietzky-Straße 9-11, 26129 Oldenburg

The acceleration dynamics of strong-field-emitted electrons from sharp metallic nano-tips sensitively depend on the carrier-envelope phase (CEP) of the incident few-cycle laser pulses [1]. Stabilising the CEP [2] thus is a step towards controlling the coherent electron motion on ultrashort time and length scales. Focussing 120-fs pulses centred at 800 nm from a regenerative titanium:sapphire chirped pulse amplification system operating at a repetition rate of 5 kHz into a sapphire crystal generates a white light continuum, which inherits the CEP of the driving pulses. Out of this spectrum both a broadband proportion in the visible and a narrowband proportion in the infrared are parametrically amplified in a non-collinear setup using the second harmonic of the driving pulses as pumping radiation. By recombining the output of these two stages via type II difference frequency generation shot-to-shot CEP fluctuations cancel out and passively CEP-stabilised

pulses tunable in a range from 1400 nm to 1800 nm with a pulse duration of 10 fs and a pulse energy of 200 nJ are produced. Here, we demonstrate the CEP stability of our system and show its importance for the electron motion around metallic nanostructures.

[1] Piglosiewicz, B. et al. Nature Photonics (2013). doi:10.1038/nphoton.2013.288
[2] Manzoni, C. et al. Opt. Lett. 29, 2668 (2004)

HL 110: Invited Talk Irene Burghardt

Time: Friday 9:30–10:00 Location: POT 051

Invited Talk HL 110.1 Fri 9:30 POT 051

Quantum dynamics of exciton migration and dissociation in functional organic polymer materials — •Irene Burghardt — Institut f. Physik. u. Theor. Chemie, Goethe Universität Frankfurt

As highlighted by recent experiments, elementary processes in organic photovoltaics can be guided by quantum coherence, despite the presence of electron-phonon coupling and static and dynamic disorder. We present quantum dynamical studies of these processes using the Multi-Configuration Time-Dependent Hartree (MCTDH) method, focusing on (i) the dynamics of exciton migration across a torsional defect that locally breaks the π-conjugation in oligo-(p-phenylene vinylene) type fragments [1], and (ii) exciton dissociation in oligothiophene-fullerene donor-acceptor complexes [2,3], i.e., models of P3HT-PCBM heterojunctions. Here, the primary exciton break-up is found to occur within 50-100 fs and exhibits a pronounced oscillatory decay profile, reflecting vibronic coherence [2]. Furthermore, rapid free carrier generation from the interfacial charge transfer (CT) state is feasible, due to an effective lowering of the Coulomb barrier as a result of charge delocalization, along with the vibronically hot nature of the primary CT state [3].

[1] R. Binder, J. Wahl, S. Römer, I. Burghardt, Faraday Discuss. 163, 205 (2013), A. N. Panda, F. Plasser, A. Aquino, I. Burghardt, H. Lischka, J. Phys. Chem. A, 117, 2181 (2013) [2] H. Tamura, R. Martinazzo, M. Ruckenbauer, I. Burghardt, J. Chem. Phys., 137, 22A540 (2012); H. Tamura, I. Burghardt, M. Tsukada, J. Phys.Chem. C, 115, 9237 (2011) [3] H. Tamura, I. Burghardt, J. Phys. Chem. C, 117, 15020 (2013), J. Am. Chem. Soc. (Comm.), 135, 16364 (2013).

HL 111: Graphene: Bi- and multi-layers (with MA/O/TT)

Time: Friday 9:30–11:00 Location: POT 081

HL 111.1 Fri 9:30 POT 081

Atomistic simulations of dislocations in bilayer graphene — •Konstantin Weber[1], Christian Dolle[2], Florian Niekiel[2], Benjamin Butz[2], Erdmann Spieker[2], and Bernd Meyer[1] — [1]Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg — [2]Center for Nanoanalysis and Electron Microscopy, FAU Erlangen-Nürnberg

The atomic structure and the properties of basal-plane dislocations in bilayer graphene, the thinnest imaginable crystal that can host such 1D defects, has been investigated by atomistic simulations based on the registry-dependent potential of Kolmogorov and Crespi [1] and the classical AIREBO potential.

Our calculations show that the dislocations lead to a pronounced buckling of the graphene bilayers in order to release strain energy, leading to a complete delocalization of the residual compressive/tensile strain in the two graphene sheets [2]. Furthermore, the absence of a stacking-fault energy, a unique peculiarity of bilayer graphene, gives rise to a splitting of the dislocations into equidistant partials with alternating Burgers vectors [2]. Thus, dislocations in bilayer graphene show a distinctly different behavior than corresponding dislocations in graphite or other 3D crystals.

[1] A. Kolmogorov, V. Crespi, *Phys. Rev. B* **71**, 235415 (2005).
[2] B.Butz, C. Dolle, F. Niekiel, K. Weber, D. Waldmann, H.B. Weber, B. Meyer, E. Spieker, *Nature*, (2013) (accepted for publication).

HL 111.2 Fri 9:45 POT 081

Study of the magnetoresistance of biased graphene bilayers — •Dmitri Smirnov[1], Galina Y. Vasileva[1,2], Yurij B. Vasilyev[2], Pavel S. Alekseev[2], Yurij L. Ivanov[2], Hennrik Schmidt[1], Alexander W. Heine[1], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover — [2]Ioffe Physical Technical Institute, Russian Academy of Sciences, St. Petersburg

We demonstrate magnetotransport behaviour of bilayer graphene. In contrast to monolayer graphene, bilayer has a parabolic band structure with a zero band gap, which can be opened by applying an electrical field perpendicular to the samples [1]. One of the consequences of such a band structure is the coexistence of two different types of charge carriers with the Fermi energy placed near the charge neutrality point.

Several bilayer graphene samples with different electrical properties (charge neutrality point, mobility) have been investigated. A positive and negative magnetoresistance is observed for electrons and holes. We can show that that the positive magnetotransport can be described well with a two carrier Drude model which allows us a new approach to probe parameters of electrons and holes separately.

[1] McCann, E., and V. Fal'ko Phys. Rev. Lett. 96, 086805 (2006)

HL 111.3 Fri 10:00 POT 081

Transport in Dual Gated Encapsulated Bilayer Graphene — •Jonas Hesselmann[1], Stephan Engels[1,2], Bernat Terrés[1,2], Kenji Watanabe[3], Takashi Taniguchi[3], and Christoph Stampfer[1,2] — [1]JARA-FIT and II. Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan

Bilayer graphene (BLG) is a promising material which combines superior electronic properties like high charge carrier mobilities with the possibility of opening a band gap. The band gap can be induced by applying a perpendicular electric field resulting in a gap in the order of a few 10 meV. This makes BLG a possible candidate for future nanoelectronic applications. Here, we present the fabrication and low temperature (T=2K) transport measurements of dual gated BLG which is encapsulated in hexagonal boron nitride serving as an atomically flat gate dielectric. We show that the investigated devices exhibit mobilities of up to 80.000 cm^2/Vs. Quantum Hall effect measurements show a distinct sequence of Hall plateaus together with a full symmetry breaking of the eightfold degenerate zero Landau level. By temperature dependent measurements we investigate the energy gap opening as function of a perpendicular electric field. We find that the transport via localized states at low temperatures exhibits a strong asymmetric behavior with respect to the sign of the applied electric field while the temperature activated transport is fully symmetric.

HL 111.4 Fri 10:15 POT 081

An emergent momentum scale and low energy theory for the graphene twist bilayer. — •Sam Shallcross, Nicolas Ray, Dominik Weckbecker, and Oleg Pankratov — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

We identify an angle dependent *momentum scale* as the fundamental property of a bilayer composed of mutually rotated graphene layers [1]. This leads to (i) a numerical method that increases, for the twist bilayer, the efficiency of the standard tight-binding method by a factor of $\approx 10^3$, at no loss of accuracy, and (ii) a low energy theory that can be deployed, without distinction, for both the low angle regime and the large angle regime. In the low angle regime this leads to a theory that is close to that of Bistritzer *et al.* [2], but differs in the choice of momentum scale. In the large angle this approach yields electronic versions of the Hamiltonians first derived on symmetry grounds by Mele [3]. We use these low energy approaches to give an overview of the $T = 0$ electronic properties of the twist bilayer system, with a

particular focus on the localization of electrons, mixing of single layer graphene states by the interaction, and low energy density of states features.

[1] S. Shallcross, S. Sharma, and O. Pankratov, *Phys. Rev. B* **87**, 245403, 2012.
[2] R. Bistritzer and A. H. MacDonald. *Proc. Natl Acad. Sci.*, **108:12233**, 2010.
[3] E. J. Mele. *Journal of Physics D Applied Physics*, **45:154004**, 2012.

HL 111.5 Fri 10:30 POT 081

RKKY interaction in the AB stacked graphene bilayer: interstitial impurities and a diverging propagator. — •Nicolas Klier, Sam Shallcross, and Oleg Pankratov — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

The interaction between spin polarised impurities in graphene displays a number of novel features that arise both from the valley degree of freedom that graphene possesses, as well as the linearly vanishing density of states at the Dirac point [1,2]. Multilayer graphene systems offer both the possibility of realistic interstitial (i.e., interlayer) impurities, as well as novel electronic features. In particular, the Bernal stacked (AB) bilayer exhibits low energy (chiral) bands as well as high energy bonding and anti-bonding bands. We demonstrate that at the bonding to anti-bonding *gap edge* there is an logarithmic divergence $\log(E - E_g)$ in the propagator on one sublattice, with E the energy and E_g the energy of the bonding to anti-bonding gap (0.38 eV). This leads to a number of dramatic consequences for the RKKY interaction, most notably: (i) a $R^{-5/2}$ impurity interaction at the gap edge, and, (ii) for interstitial impurities a discontinuous change in the Fermi surface spanning vector that drives the RKKY at the gap edge. We further derive the finite temperature behaviour of this system on the basis of finite temperature perturbation theory.

[1] M.Sherafati, and S.Satpathy, Phys. Rev. B 84, 125416, 2011.
[2] F.Parhizgar, and M.Sherafati, and R.Asgari, and S.Satpathy, Phys. Rev. B 87, 165429, 2013.

HL 111.6 Fri 10:45 POT 081

Conductivity of two-dimensional charge carriers with non-parabolic dispersion — Bretislav Sopik[1], Janik Kailasvuori[2,3], and •Maxim Trushin[4] — [1]Central European Institute of Technology, Masaryk University, Kamenice 735, 62500 Brno, Czech Republic — [2]International Institute of Physics, Universidade Federal do Rio Grande do Norte, 59078-400 Natal-RN, Brazil — [3]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany — [4]University of Konstanz, Fachbereich Physik, M703 D-78457 Konstanz

We investigate the conductivity of two-dimensional charge carriers with the non-parabolic dispersion k^N with N being an arbitrary natural number assuming the delta-shaped scattering potential as a major source of disorder. We employ the exact solution of the Lippmann-Schwinger equation to derive an analytical Boltzmann conductivity formula valid for an arbitrary scattering potential strength. We proceed further with a numerical study based on the finite size Kubo formula which assesses the applicability range of our analytical model. We find that for any $N > 1$, the conductivity demonstrates a linear dependence on the carrier concentration in the limit of a strong scattering potential strength. This finding agrees with the conductivity measurements performed recently on chirally stacked multilayer graphene [1] where the lowest two bands are non-parabolic and the adsorbed hydrocarbons might act as strong short-range scatterers.

[1] L. Zhang, Y. Zhang, J. Camacho, M. Khodas I. Zaliznyak, Nature Physics **7**, 953-957 (2011).

HL 112: Energy materials: CIGS and related photovoltaics

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

HL 112.1 Fri 9:30 POT 112

Depleted heterojunction solar cells with $CuInS_2$ and ZnO nanocrystals - optical modeling and electrical characterization — •Dorothea Scheunemann, Sebastian Wilken, Jan Keller, Michael Richter, Ingo Riedel, Holger Borchert, and Jürgen Parisi — 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. Here, we study the potential of $CuInS_2$ nanocrystals (NCs) as a relevant alternative to the toxic Pb or Cd compounds for usage in depleted heterojunction solar cells. Two different layer stacks, based on a bilayer heterojunction between CIS and ZnO NCs, were investigated by means of high resolution electron microscopy and optical modelling. We applied variable-angle spectroscopic ellipsometry to derive the optical constants of the involved layers. These data served as input parameters into optical simulations in order to estimate light absorption in the individual layers of the device stack with the transfer matrix formalism. Here, we present the simulated data in comparison with experimental results. Furthermore, we studied the dependence of the current-voltage characteristics, as well as the external quantum efficiency on illumination conditions, i.e., the presence of UV light.

HL 112.2 Fri 9:45 POT 112

Application of S^{2-} stabilized $CuInS_2$ nanocrystals in inorganic and hybrid organic/inorganic nanocrystal solar cells — •Christopher Krause, Rany Miranti, Dorothea Scheunemann, Holger Borchert, and Jürgen Parisi — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, 26129 Oldenburg

Semiconductor nanocrystals have attracted much attention for application in inorganic/organic hybrid solar cells as well as all-inorganic solar cells during past years. $CuInS_2$ (CIS) nanocrystals are especially promising for solar cell application because of their absorption extending into the near infrared region, providing a suitable overlap with the solar spectrum. The nanocrystals prepared by colloidal synthesis are usually stabilized by long-chained organic molecules hampering the charge transport between adjacent nanocrystals and the charge transfer between donor and acceptor in hybrid devices. To overcome this problem the nanocrystal surface can be exchanged by inorganic ligands, like S^{2-}-ions. These ligands are small, facilitating charge transport and provide electrostatic stabilization of the colloidal solution. In this contribution I will present the application of S^{2-} stabilized CIS nanocrystals in inorganic/organic hybrid solar cells as well as all-inorganic nanocrystal solar cells.

HL 112.3 Fri 10:00 POT 112

EDX - measurements on lamellae of CIGSe solar cells — •Sven Schönherr, Alexander Kusch, Philipp Schöppe, Michael Oertel, Udo Reislöhner, and Carsten Ronning — Institut für Festkörperphysik, Friedrich Schiller Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

$Cu(In, Ga)Se_2$ solar cells were processed in a sequential process. First, a multi-layer system containing copper, indium and gallium on top of a molybdenum back contact was deposited by DC - magnetron sputtering with different Ga profiles. Afterwards, the metallic precursor was reactively annealed in two steps in a selenium vapour atmosphere where it converted to an about 2 μm thick CIGSe absorber layer. Completing the solar cell, a CdS buffer layer was deposited via chemical bath deposition and as front contact a ZnO layer was sputtered on top. From these cells lamellae with a thickness of about 200 nm were prepared using a focused ion beam (FIB) system. The thin cross sections lead to a high spatial resolution which is mainly limited by the diameter of the electron beam. Energy dispersive X-ray spectroscopy measurements were taken at lamellae with different sputtered Ga profiles in the precursors and annealed with different selenization temperatures in the first annealing step.

HL 112.4 Fri 10:15 POT 112

X-ray fluorescence on $Cu(In,Ga)Se_2$-lamellas — •Philipp Schöppe[1], Alexander Kusch[1], Michael Oertel[1], Claudia Sarah Schnohr[1], Andreas Johannes[1], Stefanie Eckner[1], Manfred

Burghammer[2], and Carsten Ronning[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]European Synchrotron Radiation Facility, B.P. 220, F-38043 Grenoble Cedex, France

Compositional and structural properties of the absorber affect significantly the efficiency of Cu(In,Ga)Se_2 solar cells. The integral composition is commonly determined using X-ray fluorescence (XRF) with high resolution. However, the absorber is typically inhomogeneous and thus there is a particular interest in collecting information from defined spatial regions in the nanometer range. Hence, XRF mapping with an X-ray beam diameter of approximately 200 to 300 nm was used to investigate cross sections of Cu(In,Ga)Se_2 solar cells. In order to implement this improved spatial resolution in the measurement, thin lamellas were prepared using a focused ion beam. Best results were obtained using a lamella thickness of about 250 nm. This enabled us to determine quantitatively the depth dependent composition of the absorber, particularly the Ga gradient, and its spatial distribution.

HL 112.5 Fri 10:30 POT 112

Impact of Gallium on chemical gradients in Cu(In,Ga)Se_2 thin film solar cells grown on flexible polyimide substrate — •Stefan Ribbe[1,2], Andreas Rahm[1], Frank Bertram[2], and Jürgen Christen[2] — [1]Solarion AG, Ostende 5, 04288 Leipzig, Germany — [2]Institute for Experimental Physics, Otto-von-Guericke-Universität Magdeburg, Germany

Cu(In,Ga)Se_2(CIGS) thin film solar cells on polyimide substrate receive a high interest for many applications due to its flexibility and weight-lightness. Lower growth temperatures - a requirement of using polyimide substrate - are a challenge for producing high efficiency CIGS material. In particular the proper adjustment of the vertical gallium gradient directly affects amongst other properties the collection of photogenerated carriers.

CIGS layers were grown on flexible polyimide foil by using an ion-beam assisted roll-to-roll process. Sodium was provided by an additional source of NaF during the three-stage process to ensure high conversion efficiency. Gallium content was varied by the growth rate controlled by XRF (x-ray fluorenscence).

Lateral microscopical fluctuations of the GGI (Ga/(Ga+In)-ratio) and changes of the vertical gallium gradient within the CIGS absorber layers have been studied by highly spatially resolved cathodoluminescence microscopy (CL) at low temperature (T = 5K). Spectral Linescans on cross sections directly show a change of a smooth vertical gradient to a discontinuous shift of the peak wavelength in dependence of the gallium content in the CIGS layers

HL 112.6 Fri 10:45 POT 112

Band alignment at the In_2S_3/Cu(In,Ga)(S,Se)$_2$ interface in thin-film solar cells — •Dirk Hauschild[1], Katharina Treiber[1], Stephan Pohlner[2], Robert Lechner[2], Jörg Palm[2], Clemens Heske[3,4,5,6], Lothar Weinhardt[3,5,6], and Friedrich Reinert[1] — [1]Experimental Physics VII, University of Wuerzburg, Germany — [2]AVANCIS GmbH & Co. KG, Munich, Germany — [3]Institute for Photon Science and Synchrotron Radiation, KIT, Germany — [4]Department of Chemistry, University of Nevada, Las Vegas (UNLV) — [5]Institute for Chemical Technology and Polymer Chemistry, KIT, Germany — [6]ANKA Synchrotron Radiation Facility, KIT, Germany

Both on laboratory scale as well as in large area industrial production, Cu(In,Ga)(S,Se)$_2$ (CIGSSe) based solar cells have been processed for many years with a CdS buffer layer between absorber and transparent front contact, using a chemical bath deposition process. However, CdS is toxic and therefore its usage increases the production and recycling costs. A substitution of CdS by In_2S_3 provides a Cd-free alternative that can be integrated in a dry inline production. The In_2S_3/CIGSSe interface has been investigated using ultraviolet (UPS) and X-ray photoelectron spectroscopy (XPS), as well as inverse photoemission (IPES). The combination of these techniques allows the determination of the conduction and valence band extrema and reveals a complete picture of the band alignment at the In_2S_3/CIGSSe interface. In this contribution we will compare the band alignments with and without tempering of the In_2S_3/CIGSSe interface structure and discuss the implications for the performance of the device.

Coffee break (15 min.)

HL 112.7 Fri 11:15 POT 112

Transient photoluminescence investigations on meta-stable Cu(In,Ga)Se2 thin-film solar cells and absorbers — •Viktor Gerliz, Stephan Heise, Jörg Ohland, Jürgen Parisi, and Ingo Riedel — Carl von Ossietzky University of Oldenburg, Germany

Light soaking and dark annealing can significantly affect the device performance of Cu(In,Ga)Se2 (CIGSe) thin film solar cells. Depending on the conditioning time we observe considerable improvements of the device performance in effect of thermal stress at 90°C under simulated AM1.5 illumination as reflected in an increased open circuit voltage (Voc) and doping concentration (ND). Contrarily, dark annealing of devices results in an opposed trend until a relaxed state is reached. It can be speculated that the conditioning has also impact on the minority carrier decay kinetics. Thus, we studied the time-resolved photoluminescence (TR-PL) decay for CIGSe solar cells and CdS-passivated CIGSe absorbers which were light-soaked/annealed for different conditioning times. Based on our results we discuss the change of Voc and ND of completed CIGSe solar cells with respect to the corresponding TR-PL decay characteristics

HL 112.8 Fri 11:30 POT 112

Investigation of contact barriers of co-evaporated Cu(In,Ga)Se_2 and Molybdenum — •Nils Neugebohrn, Maria S. Hammer, Jürgen Parisi, and Ingo Riedel — Energy and Semiconductor Research Laboratory, Department of Physics, University of Oldenburg, 26111 Oldenburg, Germany

Cu(In,Ga)Se_2 (CIGSe) solar cells have recently reached a record efficiency of 20,8%. Nevertheless, the electronic properties of the back contact which forms between CIGSe and molybdenum are poorly understood. For this interface Schottky-type as well as ohmic behavior has been reported previously. In particular, the intermediate $MoSe_2$ layer which forms between the absorber and the metal during growth of the CIGSe layer determines the contact characteristics and might be critical for the device performance. The energy band alignment at the CIGSe/$MoSe_2$/Mo interfaces depends on the growth conditions and material properties (absorber composition, Na-content of the absorber and Mo). In this study Au/CIGSe/$MoSe_2$/Mo samples have been prepared via etching of the ZnO/CdS window layer of the complete cell and subsequent deposition of Au contacts on top of the CIGSe layer. To study a potential barrier-induced current limitation we performed temperature-dependent current-voltage measurements between 80 and 300 K. We observed an exponential dependence of the injection current indicating the presence of a contact barrier. The barrier height is determined by employing the thermionic emission model. Based on these results we will discuss the location of this barrier, e.g. at the CIGSe/MoSe2 or at the $MoSe_2$/Mo interfaces.

HL 112.9 Fri 11:45 POT 112

Systematic investigation of the influence of intentionally created shunts on the cell performance of CIGS-thin film solar cells by lock-in thermography — •Finn Babbe, Jan Keller, Ingo Riedel, Jörg Ohlad, and Jürgen Parisi — Energy- and Semiconductor Research Laboratory, Department of Physics, University of Oldenburg

The efficiency of thin film solar cells and modules can be considerably reduced by local shunts, which may have been introduced in the production process. The corresponding output losses are diverse and depend on the properties of the defect (e.g. the distance to patterning lines). To investigate the effect of its position, size and shape artificial shunts were systematically prepared with a focused ion beam. This method allows the introduction of a broad variety of defined shunt structures in the micrometer range to realize different shunt configurations. The impact of the shunts was studied by lock-in thermography. Applying this technique the local heat (power) dissipation in the modified regions, caused by illumination or bias voltage excitation, was imaged and quantified. The aim of this work is to correlate the heat signatures to the output performance (especially the open circuit voltage and shunt resistance) of CIGS solar cells.

HL 112.10 Fri 12:00 POT 112

Simulation of temperature dependent admittance spectra of Cu(In,Ga)(Se,S)2 solar cells and interpretation of capacitance steps — •Michael Richter[1], Christian Schubbert[1], Patrick Eraerds[2], Jürgen Parisi[1], Ingo Riedel[1], Thomas Dalibor[2], and Jörg Palm[2] — [1]Energy and Semiconductor Research Laboratory, Department of Physics, University of Oldenburg, Carl-von-Ossietzky-Strasse 9-11, 26129 Oldenburg, Germany — [2]AVANCIS GmbH, Otto-Hahn-Ring 6, 81739 Munich, Germany

Reproducing the complex electronic device response of Cu(In,Ga)(Se,S)2 thin film solar cells by comprehensive numerical modeling is a feasible way to gain information about the device physics. Based on extensive material and device characterization we built up a simulation model that reflects not only room-temperature measurements of the current voltage and quantum efficiency but also temperature dependent admittance spectra in the temperature range from 130 K to 330 K. The individual contributions to the device admittance could be assigned to the carrier freeze out, relaxation of defects located in the bulk and in the space charge region. One dominant signature, commonly termed N1 signature, is ascribed to a second depletion region formed by a valence-band barrier at the Cu(In,Ga)(Se,S)2/Mo(Se,S)2 interface. The latter assumption is further evidenced by the correlation of the N1 signature with the roll-over behavior in temperature dependent current-voltage measurements. Furthermore, simulation of sulfur content fluctuations at the back region of the absorber shows the dependence of the roll-over on back contact properties.

HL 112.11 Fri 12:15 POT 112

Comparative study of different extraction methods of diode parameters of chalcopyrite solar cells — •Jose Fabio Lopez Salas, Jan Keller, and Ingo Riedel — Laboratory for Chalcogenide Photovoltaics (LCP), Energy and Semiconductor Research Laboratory, Department of Physics, University of Oldenburg

The current-voltage (IV) characteristics of solar cells are typically described by Shockley's equation. Here, the ideality factor n and saturation current density J_0 determine the properties of the diode. They are usually evaluated to reveal electronic loss mechanisms of the investigated solar cell, such as the localization of dominant recombination paths. If these parameters are not properly derived, the simulated diode characteristics may not reflect the real IV characteristics which leads to misinterpretation of internal electrical losses. In this work a number of methods for extraction of the mentioned parameters are applied to different CIGS solar cells and quantitatively compared. The accuracy of the parameters is verified for the cases of light, dark, temperature-dependent and intensity-dependent measurements, while the mean square error of the corresponding fits serves as the quality indicator. The necessity of an extented two-diode model will be discussed. The objective of this work is to find a method for reliable extraction of parameters of CIGS solar cells which yields the best possible reproduction of their real IV behaviour and to quantify the inaccuracy of each approach.

HL 113: Quantum information systems II (with TT)

Time: Friday 9:30–10:45 Location: POT 151

HL 113.1 Fri 9:30 POT 151

Coherent pulse re-shaping in a semiconductor optical amplifier — •Mitra Pasche, Mirco Kolarczik, Yücel Kaptan, Nina Owschimikow, and Ulrike Woggon — Institut für Optik und Atomare Physik, Technische Universität Berlin, Germany

Recently it was demonstrated that Rabi oscillations in Quantum Dots (QDS) induce a laser pulse re-shaping in a semiconductor optical amplifier (SOA) at room temperature[1]. Here we present the results of a systematic investigation of the dependence of the pulse re-shaping on pulse power, detuning and the electrical injection level. The measurements are performed using frequency resolved optical short-pulse characterization by heterodyning (FROSCH)[1]. The method allows to observe simultaneously the amplitude and phase of the light field of the laser pulse relative to a reference pulse. In numerical simulations, we vary the parameters of the probe pulse and quantify their influence on the shape of the cross-correlation of the probe and reference pulse. We can thus assign characteristic phase jumps observed in the experiment to a coherent exchange of energy in the light-matter system.

[1] M.Kolarczik, N.Owschimikow, J.Korn, B.Lingnau, Y.Kaptan, D.Bimberg, E.Schöll, K.Lüdge, U.Woggon, *Nat. Commun.*, accepted (2013).

HL 113.2 Fri 9:45 POT 151

Ambient Temperature Spin Pumping of Silicon Carbide Quantum Defects — •Hannes Kraus[1], Franziska Fuchs[1], Daniel Riedel[1], Victor Soltamov[2], Dmitrij Simin[1], Stefan Väth[1], Andreas Sperlich[1], Pavel Baranov[2], Georgy Astakhov[1], and Vladimir Dyakonov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, Germany — [2]Ioffe Physical-Technical Institute, St. Petersburg, Russia

Silicon carbide is best known as a high performance power electronics semiconductor, although intrinsic defects in this material, particularly silicon vacancies, are very promising for quantum information processing, photonics and magnetometry [1]. This is due to the defects' intriguing quantum properties: The SiC defect spin states can be initialized and subsequently read using optically detected magnetic resonance (ODMR), and the high-spin ground state of these defects can be selectively populated by optical pumping. Similar to a lasing system, this leads to a population inversion and, consequently, to a stimulated radio emission [2]. We show this effect also works at room temperature, which opens an interesting perspective to construct low noise, low cost and low maintenance solid state radio amplifiers. Another opportunity is the defect ODMR's dependence on magnetic field orientation and temperature, suggesting SiC applications in quantum sensing.

[1] D. Riedel et al., Phys. Rev. Lett. 109, 226402 (2012)
[2] H. Kraus et al., Nature Physics (2013), doi:10.1038/NPHYS2826

HL 113.3 Fri 10:00 POT 151

Silicon Vacancies in Silicon Carbide as a Vector Magnetometer — •Dmitrij Simin[1], Franziska Fuchs[1], Hannes Kraus[1], Victor Soltamov[2], Andreas Sperlich[1], Pavel Baranov[2], Georgy Astakhov[1], and Vladimir Dyakonov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg, Germany — [2]Ioffe Physical-Technical Institute, 194021 St. Petersburg, Russia

The determination of both the magnitude and orientation of ambient magnetic fields has become a crucial convenience and safety factor in smartphones, spacecrafts, and satellites. Due to severe requirements for these devices, including compactness, temperature stability, and inexpensive fabrication, there are few devices that meet them all. In this study, we present a new approach, utilizing the spin properties of the silicon vacancies in silicon carbide [1]. Using room temperature optically detected magnetic resonance [2], we measure the change in optical emission due to vacancy specific electronic transitions that are dependent on the magnitude as well as on the direction of the external magnetic field. Using these relationships, we show how silicon carbide can be used as a compact and cost-effective solution for vector magnetometry applications with a good accuracy.

[1]Riedel et al.: Phys. Rev. Lett. 109, 226402 (2012)
[2]Kraus et al.: Nat. Phys., DOI 10.1038/nphys2826 (2013)

HL 113.4 Fri 10:15 POT 151

Spin defect engineering in silicon carbide using neutron irradiation — •Franziska Fuchs[1], Michael Trupke[2], Georgy Astakhov[1], and Vladimir Dyakonov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Vienna Center for Quantum Science and Technology, Atominstitut, TU Wien, A-1020 Wien

Atom-like defects in semiconductors are promising systems for spin-based quantum information applications. With its advanced growth and device technologies, Silicon carbide (SiC) is an eligible host for such defects, e.g. silicon vacancies (V_{Si}). This spin-$\frac{3}{2}$ system can be addressed and manipulated [1] and could serve as a room temperature source for single photons [2] or a room temperature maser amplifier [3]. With these applications in mind, one main challenge is to thoroughly create, isolate, and control the defects. Here, we report defect engineering of V_{Si} defects in SiC by means of neutron irradiation. Our photoluminescence measurements show that the defect density is well controllable via the irradiation dose. The irradiation flux has been varied over 10 orders of magnitude, from 10^8 to 10^{18} neutrons/cm^2. Two specific cases are of interest. The generation of the maximum V_{Si} concentration possible without destroying the crystal structure is required for the implementation of maser amplifiers. On the other hand, the creation of very few, isolated defects is crucial for the realization of single photon sources. [1] Riedel et al.: Phys. Rev. Lett. 109, 226402 (2012), [2] Castelletto et al.: Nat Mat 12 (2013), DOI 10.1038/namt3806 [3]

Kraus et al.: Nat Phys (2013), DOI 10.1038/nphys2826

HL 113.5 Fri 10:30 POT 151

Mapping the D1-transition of Caesium by dressed-state resonance fluorescence from a single (In,Ga)As quantum dot — •Sven M. Ulrich[1], Markus Oster[1], Michael Jetter[1], Alban Urvoy[2], Robert Löw[2], Tilmann Pfau[2], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]5. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Hybrid quantum systems combining semiconductor quantum dots (QDs) and atomic vapors promise interesting applications in quantum information technology. Recent research in this field has explored the resonant coupling between single GaAs QDs and Rubidium gas to generate e.g. frequency-stabilized non-classical emission ($\sim$ 780 nm) as well as slow light for qubit storage/retrieval operations.

As an alternative hybrid approach we use a cw laser-driven single (In,Ga)As QD (4 K) in the "dressed state" resonance fluorescence (RF) regime to address the D_1 transitions of atomic Caesium (Cs) vapor (300 K). QD-atom resonance is achieved by tuning the frequency of the dressing laser close to the QD ground state $\nu_0 \approx 335.116$ THz (894.592 nm) and shifting the narrow-band center and side channels of the QD Mollow triplet. Using this laser frequency controlled QD probe light for absorption measurements allows to precisely identify all four Cs hyperfine-split transitions. Therefore, narrow-band (In,Ga)As QD RF is demonstrated as suitable to optically address individual channels of the D_1 quadruplet without magnetic field or electric field tuning.

HL 114: Oxides: Bulk, films and interfaces

Time: Friday 9:30–12:45 Location: POT 251

HL 114.1 Fri 9:30 POT 251

Structural and Electronic Properties of Si/ZnO Interfaces from ab-initio Quasiparticle Calculations — •Benjamin Höffling and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena

Transparent conducting oxides like ZnO are widely used in Si-based photovoltaics. The fundamental properties of the Si/ZnO interface, however, remain poorly understood. We have employed Density Functional Theory and modern many-body perturbation theory using nonlocal exchange-correlation functionals and Hedin's GW method to a model interface derived from lattice coincidence considerations and the minimization of dangling bonds. We present results describing the atomic structure, electronic band offsets, interface states and the influence of passivation at the interface. We also discuss how band offsets derived from mesoscopic alignment methods like the Shockley-Anderson model or Tersoff's branch point method compare to the microscopic results.

HL 114.2 Fri 9:45 POT 251

Response of titanium dioxide after fs-laser excitation using ab-initio MD-simulations — •Sergej Krylow, Fairoja Cheenicode Kabeer, Eeuwe S. Zijlstra, and Martin E. Garcia — Theoretical Physics, University of Kassel, Heinrich-Plett-Str. 40, 34132 Kassel

We determined the response of titanium dioxide supercells using our in-house Code for Highly-excIted Valence Electron Systems(CHIVES), which is an implementation of electronic temperature dependent density functional theory using pseudopotentials and localized atom-centered basis functions. In particular, we are interested in the decay of the A1g-phonon mode as a function of time as well as the phonon-phonon interactions, which are causing the decay. We demonstrate that there is a dependence of the dynamics on the applied fs-laser laser fluence. We also compare our results to recent experiments[1], showing the accuracy of CHIVES.

[1] Bothschafter, E. M. and Paarmann, A. and Zijlstra, E. S. and Karpowicz, N. and Garcia, M. E. and Kienberger, R. and Ernstorfer, R: Ultrafast Evolution of the Excited-State Potential Energy Surface of TiO_2 Single Crystals Induced by Carrier Cooling, Phys. Rev. Lett. 110, 067402 (2013)

HL 114.3 Fri 10:00 POT 251

Diameter-dependent Absorption Edges of One-dimensional TiO2 Nanotube Arrays by Atomic Layer Deposition — •Ahmed Al-Haddad[1,2], Samar Tarish[1,2], Ranjith Vellacheri[1], Wenxin Wang[1], Fabian Grote[1], Zhibing Zhan[1], and Yong Lei[1] — [1]Ilmenau University of Technology, Institute of Physics & IMN MacroNano (ZIK) Prof. Schmidt-Str. 26, 98693 Ilmena,Germany. — [2]Department of Physics, College of Science, The University of Mustansiryah, Baghdad, Iraq.

Free standing one-dimensional (1-D) TiO2 nanotube arrays (TNAs) were fabricated by atomic layer deposition (ALD) with the assistant of anodic aluminum oxide templates at 350 °C. The wall thickness of nanotubes can be precisely controlled using ALD recipe. The intensities of the UV-Vis absorption were enhanced with increasing the diameter of nanotube while the thickness of the nanotubes walls was kept constant. A blue-shift was observed when decreasing the diameter of nanotubes, indicating a change of band gap and the shift of absorption edges towards shorter wavelengths were ascribed to the quantum effect of nanotube wall. Furthermore, the structure and surface morphology of the TNAs were examined by Raman spectroscopy and scanning electron microscopy, respectively.

HL 114.4 Fri 10:15 POT 251

Heteroepitaxial ZnO films on diamond — Fabian Schuster[1], •Martin Hetzl[1], Cesar Magén[2,3], Jordi Arbiol[4,5], Jose Garrido[1] und Martin Stutzmann[1] — [1]Walter Schottky Institut, Technische Universität München, Garching, Germany — [2]Laboratorio de Microscopías Avanzadas (LMA) - Instituto de Nanociencia de Aragon (INA) and Departamento de Física de la Materia Condensada, Universidad de Zaragoza, Spain — [3]Fundación ARAID, Zaragoza, Spain — [4]Institut de Ciència de Materials de Barcelona, ICMAB-CSIC, Bellaterra, Spain — [5]Institució Catalana de Recerca i Estudis Avancats (ICREA), Barcelona, Spain

The growth of heteroepitaxial ZnO films on (110) diamond substrates is demonstrated by molecular beam epitaxy. Structural characterization is performed by means of X-ray diffraction and scanning transmission electron microscopy imaging (STEM), where single domain growth is observed. The growth direction is found to be along the polar c-axis with Zn-polarity, deduced from annular bright field STEM. Photoluminescence and absorption studies reveal good optical properties as well as amplified spontaneous emission for optical excitation above a threshold of 30 kW/cm2. In addition, electronic band structure simulations are presented, showing that the ZnO polarity dominates the electronic structure of the interface: the formation of a 2DEG on the ZnO side or a 2DHG on the diamond side are predicted for Zn- and O-polarity, respectively.

HL 114.5 Fri 10:30 POT 251

A comprehensive study on ion-implantation induced defects in ZnO thin films — •Florian Schmidt[1], Stefan Müller[1], Holger von Wenckstern[1], Robert Röder[2], Sebastian Geburt[2], Carsten Ronning[2], and Marius Grundmann[1] — [1]Universität Leipzig, Institut für Experimentelle Physik II, Abteilung Halbleiterphysik, Linnéstraße 5, 04103 Leipzig — [2]Friedrich-Schiller-Universität Jena, Institute for Solid State Physics, D-07743 Jena

Deep defects levels in semiconductors have significant impact on material properties and device performance. Therefore a profound understanding of such defects is helpful for device optimization. Devices based on the semiconductor ZnO has been reported in the last years and even simple transparent circuitry have been demonstrated [1].

Here we present characterization of deep-level defects introduced by implantation of Ar^+, Ne^+, Zn^- and O^- by means of deep-level transient spectroscopy (DLTS) and optical DLTS (ODLTS). Independent of the implanted ion defect levels with thermal activation energies of $E_a \approx 1000$ meV and ≈ 1200 meV were introduced. A defect level with the thermal activation energy of 388 meV was only detectable after oxygen ion implantation. We will present for each ion implanted the density of the defects introduced.

[1] H. Frenzel *et al.*, phys. stat. sol. RRL **7** (9), 605 (2013).

HL 114.6 Fri 10:45 POT 251

Influence of deposition parameters on p-NiO/n-ZnO heterojunctions — •Paul Räcke, Robert Karsthof, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstraße 5, 04103 Leipzig, Germany

An ideal transparent solar cell completely transmits the visible part of the solar spectrum. At the same time, the energy of the rest of the solar spectrum is converted into electric power as efficiently as possible. A few wide-gap transparent semiconductors are candidates for the construction of a photovoltaic cell that absorbs radiation in the UV spectral range.

In this work the optical and electrical properties of zinc oxide-nickel oxide thin film heterojunctions were studied. The p-type NiO was grown by reactive DC sputter deposition onto pulsed laser deposited (PLD) n-type ZnO with a highly transparent ZnO:Al back contact on a-sapphire. A very thin gold layer on top of the NiO works as hole extraction layer. The result is a semi-transparent cell stack for which the transmission is mainly limited by the NiO layer and depends on its thickness and stoichiometry.

We investigated the influence of the NiO film thickness on the transmission spectrum and the IV characterstics including photovoltaic parameters. Furthermore, the transmission by the NiO was improved tremendously by annealing the cell stack in an oxygen ambient. The changes in the IV characteristics will be discussed as well.

Coffee break (15 min.)

HL 114.7 Fri 11:15 POT 251

Formation of stable bound magnetic polarons in depleted ZnCoO films — •T. Kaspar[1], D. Bürger[1], I. Skorupa[2], O.G. Schmidt[1,3], and H. Schmidt[1] — [1]TU Chemnitz, 09111 Chemnitz, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [3]IFW Dresden, 01069 Dresden, Germany

Metal-semiconductor field effect transistors (MESFET) with a paramagnetic ZnCoO [1] channel and a free charge carrier concentration below the metal insulator transition [2] have been fabricated by pulsed laser deposition on c-plane sapphire substrates. The unstructured ZnCoO films reveal a positive magnetoresistance due to s-d- exchange interaction effects. We show that the formation of stable BMPs with a stable defect [3] is responsible for switching depleted ZnCoO from a low into a high resistance state by applying an external magnetic field. The high resistance state is persistent until the MESFET is heated up to 300 K and is caused by the formation of stable bound magnetic polarons (BMPs) in depleted ZnCoO. This effect could be possibly used for the realization of nonvolatile spin valves in ZnCoO films with two gate contacts. [1] T. Kaspar et al., IEEE 34, 1271 (2013) [2] Q.Y. Xu et al., J. Appl. Phys. D-Appl. Phys. 42, 085001 (2009); Phys. Rev. B 73, 205342 (2006); Phys. Rev. B. 76, 134417 (2007) [3] H. Schmidt et al., Appl. Phys. Lett. 91, 232110 (2007).

HL 114.8 Fri 11:30 POT 251

Structure dependent magnetic properties of Co implanted TiO2 — •Oguz Yildirim[1,2], Steffen Cornelius[1], Maik Butterling[3], Wolfgang Amwand[3], Andreas Wagner[3], Alevtina Smekhova[4], and Kay Potzger[1] — [1]Institute for Ion Beam Physics and Materials Research, HZDR, Dresden, Germany — [2]Institute for Physics of Solids, TU Dresden, Zellescher Weg 16, 01069 Dresden, Germany — [3]Institute for Radiation Physics , HZDR, Dresden, Germany — [4]Lomonosov Moscow State University, MSU, Faculty of Physics, Moscow, Russia

Magnetic and structural properties of amorphous and anatase TiO2 thin films implanted with Co ions have been investigated. Implantation induced defects have been characterized using positron annihilation spectroscopy (PAS) while for magnetic chracterization we have used magnetometry. Up to a doping level of 2.5 at.%, only a paramagnetic contribution has been detected. The susceptibility strength , however, depends on the structure of the unimplanted film. Results on the formation of secondary phases at higher doping level will also be presented.

This work is supported by the Initiative and Networking Fund of the German Helmholtz Association, Helmholtz-Russia Joint Research Group HRJRG-314, and the Russian Foundation for Basic Research, RFBR 12-02-91321-SIG, Start: 01.02.2012

HL 114.9 Fri 11:45 POT 251

Multicentric coordination of hydrogen in the metal oxides ZnO and MgO — •Sandro G. Koch, Edward V. Lavrov, and Jörg Weber — Technische Universität Dresden, 01062 Dresden, Germany

Hydrogen is an inherent impurity in ZnO and MgO. The formation of shallow hydrogen donors and the passivation of acceptors as well as F-centers significantly influence the optical and electrical properties of these materials. Calculations by Janotti and Van de Walle suggested that hydrogen substituting for oxygen (H_O) in ZnO and MgO binds equally to all metal neighbors resulting in a lower local vibrational mode (LVM) frequency compared to a two-center bond. The authors introduced the concept of the hydrogen multicenter bond in solids to visualize their results [1]. An experimental verification of this hypothesis is challenging, since the predicted LVM frequencies are located in a multi-phonon absorption region.

Here, we present an experimental approach to overcome the LVM detection limitation in strongly absorbing spectral regions. Using the photoconductivity technique we show that H_O in ZnO is tetrahedrally coordinated with LVMs at 742 and 792 cm^{-1} [2]. First preliminary results on H_O in MgO are also presented .

[1] A. Janotti and C. Van de Walle, Nat. Mater. **6**, 44 (2007).
[2] S. G. Koch *et al.*, Phys. Rev. Lett. **108**, 165501 (2012).

HL 114.10 Fri 12:00 POT 251

Recharging behaviour of nitrogen-centers in ZnO — •Jan M. Philipps[1], Bruno K. Meyer[1], Detlev M. Hofmann[1], and Matt McCluskey[2] — [1]Institute of Physics I, Heinrich-Buff-Ring 16, Justus-Liebig-University Giessen, D-35392 Giessen, Germany — [2]Department of Physics and Astronomy, Washington State University, Pullman, WA 99164-2814, USA

Nitrogen was quoted to be a candidate to obtain p-type conductive ZnO. One assumes in a simple model that nitrogen substitutes an oxygen atom in the crystal lattice and thus causes an acceptor. The hope was that the recharging level of the nitrogen acceptors is shallow enough to accept electrons from the valence band and thus to promote hole conductivity. Unfortunately, it turned out that this model was too simple, electron paramagnetic resonance experiments (EPR) revealed that substitutional nitrogen centers (N_O) are deep defects with a recharging level 1.3 eV above the valence band.

In the following it was speculated that nitrogen-pair centers or complexes consisting of nitrogen and vacancies could act as shallow acceptors. Again EPR was successful to identify N_2-centers in ZnO by the observation of a 5-line spectrum caused by the hyperfine interaction of two nitrogen nuclei. The recharging of this center exhibits two steps, a weak onset at about 1.4 eV and a strongly increasing signal for photon energies above 2.1 eV. The later energy coincides with the recharging energy of the N_O-centers. These results indicate that also the N_2-centers are deep level defects and not suitable to cause significant hole-conductivity at room temperature.

HL 114.11 Fri 12:15 POT 251

Highly rectifying contacts on amorphous zinc-tin-oxide thin films consisting of metals and p-type zinc-cobalt-oxide — •Peter Schlupp, Friedrich-Leonhard Schein, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Leipzig, Deutschland

In order to provide cost-efficient and homogeneous oxide thin films for electronic devices it is desirable to use amorphous materials which can be deposited at room temperature (RT). Zinc-tin-oxide (ZTO) is a promising n-type semiconducting material in which only abundent materials are contained. To produce MESFETs or JFETs highly rectifying Schottky contacts or pn-heterodiodes are needed. The latter could be realized with p-type semiconductors like zinc-cobalt-oxide (ZCO).

We present electrical properties of highly rectifying contacts on amorphous ZTO layers. Our first metal-semiconductor structures showed only weakly rectifying behavior due to trap-assisted tunnel currents. In order to improve rectification, we introduced a thin insulating ZTO layer between the metal and the thin film. Optimized Schottky contacts on this structure exhibit current on/off-ratios up to 10^7 at $\pm 2\,V$. Using p-type ZCO we fabricated all-amorphous oxide heterodiodes. Again, we introduced an insulating ZTO layer on the n-side of the heterointerface and obtained pin-diodes having current on/off ratios up to 5×10^6 at $\pm 1.6\,V$. Thus they widely outperform the previously best fully amorphous TSO pn-junctions. Temperature dependent current-voltage characteristics and the current transport mechanism across the heterointerface will be discussed.

HL 114.12 Fri 12:30 POT 251

Transparent photovoltaics: ZnO/NiO heterojunctions working as UV solar cells — •Robert Karsthof, Paul Räcke, Zhipeng Zhang, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Insitut für Experimentelle Physik II, Linnéstraße 5, 04103 Leipzig, Germany

A solar cell transmitting visible light rather than absorbing it seems to contradict the general idea of efficient energy conversion. However, it has been shown recently [1] that a device which only absorbs photons from the IR and UV range of the solar spectrum can reach conversion efficiencies up to 37% (Shockley-Queisser limit). PV modules consisting of such cells could be used to generate electric power e.g. on large window areas on office buildings without reducing the daylight illumination of the interior – in contrast to conventional technologies.

In this work we present an approach based on zinc oxide-nickel oxide thin film heterojunctions. We grew *p*-type NiO by reactive DC and RF sputter deposition on top of pulsed laser deposited (PLD) *n*-type ZnO on *a*-sapphire to produce semi-transparent *pn*-junctions. A highly Al-doped PLD-grown ZnO layer was used as transparent back contact. The completed cell stack showed a high transmission of 50% and above. The cells were characterized by means of *IV* and external quantum efficiency (EQE) measurements. We could confirm that with this approach energy conversion efficiencies above 1% and EQE around 100% in the UV range are already feasible.

[1] R. Lunt: *Appl. Phys. Lett.* **101**, 043902 (2012)

HL 115: Symposium SYOM: One-dimensional metals - Reality or fiction?

Time: Friday 9:30–12:30 Location: HSZ 02

Invited Talk HL 115.1 Fri 9:30 HSZ 02

Atomic-scale dopant wires for quantum computer architectures — •Michelle Y Simmons — Centre of Excellence for Quantum Computation and Communication Technology, University of New South Wales, Sydney, NSW 2052, Australia

Down-scaling has been the leading paradigm of the semiconductor industry since the invention of the first transistor in 1947. As silicon electronics approaches the atomic scale, interconnects and circuitry become comparable in size to the active device components. Maintaining low electrical resistivity at this scale is challenging because of the presence of confining surfaces and interfaces. We report on the fabrication of wires in silicon-only one atom tall and four atoms wide-with exceptionally low resistivity ˜ 0.3 milliohm-centimeters. By embedding phosphorus atoms within a silicon crystal with an average spacing of less than 1 nanometer we achieved a diameter-independent resistivity [1]. Atomistic tight-binding calculations confirm the low resistivity of these atomic-scale wires [2], which pave the way for single-atom device architectures for both classical and quantum information processing. I will demonstrate how we have incorporated these wires into single atom transistors [3] and performed single-shot spin read-out of precisely-positioned P donor electron spins as potential qubits in Si [4].

[1] B. Weber et al., Science 335, 6064 (2012). [2] H. Ryu et al., Nanoscale 5, 8666 (2013). [3] M. Fuechsle et al., Nature Nanotechnology 7, 242 (2012). [4] H. Buch et al., Nature Communications 4, 2017 (2011).

Invited Talk HL 115.2 Fri 10:10 HSZ 02

$1 + \delta$: Tuning the Dimensionality of Organic Conductors — •Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart

Organic charge-transfer salts are prime candidates for tuning the dimension by applying pressure. Strictly one-dimensional systems, such as the Fabre salts $(TMTTF)_2X$, are Mott insulators that undergo a deconfinement transition towards a Luttinger liquid and eventually a two-dimensional Fermi liquid if the interchain interaction increases with pressure. The deconfinement transition can be identified when the transverse hopping integral $2t_\perp = \Delta_\rho$, the Mott gap. Ab-initio density functional theory allows us to study the influence of temperature and pressure on the electronic band structure.

Quasi-one-dimensional organic conductors, like the Bechgaard salts $(TMTSF)_2X$, exhibit a cross-over from a Luttinger liquid to a Fermi liquid behavior upon cooling and application of external pressure. Frequency and temperature dependent transport measurement yield a change in power-laws and Luttinger exponent.

Often the metallic phase is not stable in reduced dimensions: at low temperatures the electronic charges and spins tend to arrange themselves in an orderly fashion due to relatively strong correlations. There are a growing number of molecular materials where electronic degrees of freedom and electronic interactions are directly responsible for electric polarization and ferroelectric transition, termed electronic ferroelectricity. Recently, it was discovered that charge order not only produces ferroelectricity but also breaks the symmetry of the magnetic degree of freedom in organic quantum spin chains.

Coffee break (20 min)

Invited Talk HL 115.3 Fri 11:10 HSZ 02

Spectral and transport properties of one-dimensional correlated electrons — •Volker Meden — Institut für Theorie der Statistischen Physik, RWTH Aachen University

Two-particle interactions strongly alter the low-energy physics of electrons confined to one spatial dimension. Excitations cannot be described by fermionic quasi-particles. Metallic systems of this type fall into the Luttinger liquid universality class and are characterized by power-law decay of correlation functions. I will give an overview over the one-particle spectral and transport properties of such systems including a discussion of the model dependent low-energy scale beyond which Luttinger liquid power laws are observable. Leaving the framework of equilibrium physics I will report on recent progress in understanding the non-equilibrium steady state as well as relaxation dynamics of isolated and contacted quantum wires.

Invited Talk HL 115.4 Fri 11:50 HSZ 02

Atomic nanowires on surfaces: Spectroscopic reality versus theoretical fiction — •Ralph Claessen — Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Solids with electrons confined to only one spatial dimension are predicted to behave quite different from conventional metals. Many-body theory finds that electronic interactions may lead to Peierls-type instabilities or even a breakdown of Landau's quasiparticle picture, which works so well in higher dimensions. Atomic nanowires formed by self-organized growth of metal atoms on suitable semiconductor surfaces can be viewed as closest approach to perfect 1D electron confinement, and therefore serve well as model systems for experimental tests of the expected 1D physics. In my presentation I will discuss current experiments on atomic nanowires, using photoelectron spectroscopy and scanning tunneling microscopy as experimental probes, and compare the results to corresponding theoretical predictions. Examples include the observation of Tomonaga-Luttinger behavior as well as the possible detection of (quasi-)1D antiferromagnetic order.

HL 116: Topological insulators (organized by MA)

Time: Friday 9:30–12:00 Location: HSZ 04

HL 116.1 Fri 9:30 HSZ 04

Experimental characterization and simulation of quasi-particle-interference in the Bi-bilayer topological insulator — •Matteo Michiardi[1], Andreas Eich[2], Gustav Bihlmayer[3], Alex A. Khajetoorians[2], Jens Wiebe[2], Jianli Mi[4], Bo B. Iversen[4], Philip Hofmann[1], and Roland Wiesendanger[2] — [1]Department of physics and astronomy, Aarhus University, Denmark — [2]Institute of Applied Physics, University of Hamburg, Germany — [3]Peter Grünberg Institut, Forschungszentrum Jülich, Germany — [4]Center for Materials Crystallography, Aarhus University, Denmark

Topological insulators (TI) are a new class of materials that host gapless surface states with spin helicity. While several 3D TIs have been discovered, the interest in 2D TI systems that can host topological edge state is rising. A single bilayer of bismuth is predicted to be such a 2D TI. Here we present an experimental and theoretical study of a Bi-bilayer grown on 3D TI Bi_2Se_3. The use of Bi_2Se_3 as substrate allows the epitaxial growth of the bilayer in the rhombohedral structure, as shown by Scanning Tunnelling Microscopy. We calculate the band structure of the Bi-bilayer/Bi_2Se_3 system by Density Function Theory (DFT) and experimentally study the quasi particle interference (QPI) on the bilayer. In order to clarify the scattering channels responsible for the QPI, we perform simulations based on the Joint Density of States method starting from our DFT calculations. The comparison with the experimental results reveals a good match for a wide range of binding energies for both occupied and unoccupied states.

HL 116.2 Fri 9:45 HSZ 04

Quasiparticle self-consistent *GW* study of bismuth under strain — •Irene Aguilera, Christoph Friedrich, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

It has been recently claimed on the basis of ARPES measurements that bulk bismuth is a topological semimetal. The discrepancies between this result and previous *ab-initio* calculations were attributed to the failure of density functional theory (DFT) in the prediction of band gaps, because the topological or trivial character of Bi depends only on the "sign" of the very small direct band gap at the L point. We show that bulk Bi is indeed predicted by DFT in the local-density approximation (LDA) to be a trivial semimetal, with a surprisingly overestimated gap at L. We have performed quasiparticle self-consistent *GW* (QS*GW*) calculations for bulk bismuth that support its trivial character. The QS*GW* gap at L as well as the energy overlap between the electron and hole pockets are in much better agreement with experiments than the LDA ones. Thus, the QS*GW* approach appears as the right tool to study the trivial-to-topological transition that Bi experiences under stress, as a result of a change of sign of the gap at L. We have analyzed the effect of strain on the topological properties of bulk Bi. Whereas LDA predicts that an impractical stress is needed for such a transition, QS*GW* shows that bulk Bi becomes a topological semimetal already under very small stress. This work is supported by the Helmholtz Virtual Institute for Topological Insulators (VITI).

HL 116.3 Fri 10:00 HSZ 04

Combined STM/STS- and ARPES-investigation of the quaternary Topological Insulator $Bi_{1.5}Sb_{0.5}Te_{1.8}Se_{1.2}$ — •Thomas Bathon[1], Felix Reis[1], Christoph Seibel[2], Hendrik Bentmann[2], Paolo Sessi[1], Friedrich Reinert[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Physikalisches Institut, Experimentelle Physik VII, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We present a combined scanning tunneling microscopy/spectroscopy (STM/STS) and angular-resolved photoemission spectroscopy (ARPES) characterization of the electronic properties of the quaternary compound $Bi_{1.5}Sb_{0.5}Te_{1.8}Se_{1.2}$. ARPES-data evidence that this compound is still a Topological Insulator (TI) with a single Dirac cone, which is characteristic for the Bi_2X_3-class. The topological properties of the surface state, i.e. forbidden backscattering, have been confirmed by Fourier-transformed differential conductance (dI/dU) maps. Measurements performed both above and below the Fermi level allow us to determine the energy dispersion relation, the carrier velocity, and—by extrapolation to zero momentum—the position of the Dirac point. The observed scattering vectors are not as well-defined as those observed in binary compounds, probably due to substitutional disorder which results in a spatial fluctuation of the chemical potential. Our investigations illustrate how the properties of the well-known TI Bi_2Te_3 can be changed by chemical substitution.

HL 116.4 Fri 10:15 HSZ 04

Surface and bulk contributions to the electronic structure of the topological insulator Sb_2Te_3(0001) — •Christoph Seibel[1,2], Hendrik Bentmann[1,2], Henriette Maass[1,2], Jürgen Braun[3], Jan Minár[3], Kenya Shimada[4], and Friedrich Reinert[1,2] — [1]Experimentelle Physik VII, Universität Würzburg, D-97074 Würzburg — [2]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie KIT, D-76021 Karlsruhe — [3]Department Chemie, Physikalische Chemie, Universität München, Butenandtstraße 5-13, D-81377 München — [4]Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima 739-0046, Japan

Photon energy dependent angle-resolved photoemission measurements were performed to disentangle surface and bulk contributions to the electronic structure of the 3D topological insulator (TI) Sb_2Te_3. We discover a penetration of the topological surface state (TSS) into the bulk valence band regime where it coexists with bulk states without considerable hybridization. Our results indicate an emerging $k_\perp$-dispersion of the TSS at higher binding energies, which we attribute to an increasing bulk character. These observations deviate from previous findings for the isostructural TIs Bi_2Se_3 and Bi_2Te_3. Our results are supported by fully relativistic one-step photoemission calculations. [1] Seibel *et al.* PRB 86, 161105(R) (2012)

15 min. break

HL 116.5 Fri 10:45 HSZ 04

Spin-dependent unoccupied electronic structure of the topological insulator Sb_2Te_3 — •Anna Zumbülte[1], Anke B. Schmidt[1], Markus Donath[1], Peter Krüger[2], Gregor Mussler[3], and Detlev Grützmacher[3] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany — [2]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, Germany — [3]Peter Grünberg Institut, Forschungszentrum Jülich, Germany

Studies on three-dimensional topological insulators focus mainly on the well-known systems of Bi_2Se_3 and Bi_2Te_3 and the related ternary compounds. Theoretical predictions of chalcogenides as topological insulators with a single Dirac cone [1] include an additional compound, Sb_2Te_3. There, due to p-type doping of the available samples, the Dirac point lies above the Fermi level, making it inaccessible to photoemission experiments unless the surface is modified with an adsorbate [2]. Consequently, the electronic structure of this system has been left almost unstudied.

We present spin- and angle-resolved inverse-photoemission measurements of the unoccupied electronic states of Sb_2Te_3. In addition to the Dirac state, further spin-dependent features have been obtained which show a distinct Rashba splitting. The experimental data will be discussed along with bandstructure calculations.

[1] H. Zhang *et al.*, Nat. Phys. **5**, 438 (2009)
[2] C. Seibel *et al.*, Phys. Rev. B **86**, 161105 (2012)

HL 116.6 Fri 11:00 HSZ 04

Comparitive study of the ternary topological insulators Bi_2Se_2Te and Bi_2Te_2Se — •Felix Reis[1], Thomas Bathon[1], Christoph Seibel[2], Hendrik Bentmann[2], Paolo Sessi[1], Friedrich Reinert[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Physikalisches Institut, Experimentelle Physik VII, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The 3D topological insulators Bi_2Se_2Te and Bi_2Te_2Se have been investigated by combining the complementary experimental techniques scanning tunneling microscopy (STM/STS) and angular-resolved photoemission spectroscopy (ARPES). With low temperature STM/STS technique we investigate the structural and electronic properties of both systems. Fourier-transformed quasi-particle interference (QPI)

maps give access to the scattering events within the topological surface state. Taking QPI maps for several energies allows us to obtain information on the position of the Dirac point and the carrier velocity by fitting the linear energy dispersion relation of the Dirac fermions. These results will be compared with the band structure as obtained by ARPES measurements.

HL 116.7 Fri 11:15 HSZ 04

A large-energy-gap oxide topological insulator based on the superconductor BaBiO3 — •Binghai Yan[1,2,3], Martin Jansen[1], and Claudia Felser[1,3] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden — [3]Institute for Inorganic and Analytical Chemistry, Johannes Gutenberg University of Mainz, 55099 Mainz

Topological insulators are a new class of quantum materials that are characterized by robust topological surface states (TSSs) inside the bulk-insulating gap, which hold great potential for applications in quantum information and spintronics as well as thermoelectrics. One major obstacle is the relatively small size of the bulk bandgap, which is typically around 0.3eV for the known topological insulator materials. Here we demonstrate through ab initio calculations that a known superconductor BaBiO3 (BBO) with a Tc of nearly 30 K emerges as a topological insulator in the electron-doped region. BBO exhibits a large topological energy gap of 0.7 eV, inside which a Dirac type of TSSs exists. As the first oxide topological insulator, BBO is naturally stable against surface oxidization and degradation, distinct from chalcogenide topological insulators. An extra advantage of BBO lies in its ability to serve as an interface between TSSs and superconductors to realize Majorana fermions for future applications in quantum computation.

Reference: B. Yan, M. Jansen, C. Feler, Nature Physics 9, 709*711 (2013) (arXiv:1308.2303).

HL 116.8 Fri 11:30 HSZ 04

Topological surface states of HgTe and Heulser compounds — •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 Complex Systems, Dresden, Germany.

We studied the topological electronic structures of HgTe and half Heusler compounds (e.g.: XYZ, X = rare earth elements, Y = trasition metal and Z = main group elements) by both *ab initio* calculations. The topological surface structures were investigated by the Wannier function based tight-binding method. The effects of external strains induced from the substrate and surface terminations are taken into account by the atomic positions. Our results agree well with recent photoemission experiments.

HL 116.9 Fri 11:45 HSZ 04

Sputter Deposition of Half-Heusler Topological Insulators — •Benedikt Ernst, Daniel Ebke, Stanislav Chadov, Gerhard Fecher, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany

Heusler compounds have exhibited manifold physical properties in the recent years and attracted a lot of interest in the field of spintronic applications due to their half-metallic properties. Recently, a topological insulating state has been predicted by theory for some of these compounds.

In this work, we have prepared Heusler materials such as LaPdBi and LaPtBi for which a topological insulating behavior was predicted. Co-deposition by DC- and RF magnetron sputtering was used to prepare corresponding thin films. To realize an epitaxial film growth in the crystallographic $C1_b$ structure on MgO-substrates, a buffer layer was applied and optimized. Initial transport properties will be discussed with regard to the film composition and the crystallographic properties.

HL 117: Organic semiconductors: Material properties (with CPP/DS)

Time: Friday 10:15–12:30 Location: POT 051

HL 117.1 Fri 10:15 POT 051

Pressure dependent Electronic Structure 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, USA

The electronic properties of organic semiconductors typically exhibit a significant dependence on the strain, stress and pressure [1]. To clarify the role of these effects electronic-structure theory is uniquely suited. However, standard density-functional theory approaches that neglect van-der-Waals interactions and that treat exchange and correlation in a semi-local approximation often fail to describe organic materials properly. To overcome this limitation, we have extended our implementation of the analytical strain derivatives (stress tensor) to include the contributions that stem from (a) the van-der-Waals interaction [2] and (b) the Fock-exchange in hybrid functionals. We discuss the details of our implementation that is based on a local resolution of identity (LVL) of the Coulomb matrix [3]. We validate our approach by investigating the geometric and electronic changes that occur in polyacetylene, polyaniline, and anthracene under 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.

[1] J. H. Kim, S. Seo, and H. H. Lee, Appl. Phys. Lett. **90**, 143521 (2007).
[2] A. Tkatchenko, and M. Scheffler, PRL **102**, 073005 (2009)
[3] A. Sodt, and M. Head-Gordon, J. Chem. Phys. **128**, 104106 (2008)

HL 117.2 Fri 10:30 POT 051

DFT study of vibronic properties of partially fluorinated nickel phthalocyanine — •Davoud Pouladsaz — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Since fluorinated phthalocyanines are shown to be sensitive to reducing gases due to the withdrawing effect of fluorine atoms, by means of density functional theory, we have investigated the effect of fluorination on the vibronic couplings and ionization potential in nickel phthalocyanine.

HL 117.3 Fri 10:45 POT 051

Ab-initio investigation of Charge and Spin transport properties of Organic Semiconductors. — •Sandip Bhattacharya and Stefano Sanvito — School of Physics and CRANN, Trinity College Dublin, Ireland

In this talk I will describe in detail our procedure to explore the spin and charge transport properties of organic single-crystal semiconductors from first principles. Our technique involves representing the organic semiconductor with a tight-binding model, including coupling of the charge carrier to phonons and spin relaxation due to hyperfine and spin-orbit coupling interaction. The ab-initio Hamiltonian parameters are extracted from DFT and the maximally localized Wannier functions scheme. We evolve the classical fields in the Hamiltonian via Monte Carlo simulations, and then compute the mobility from Kubo formula and the spin-diffusion length from a Landauer-Buettiker approach. We shall demonstrate calculated charge carrier mobilities very close to those measured in single-crystal rubrene-based organic field effect transistors and spin-diffusion length quite close to that estimated in experiments on rubrene-based spin valves. In the second part of my talk, I shall discuss the use of a similar procedure to predict the ab-initio spin and charge transport characteristics of Triarylamine-based organic nanowires, recently synthesized. We obtain quite superior estimates for hole mobilities as well as spin-diffusion lengths in such organic nanowires, corroborating the experimental find of exceptional conductance through nanodevices made out of such nanowires.

HL 117.4 Fri 11:00 POT 051

Growth control of AgTCNQ nanowire arrays by using template-assisted electro-deposition method — •Chengliang Wang[1], Liaoyong Wen[1], Thomas Kups[2], Ranjith Vellacheri[1], Yaoguo Fang[1], Peter Schaaf[2], Huaping Zhao[1], and Yong Lei[1] — [1]Institute for Physics and IMN MacroNano(ZIK), Ilmenau University of Technology, Ilmenau 98693, Germany — [2]Institute of Materials Engineering and IMN MacroNano(ZIK), Ilmenau University of Technology, Ilmenau 98693, Germany

One dimensional (1D) organic semiconductor nanostructures, espe-

cially their aligned arrays, have attracted extensive attention due to their potential application in organic optoelectronics, and template-assisted methods have been proved to be one of the most powerful methods to achieve this kind of arrays. Due to the small size of the AAO nanopores, diffusion of the objects into the nanopores is one of the crucial issues to achieve nanowire arrays. Here, the growth control of AgTCNQ (TCNQ: 7,7,8,8-tetracyanoquinodimethane) nanowire arrays is achieved by using template-assisted electro-deposition methods. We find that the diffusion of the electrolyte into the nanopores takes an important role in the electro-deposition process and the equilibrium between the reduction and the diffusion is necessary to achieve continuous AgTCNQ nanowire arrays. We believed that the analysis of the equilibrium between the deposition and the diffusion and the controllable synthesis of organic semiconductor arrays will benefit the preparation of other semiconductor arrays.

HL 117.5 Fri 11:15 POT 051

Energy-transfer in ZnO/ladder-type oligophenylenes hybrid structures — •Francesco Bianchi[1], Sylke Blumstengel[1], Fritz Henneberger[1], Björn Kobin[2], Stefan Hecht[2], Rafael Schlesinger[1], and Norbert Koch[1] — [1]Institut für Physik Humboldt-Universität, Berlin, Germany — [2]Department of Chemistry Humboldt-Universität, Berlin, Germany

Inorganic/organic hybrid systems designed to inherit the advantageous properties of each of their constituents are of great interest both to basic science as well as for optoelectronic applications. In this regard it is required to find an organic material that exhibits specific properties like narrow transitions, large dipole moment, small emission-absorption Stokes shift and an optical gap that corresponds to the inorganic material. The design we use consists in a three spiro-bridged ladder-type quarter-phenyl (SP3-L4P) grown on ZnO-based single quantum wells (SQW) to obtain incoherent coupling. In such a setting, it should be possible to convert Wannier excitons of the SQW into Frenkel excitons of the organic layer via a Förster type energy transfer (FRET).

We investigate the FRET between SQW with different cap thickness and a 3Sp-L4P thin layer evaporated on top of them. With photoluminescence excitation and time-resolved spectroscopy we demonstrate that these hybrid structures exhibit energy transfer with an efficiency up to 65%. Despite the high efficiency, UPS measurements show a type II interface between ZnO and the molecules layer, leading to a charge separation process that limits the light emitted. Finally we investigate on the use of high gap material spacer to reduce this effect.

HL 117.6 Fri 11:30 POT 051

Temperature dependent PL measurements of rubrene single crystals with μm-resolution — •T. Schmeiler[1], J. Gabel[1], R. Claessen[1], and J. Pflaum[1,2] — [1]Inst. Exp. Phys. VI/IV, University of Würzburg, 97074 Würzburg — [2]ZAE Bayern e.V., 97074 Würzburg

Our previous demonstration of spatial confinement effects on exciton dynamics in rubrene (rub) single crystals, microcrystals and amorphous films [1] has raised fundamental questions on excitonic processes occurring at surfaces and interfaces of molecular stacks. We address this topic by analyzing the temperature dependent PL characteristics of rub single crystals on μm-length scales and under various boundary condition by e.g. capping them with thin films of different polarizability such as Au or LaVO. At first, a pronounced enhancement of the total PL intensity of up to two orders of magnitudes was observed in case of the Au top layer which can be attributed to a resonant coupling of the excited rub states to the surface plasmon modes of the metal. This coupling phenomenon is further corroborated by relative intensity changes within the PL spectra of the Au covered rub upon cooling below 100K. In case of a LaVO capping layer, providing high polarizability without significant contributions by exciton quenching, a strong temperature dependent influence in the rub PL peaks at short wavelengths is observed. This behavior will be discussed in the context of temperature dependent changes of the LaVO layer itself as well as different coupling mechanism for the interfacial excitonic species. Financial support by the DFG research unit FOR 1809 (project PF385/6) is gratefully acknowledged. [1] B. Gieseking et al., arXiv:1309.1107

HL 117.7 Fri 11:45 POT 051

Optical absorption and photoluminescence properties of perylene single-crystals — •Andre Rinn, Niklas Kraus, André Pick, Gregor Witte, and Sangam Chatterjee — Phillips Universität Marburg, Marburg, Germany

Organic semiconductors are considered promising candidates for next-generation optical devices. However, a detailed systematic understanding of the electro-optical response is in a much less holistic state than for inorganic materials such as Si or GaAs. Therefore, we investigated the two crystalline phases of perylene as model organic semiconductors and gain further insight in their optical response. This system crystallizes in two different phases: the beta-phase has a monomeric herringbone structure with two molecules per primitive unit cell, whereas the alpha phase grows in a dimeric herringbone configuration with four molecules per unit cell. The single -crystalline samples have been grown in silicon oil, which results in microcrystals of excellent quality. Hence, we can investigate the consequences of the respective crystal orientation on the Davydov splitting of the excitons as well as excimer formation. Both configurations have been investigated with polarization resolved absorption spectroscopy and time resolved luminescence experiments. Absorption spectroscopy reveals results with significant deviations from the widespread Davydov picture. The data obtained by time resolved luminescence shows characteristic excimer behavior. Additionally, the optical spectra are compared to the response of perylene in solution and the vapour phase.

HL 117.8 Fri 12:00 POT 051

Direct measurement of the charge carrier mobility in organic donor-acceptor blend in device geometry – including extreme stoichiometry — •Johannes Widmer[1], Janine Fischer[1], Christian Koerner[1], Karl Leo[1], and Moritz Riede[1,2] — [1]Institut für Angewandte Photophysik (IAPP), TU Dresden, Germany — [2]Current address: Clarendon Laboratory, UK

Blend layers of an organic donor (D) and a fullerene acceptor (A) are a key component of highly efficient organic solar cells. The charge carrier mobility in the blend sensibly affects the device efficiency concerning transport and recombination of charge carriers.

The applied method "POEM" – potential mapping by thickness variation – is a direct measurement giving model-free experimental access to the effective mobility $\mu(F, n)$ as a function of the electric field F and the charge carrier density n. It is based on a novel evaluation strategy for space-charge limited current (SCLC) in single carrier devices in a vertical device geometry.[Widmer et al., Org. El. (2013)]

Here, we apply POEM to characterize the hole transport in D:A blends of small molecules with different blend ratios. The measurements cover common ratios as well as strongly diluted blends with only $\approx 1\,\%$ donor content, which are known to yield efficient solar cells. Beyond characterizing disorder and trap states, which influence μ, the POEM measurements reveal that also in the diluted blend effective hole transport is possible, but takes place not only on the donor.

The obtained $\mu(F, n)$ functions allow for an advanced understanding of charge transport in D:A blends – also in moderate blend ratios.

HL 117.9 Fri 12:15 POT 051

Polymer aggregation control in polymer: PCBM bulk heterojunctions adapted from solution — •Christian Kästner[1], Daniel Egbe[2], and Harald Hoppe[1] — [1]Ilmenau University of Technology, Ilmenau, Germany — [2]Linz Institute for Organic Solar Cells, Linz, Austria

It is common knowledge that the polymer conformation and its phase separation with fullerene derivatives are delicate issues crucially impacting on the photovoltaic parameters of polymer based solar cells. Whereas strongly intermixed polymer:fullerene phases provide large interfacial area and consequently a high quantum efficiency of exciton dissociation, pristine and primarily ordered polymer and fullerene domains support efficient charge transport and percolation. To study the aggregation and phase separation in polymer solar cells we investigated counterbalancing influences of polymer solution concentration and PCBM ([6,6]-phenyl-C61-butyric acid methyl ester) blending ratio on the basis of a semi-crystalline anthracene-containing poly(p-phenylene-ethynylene)-alt-poly(p-phenylene-vinylene) (PPE-PPV) copolymer statistically bearing either branched 2-ethylhexyloxy or linear octyloxy side-chains (AnE-PVstat). The polymer aggregation varied with both, solution and PCBM concentrations, yielding a specific maximum within the parameter range. We explicitly demonstrate the counterbalancing effect on charge generation and transport for increasing polymer aggregation. Furthermore the influence of polymer aggregation on fundamental optoelectronic properties is discussed, providing detailed understanding of resulting photovoltaic parameters.

HL 118: Graphene: Interaction with the substrate (with DY/MA/O/TT)

Time: Friday 11:15–13:00 Location: POT 081

HL 118.1 Fri 11:15 POT 081

Phonons of graphene on metallic and semiconductor surfaces, an ab-inito approach — •Alejandro Molina-Sanchez and Ludger Wirtz — Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg

The interaction of graphene with substrates can alter its electronic and vibrational properties and is relevant for the practical use of graphene. In this work, we describe the graphene-substrate interaction through the theoretical study of the vibrational properties. We focus on three paradigmatic cases where the interaction strength changes gradually: graphene@BN, graphene@Ir(111), and graphene@SiC (i.e., the buffer layer). We use ab-initio methods to obtain the phonon modes, the density of states, and the strength of the electron-phonon coupling. When we deal with large supercells, we use an unfolding scheme to visualize the phonon bands in the primitive unit cell. Thus, we can distinguish clearly the changes in the phonon dispersion of perturbed-graphene with respect to the one of pristine graphene. Graphene on boron nitride exhibits a weak interaction but a non-negligible shift of the 2D Raman band. We explain this observation as due to a weakening of the electron-phonon interaction via screening of electron-electron correlation by the dielectric substrate. Graphene on iridium, also displays weak interaction but the underlying material is a metal. This leads to an even more pronounced screening of the electron-electron interaction in graphene. In the last case, we study the buffer layer of graphene on silicon carbide. The hybridization of graphene with silicon carbide changes the electronic structure of graphene and the phonon bands.

HL 118.2 Fri 11:30 POT 081

The (3×3)-SiC($\bar{1}\bar{1}\bar{1}$) reconstruction: Surface phase equilibria near the graphene formation regime on 3C-SiC($\bar{1}\bar{1}\bar{1}$) — •Lydia Nemec[1], Florian Lazarevic[2], Patrick Rinke[1], Volker Blum[3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]AQcomputare GmbH, Chemnitz — [3]MEMS Department, Duke University, Durham, NC, USA

To refine the growth quality of epitaxial graphene on the C-side of SiC and improve the resulting electronic character of these films, it is important to understand the atomic- and electronic-structure of the interface. A phase mixture of different surface phases is observed just when surface graphitization first sets in. However, the atomic structure of some of the competing surface phases, as well as of the SiC-graphene interface, is unknown.

We performed a density functional theory study on the C-side of the polar SiC($\bar{1}\bar{1}\bar{1}$) surface using the all-electron, numeric, atom-centered basis function code FHI-aims. The formation energy of different reconstructions and model systems for the interface is presented within the thermodynamically allowed range.

The surface energies of the known (2×2) phase is compared with several structural models of the (3×3) phase proposed in the literature. In comparison all the previously suggested (3×3) models are higher in energy than the known (2×2) phase. We present a new model for the (3×3) reconstruction. Its formation energy crosses that of the (2×2) phase just at the carbon rich limit of the chemical potential, which could explain the observed phase mixture.

HL 118.3 Fri 11:45 POT 081

Reststrahl band assisted photocurrents in epitaxial graphene layers — •P. Olbrich[1], C. Drexler[1], L.E. Golub[2], S.N. Danilov[1], V.A. Shalygin[3], V.A. Shalygin[3], R. Yakimova[4], S. Lara-Avila[5], S. Kubatkin[5], B. Redlich[6], R. Huber[1], and S.D. Ganichev[1] — [1]University of Regensburg, Regensburg, Germany — [2]Ioffe Institute, St. Petersburg, Russia — [3]State Polytechnic University, St. Petersburg, Russia — [4]Linköping University, Linköping, Sweden — [5]Chalmers University of Technology, Göteborg, Sweden — [6]FOM Institute for Plasma Physics, Nieuwegein, The Netherlands

We report on the observation of reststrahl band assisted photocurrents in epitaxial graphene on SiC. The samples were excited by the infrared radiation from the tunable free electron laser "FELIX" and a CO_2 gas laser [1]. We show that the photoresponse due to linearly (circularly) polarized mid-infrared light is strongly enhanced (suppressed) in the vicinity of the reststrahl band of SiC. Our data, in particular a complex spectral behavior, are well described by the developed theory taking into account photon drag and photogalvanic effects affected by an enhanced light-matter interaction in the range of substrate's negative dielectric function in its reststrahl band. Moreover, our work demonstrates that substrate phonons strongly influence the transport properties of the carriers in graphene.

[1] P. Olbrich *et al.*, arXiv:1308.0123

HL 118.4 Fri 12:00 POT 081

Towards superlattices: Lateral bipolar multibarriers in graphene — •Martin Drienovsky[1], Franz-Xaver Schrettenbrunner[1], Andreas Sandner[1], Ming-Hao Liu[2], Fedor Tkatschenko[2], Klaus Richter[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Institut für Experimentelle und Angewandte Physik Universität Regensburg — [2]Institut für Theoretische Physik Universität Regensburg

We report on transport properties of monolayer-graphene (MLG) with a laterally modulated charge carrier density profile. For that we employed a planar back gate and striped top gate electrodes of 25 nm width and a spacing of 100 nm up to 200 nm, separated from the MLG by an Al_2O_3 dielectric. Tuning of top and back gate voltages gives rise to multiple potential barriers and wells, enabling the investigation of resistance either in the unipolar or the bipolar transport regime. In the latter pronounced single- and multibarrier Fabry-Pérot (FP) resonances are observed. The experimental data of different devices with alternating numbers of top gate stripes and pitch, taken at different temperatures, is consistent with a ballistic transport calculation, employing a realistic potential profile, extracted from classical electrostatic simulation combined with the quantum capacitance model. The origin of resistance oscillations in our multibarrier graphene system can be explained in the FP-picture, without resorting to an artificial band structure.

HL 118.5 Fri 12:15 POT 081

Scanning Tunnelling Spectroscopy of Moiré Patterns on Graphene/Rh(111) — •Anne Holtsch, Tobias Euwens, Hussein Schanak, and Uwe Hartmann — Institut für Experimentalphysik, Universität des Saarlandes, Saarbrücken

The lattices of graphene and Rh(111) provide a difference of approximately 9% between the two lattice constants. This mismatch results in the formation of a Moiré pattern with a lattice constant of 2.9 nm. Each unit cell of the pattern exhibits four regions where the graphene lattice is aligned differently with respect to the Rh(111) atoms. Scanning tunnelling microscopy and spectroscopy are used to investigate changes in the electronic properties at the four regions of the Moiré unit cell. Density functional theory (DFT) calculations show that a decreasing C-Rh distance at different symmetry points coincides with an increasing interaction strength between graphene and Rh(111) [1]. The locations of the minima in the dI/dV curves are identical for the different symmetry regions. Beyond the minimum, the symmetry points show differences in the dI/dV curves according to the C-Rh interaction strength.

[1] M. Iannuzzi and J. Hutter, Surf. Sci. 605, 1360 (2011).

HL 118.6 Fri 12:30 POT 081

Varied Moiré patterns of graphene/Rh(111) measured by scanning tunnelling microscopy — •Tobias Euwens, Anne Holtsch, Hussein Schanak, and Uwe Hartmann — Institute of Experimental Physics, Saarland University, P.O. Box 151150, D-66041 Saarbrücken

Scanning tunnelling microscopy measurements on graphene deposited on a Rh(111) surface are conducted to investigate the superstructures that originate from the different lattice parameters of the graphene and the substrate. Different kinds of superstructures, also called Moiré patterns, can be seen in the resulting images. Their origin lies in either the surface inhomogenities of the Rh(111) substrate or in the form of folds and steps in the graphene itself. Knowing the properties of the growth of graphene on the rhodium surface is important for the construction of more complex graphene-based electronics. Understanding the specific structure of the Moiré patterns can help in that regard as it relays information about the angle between the carbon and the rhodium lattice and potential reasons for the twisting between the two lattices.

HL 118.7 Fri 12:45 POT 081

Impact of the substrate on the electronic properties of graphene — •Hussein Shanak, Anne Holtsch, Tobias Euwens, and Uwe Hartmann — Institute of Experimental Physics, Saarland University, P.O. Box 151150, D-66041 Saarbrücken

Electronic properties of graphene grown on different substrates such as Rh, Cu and SiO2 were investigated using scanning tunnelling microscopy and spectroscopy. The different kinds of substrates result in different types of superstructures due to the mismatch between graphene and substrate. Comparison of the electronic properties obtained for graphene on the different substrates leads to a better understanding of the graphene doping behaviour. Additionally, the existence of different superstructures leads to different growing properties of the materials on top of graphene itself.

HL 119: Invited Talk Michael Leuenberger

Time: Friday 11:00–11:30 Location: POT 006

Invited Talk HL 119.1 Fri 11:00 POT 006

A 3D topological insulator quantum dot for optically controlled quantum memory and quantum computing — Hari P. Paudel and •Michael N. Leuenberger — NanoScience Technology Center, University of Central Florida, Orlando, FL 32826, USA

We present the model of a quantum dot (QD) consisting of a spherical core-bulk heterostructure made of 3D topological insulator (TI) materials, such as the narrow-bandgap semiconductor $Pb_{1-x}Sn_xTe$, with bound massless and helical Weyl states existing at the interface and being confined in all three dimensions. The number of bound states can be controlled by tuning the size of the QD and the magnitude of the core and bulk energy gaps, which determine the confining potential. We demonstrate that such bound Weyl states can be realized for QD sizes of few nanometers. In contrast to topologically trivial semiconductor QDs, the confined massless Weyl states in 3D TI QDs are localized at the interface of the QD and exhibit a mirror symmetry in the energy spectrum. We find that strict optical selection rules give rise to the Faraday effect due to Pauli exclusion principle. We show that the semi-classical Faraday effect can be used to read out spin quantum memory. When a 3D TI QD is embedded inside a cavity, the single-photon Faraday rotation provides the possibility to implement optically mediated quantum information processing.

HL 120: Ultra-fast phenomena II

Time: Friday 11:30–12:45 Location: POT 006

HL 120.1 Fri 11:30 POT 006

High-harmonic generation by extreme nonlinear terahertz excitation of semiconductors — •Ulrich Huttner[1], Mackillo Kira[1], Stephan W. Koch[1], Olaf Schubert[2], Matthias Hohenleutner[2], Fabian Langer[2], Benedikt Urbanek[2], Christoph Lange[2], and Rupert Huber[2] — [1]Department of Physics, Philipps-University Marburg, 35032 Marburg, Germany — [2]Department of Physics, University of Regensburg, 93040 Regensburg, Germany

Combining theory and experimental results we demonstrate that one can access the regime of ultrafast coherent charge transport in semiconductors by applying extremely strong and ultrashort terahertz (THz) pulses with stable carrier envelope phase (CEP). Since the bandgap in semiconductors is typically much larger than the THz-photon energy, the THz excitation nonresonantly excites coherent polarization and currents. Modeling these processes with the semiconductor Bloch equations [1,2], we find that the strong THz field leads to intense high-harmonic generation (HHG) and dynamical Bloch oscillations [3]. Our experiments with a GaSe sample show harmonics up to the 22nd order. The HHG is strongly influenced by the dynamical Bloch oscillations that can be controlled via the CEP of the exciting THz-pulse.

[1] Golde, D. et al. - phys. stat. sol. b 248, 863-866 (2011).

[2] Kira, M. & Koch, S. W. - Semiconductor Quantum Optics: (Cambridge University Press, 2011).

[3] Schubert, O. et al. - Sub-cycle control of terahertz high-harmonic generation by dynamical Bloch oscillations, 2013, accepted for publication.

HL 120.2 Fri 11:45 POT 006

Phonon hardening and softening in femtosecond-laser-excited metals — •Naira S. Grigoryan, Fairoja C. Kabeer, Eeuwe S. Zijlstra, and Martin E. Garcia — Theoretische Physik, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

Many ultrafast structural phenomena in solids at high fluences are related to changes in the phonon frequencies at lower fluences. Here we studied the response of representative phonon modes of Mg and Cu to femtosecond-laser excitation using electronic-temperature-dependent density functional theory. We found softening of some and hardening of other lattice modes, where some modes even showed both behaviors as a function of the excitation strength. We relate the laser-induced changes in the phonon frequencies to changes in the ground-state electronic density of states following atomic displacement patterns in the directions of a phonon eigenmode. Using this relationship we established a general connection between the unexcited electronic structure of a material and the structural response to intense femtosecond-laser excitation.

HL 120.3 Fri 12:00 POT 006

Femtosecond Transmission Electron Diffraction on Single Crystalline Graphite — •Silvio Morgenstern, Christian Gerbig, Cristian Sarpe, Marlene Adrian, Arne Senftleben, and Thomas Baumert — University of Kassel, Institute of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), D-34132 Kassel, Germany

In carbon layered materials (graphite, graphene) the electron subsystem, stimulated by optical excitations, is strongly coupled to a small set of optical phonons which limits the ballistic conductance. A detailed understanding of phonon decay mechanism is thus essential in improving the performance of carbon-based electronic devices [1,2]. Time-resolved electron diffraction has become a promising technique to observe dynamics at the molecular level with ultrafast precision [3,4]. We use a fs-transmission electron diffractometer to study the evolution of phonon decays in single crystalline graphite after ultrashort laser excitation. Our compact setup is well characterized [4] with excellent spatial-temporal resolution (coherence length > 8 nm, e-pulse duration < 200 fs [5]). In this contribution the generation and decay of coherent acoustic and optical phonons are discussed in dependence of film thickness down to few-layer graphene [6]. [1] T. Kampfrath et al., Phys. Rev. Lett. 95, 187403 (2005) [2] S. Schäfer et al., New J. Phys. 13, 063030 (2011) [3] M. Chergui & A. H. Zewail, Chem. Phys. Chem. 10, 28 (2009) [4] G. Sciaini & R. J. D. Miller, Rep. Prog. Phys 74, 096101 (2011) [5] C. Gerbig et al., submitted (2013) [6] C. Gerbig et al., in preparation (2013)

HL 120.4 Fri 12:15 POT 006

Effective potential for femtosecond-laser-excited silicon — •Bernd Bauerhenne, Eeuwe S. Zijlstra, and Martin E. Garcia — Theoretische Physik - Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

Effective potentials are a powerful tool for modeling femtosecond-laser materials processing where the spatial geometry of the laser is important and therefore a huge number of atoms must to be taken into account, like, ablation or spallation. Here we present a new effective potential for femtosecond-laser-excited silicon, which we test by accurately reproducing the physics of ultrafast melting.

HL 120.5 Fri 12:30 POT 006

Fractional diffusion in laser-excited silicon — •Tobias Zier, Eeuwe S. Zijlstra, and Martin E. Garcia — Theoretical Physics,

University of Kassel, Germany

With an intense ultrashort-laser pulse excitation of crystalline Si one creates a highly nonthermal state, which is characterized by electrons with a temperature of several 10 000 K and ions close to room temperature. Due to this the interatomic bonds can soften or even break for sufficiently high excitations. In the latter case the crystalline structure disorders within several hundreds of femtoseconds. Therefore, this process is called ultrafast melting. The results of our performed ab initio MD-Simulations with supercells containing up to 800 atoms show for the first time that the atoms exhibit fractional diffusion during the ultrafast melting process, a behavior that was up to now only known for big molecules in solutions [1].

[1] E. S. Zijlstra, et al., Adv. Mater. 25, 5605 (2013)

HL 121: Graphene (organized by DS)

Time: Friday 11:30–13:15 Location: CHE 89

HL 121.1 Fri 11:30 CHE 89

Plasma-enhanced chemical vapor deposition of graphene on copper substrates — •Nicolas Wöhrl, Oliver Ochedowski, Steven Gottlieb, and Volker Buck — Universität Duisburg-Essen und CENIDE, 47057 Duisburg, Germany

In this work we present the synthesis of graphene on copper 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. The PE-CVD process uses hydrogen and methane as reaction gases exactly like thermal CVD process does. The gaseous precursors are decomposed in the plasma and the catalytic influence of copper and the minor solubility of carbon in copper lead to the growth of one monolayer of graphene. Plasma parameters are varied to investigate the influence on the graphene properties. Raman spectroscopy and AFM measurements are used as nondestructive tools for the characterization of the synthesized graphene films. Especially Raman spectroscopy is used as an efficient 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 a copper based substrate. This technology can help to make graphene available for industrial applications.

HL 121.2 Fri 11:45 CHE 89

Continuous wafer-scale graphene on cubic-SiC(001) — •Victor Aristov[1,2], Olga Molodtsova[2], Alexei Zakharov[3], Dmitry Marchenko[4], Jaime Sánchez-Barriga[4], Andrei Varykhalov[4], Marc Portail[5], Marcin Zielinski[6], Igor Shvets[7], and Alexander Chaika[1,7] — [1]ISSP RAS, Chernogolovka, Moscow dist. 142432, Russia — [2]HASYLAB at DESY, D-22607 Hamburg, Germany — [3]MAX-lab, Lund University, Box 118, 22100 Lund, Sweden — [4]HZB für Materialien und Energie, D-12489 Berlin, Germany — [5]CNRS-CRHEA, 06560 Valbonne, France — [6]NOVASiC, BP267-F73375 Le Bourget du Lac Cedex, France — [7]CRANN, School of Physics, Trinity College, Dublin 2, Ireland

The atomic and electronic structure of graphene synthesized on commercially available cubic SiC(001)/Si(001) wafers have been studied. LEED, LEEM, PEEM, STM and ARPES data prove the wafer-scale continuity and uniform thickness of the graphene overlayer and reveal that the graphene overlayer consists of only a few monolayers with physical properties of quasi-freestanding graphene: atomic-scale rippling, asymmetric distributions of carbon-carbon bond lengths etc. In addition, graphene overlayer consists of rotated nanometer-sized ribbons with four different lattice orientations connected through the grain boundaries. Thus, this graphene could be adapted for graphene-based electronic technologies and directly patterned using Si-electronic lithographic process. Supported by RFBR grant 14-02-00949, by Marie Curie IIF grant (7th ECFP) and by SPP 1459 of DPG.

HL 121.3 Fri 12:00 CHE 89

Characterization of single and few layer of molybdenum disulfide with spectroscopic imaging ellipsometry — •P. H. Thiesen[1], B. Miller[2], C. Röling[1], E. Parzinger[2], A. W. Holleitner[2], and U. Wurstbauer[2] — [1]Accurion GmbH, Göttingen, Germany — [2]Technische Universität München, Walter Schottky Institut, 85748 Garching, Germany

Molybdenum disulfide is a layered transition metal dichalcogenide. From the point of current research, 2D-materials based on MoS2 are very promising because of the special semiconducting properties. The bulk material has an indirect 1.2 eV electronic bandgap, but single layer MoS2 has a direct 1.8 eV bandgap. The monolayer can be used in prospective electronic devices like transistors or photo detectors. Like in the initial period of graphene research, the issue is to identify and characterize MoS2 crystallites of microscopic scale. Imaging ellipsometry is a nondestructive optical method in thin film metrology with a lateral resolution down to 1 micro meter. Imaging ellipsometry has been applied to characterize graphene flakes of few micrometer size [1],[2] and also to identify single layer steps in multilayer graphene/graphite stacks [3]. Delta and Psi Spectra of MoS2 monolayers as well as maps of the ellipsometric angles will be presented. The practical aspect of single layer identification will be addressed and the capability of ellipsometric contrast micrographs as a fast tool for single layer identification will be demonstrated. [1] Wurstbauer et al., Appl. Phys. Lett. 97, 231901 (2010) [2] Matkovic et al. J. Appl. Phys. 112, 123523 (2012) [3] Albrektsen et al. J. Appl. Phys. 111, 064305 (2012)

HL 121.4 Fri 12:15 CHE 89

Charge and Spin Transport in Turbostratic Graphene and Graphene Nanoribbons — •Nils Richter[1], Sebastian Schweizer[2], Ajit Kumar Patra[2], Yenny Hernandez[3], Akimitsu Narita[3], Xinliang Feng[3], Petr Ostrizek[1], Klaus Müllen[3], and Mathias Kläui[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, 55099 Mainz, Germany — [2]FB Physik, Universität Konstanz, 78457 Konstanz, Germany — [3]Max Planck Institute for Polymer Research, 55128 Mainz, Germany

We present two specially selected allotropes of graphene: Turbostratic graphene (TG) and graphene nanoribbons (GNRs).

TG discs are graphitic microstructures where the twisting of adjacent layers leads to an electronic decoupling. Electrical transport measurements reveal quantum effects such as weak localization and huge charge carrier mobilities (100,000 cm^2/Vs) in protected bulk layers [1]. In non-local spin valves we find efficient spin injection over micrometer distances showing large spin diffusion lengths.

Using electromigrated nanojunctions we are able to investigate electrical and spin transport in chemically synthesized GNRs. As they are dispersed in a solvent [2] they can be drop cast on such junctions. With GNRs of different widths and edge geometries we will probe the exciting unconventional properties that have been predicted for these nanostructures [3].

[1] Y. Hernandez et al., arXiv:1301.6087 (under review 2013). [2] A. Narita et al., Nature Chem., in press, DOI: 10.1038/NCHEM.1819. [3] O. Yazyev, Rep. Prog. Phys. 73, 056501 (2010).

HL 121.5 Fri 12:30 CHE 89

Graphene functionalisation with N and O: reversible or permanent modification of the electronic properties? — •Peter Brommer[1,2], Alex Marsden[1], Neil Wilson[1], Gavin Bell[1], and David Quigley[1,2] — [1]Department of Physics, University of Warwick, Coventry, UK — [2]Centre for Scientific Computing, University of Warwick, Coventry, UK

For many applications it is essential to modify the electronic properties of graphene in a controlled fashion. This can be achieved via oxygen and nitrogen functionalisation in ultra-high vacuum, leading to a system in which electronic and structural properties can be systematically studied. Low dose oxygen functionalisation ($<$ 5 atomic percent) can be reversed completely by annealing at 200 °C, while nitrogen permanently integrates itself into the material. Here we present insights from DFT calculations on this system, such as the low-energy configurations and simulated transmission electron microscopy (TEM) images, binding energies and effective band structures of the N and O decorated graphene sheets. We directly compare our results with experiments on CVD grown graphene. Angle-resolved photoemission spectroscopy (ARPES) resolves the band structure changes on func-

tionalization, whilst X-ray photoelectron spectroscopy (XPS) provides information about the chemical environment of the defect atoms. Combined, the computational and experimental data can offer insights into the structural changes induced by the functionalisation process and their consequences on the electronic properties of the material.

HL 121.6 Fri 12:45 CHE 89

Revealing the ultrafast process behind the photoreduction of graphene oxide — •Daniel S. Badali[1], Regis Y.N. Gengler[1], Dongfang Zhang[1], Kostantinos Dimos[2], Kostantinos Spyrou[2], Dimitrios Gournis[2], and R.J. Dwayne Miller[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, Hamburg Center for Ultrafast Imaging, University of Hamburg, Hamburg, Germany — [2]Department of Material Science and Engineering, University of Ioannina, Ioannina, Greece

Because of its unique electronic and structural properties, graphene has brought two-dimensional materials to the foreground of material science and nanoelectronic research. As such, reliable methods for producing graphene are in demand and have significant impact on the field of thin films. In recent years it has been found that irradiating dispersions of graphene oxide in water with ultraviolet light has led to the production of graphene. Although this has been observed in a variety of experimental conditionals, the exact mechanism of the reduction has remained elusive until now. To this end, we have performed careful optical pump-probe measurements which have revealed the chemistry of this process: rather than direct photoreduction, the reduction is mediated by solvated electrons which have been liberated from water molecules by the ultraviolet light. We show that this occurs on an ultrafast timescale in the tens of picoseconds range. Characterization of the final product confirms the removal of oxygen containing groups and the restoration of the honeycomb carbon network of graphene.

HL 121.7 Fri 13:00 CHE 89

Tuning of structural, electronic and optical properties in twisted bilayer MoS_2 — •Jens Kunstmann[1], Arend M. van der Zande[1], Alexey Chernikov[1], Daniel A. Chenet[1], YuMeng You[1], XiaoXiao Zhang[1], Timothy C. Berkelbach[1], Pinshane Y. Huang[2], Lei Wang[1], Fan Zhang[1], Mark Hybertsen[1,3], David A. Muller[2], David R. Reichman[1], Tony F. Heinz[1], and James C. Hone[1] — [1]Columbia University, New York, New York, 10027, USA — [2]Cornell University, Ithaca, New York, 14853, USA — [3]Brookhaven National Laboratory, Upton, New York 11973, USA

With the rise of graphene, atomically thin 2D materials have become the focus of many researchers worldwide. Among them, group 6 transition metal dichalcogenides, such as MoS_2 are new 2D direct gap semiconductors, have been used as field effect transistors and are promising for applications in valleytronics. However, little is understood about the interlayer interactions between 2D materials. We measured dozens of MoS_2 bilayers with well-defined twist angle by stacking single crystal monolayers using ultraclean transfer techniques. We observe that continuous changes in the interlayer twist angle lead to strong, continuous tuning in the indirect optical transitions, the Raman modes, the second harmonic generation, and the reflection spectra. We use electronic structure calculations to show that the tuning in the indirect band transitions arise from an increase of the bilayer separation caused by the van der Waals repulsion of sulfur atoms. These results indicate the possibility of producing new 2D materials with desired properties by tailoring the interlayer alignment in 2D heterostructures.