Semiconductor Physics Division
Fachverband Halbleiterphysik (HL)

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Overview of Invited Talks and Sessions

(Lecture Rooms H2, H3, H13, H14, H15, H16, and H17; Poster A)

Invited Talks

HL 14.1	Mon	13:30–14:00	H2	**Complex oxides for next-generation electronics** — •Chris G. Van de Walle
HL 19.1	Mon	15:00–15:30	H17	**Relaxation dynamics in graphene close to the Dirac point** — •Stephan Winnerl
HL 33.1	Tue	9:30–10:00	H13	**Acoustic nanoquakes dynamically control optical nanosystems** — •Hubert Krenner
HL 42.1	Tue	12:30–13:00	H2	**MBE growth of topological insulator films and ARPES measurements** — •Gregor Mussler, Jörn Kampmeier, Svetlana Borisova, Detlev Grützmacher
HL 43.1	Tue	15:00–15:30	H2	**Single phonon quantum interference and back-action in quantum-dot electrical circuits** — Ghislain Granger, Daniela Taubert, Carolyn Young, L. Gaudreau, A. Kam, S. Studenikin, D. Harbusch, Dieter Schuh, Werner Wegscheider, Zbigniew Wasilew, Aashish Clerk, Andrew Sachrajda, •Stefan Ludwig
HL 47.1	Tue	15:30–16:00	H2	**Compact physics-based modeling of semiconductor devices for circuit** — •Mitiko Miura-Mattausch
HL 51.1	Wed	9:30–10:00	H15	**Nano-scale characterization of semiconductors using helium temperature scanning transmission electron microscopy cathodoluminescence** — •Jürgen Christen, Gordon Schmidt, Peter Veit, Frank Bertram, Marcus Müller

Invited Talks in Focus Sessions

HL 3.1	Mon	9:30–10:00	H13	**Ultrafast processes in carbon nanotubes and quantum dots** — •Ulrike Woggon
HL 3.3	Mon	10:15–10:45	H13	**Quantum dots - artificial atoms, molecules or small pieces of bulk? Nonadiabatic molecular dynamics in the Kohn-Sham representation.** — •Oleg Prezhdo, Heather Jaeger, Long Run, Amanda Neukirch, Kim Hyeon-Deuk
HL 3.5	Mon	11:00–11:30	H13	**Out-of-equilibrium carrier dynamics in semiconductors: a novel approach** — •Andrea Marini
HL 3.6	Mon	12:30–13:00	H13	**The role of phonons for exciton and biexciton generation in a quantum dot driven by adiabatic rapid passage** — •Tilmann Kuhn
HL 3.8	Mon	13:15–13:45	H13	**Spin lifetime and electron-phonon interaction in graphene** — •Guido Burkard
HL 15.1	Mon	15:00–15:30	H2	**Optical absorption and radiation damage in transparent conducting oxides** — •Andre Schleife, Friedhelm Bechstedt, Alfredo Correa, Yosuke Kanai

HL 15.3	Mon	15:45–16:15	H2	**Growth from the melt of high-quality In2O3 and Ga2O3 single crystals** — •Roberto Fornari, Zbigniew Galazka, Reinhard Uecker, Klaus Irmscher
HL 15.5	Mon	16:45–17:15	H2	**Development of gallium oxide power devices** — •Masataka Higashiwaki, Kohei Sasaki, Akito Kuramata, Takekazu Masui, Shigenobu Yamakoshi
HL 15.9	Mon	18:15–18:45	H2	**Surface electron accumulation layers in oxide semiconductors** — •Tim Veal
HL 31.1	Tue	9:30–10:00	H2	**Localization at graphene system and topological insulator edges** — •Markus Buttiker
HL 31.2	Tue	10:00–10:30	H2	**Controlling Quantized Edge Transport in Two-dimensional Topological Insulators** — Viktor Krueckl, Sven Essert, •Klaus Richter
HL 31.3	Tue	10:30–11:00	H2	**First-principles studies of Dirac-cones in graphene and 3D topological insulators** — •Gustav Bihlmayer
HL 31.4	Tue	11:15–11:45	H2	**Lifetime broadening of topological surface states with and without magnetic moments** — •Oliver Rader, Markus Scholz, Jaime Sánchez-Barriga, Andrei Varykhalov, Dmitry Marchenko, Emile Rienks, Andrey Volykhov, Lada Yashina
HL 31.5	Tue	11:45–12:15	H2	**Transport in topological insulators - experiments** — •Christoph Brüne
HL 58.1	Wed	15:00–15:30	H13	**Potential and possibilities of copper oxide compounds** — •Bruno K. Meyer
HL 58.2	Wed	15:30–16:00	H13	**Intrinsic and hydrogen related impurities in Cu_2O** — •Graeme Watson
HL 58.4	Wed	16:45–17:15	H13	**Accelerating efficiency enhancements in cuprous oxide thin films by applying a structured approach** — •Tonio Buonassisi
HL 58.5	Wed	17:15–17:45	H13	**Photoemission Spectra of CuO from First Principles: Quasiparticle Excitations and Beyond** — •Claudia Rödl, Francesco Sottile, Lucia Reining
HL 60.1	Wed	15:00–15:30	H16	**Direct observation of coherent light matter interaction in room temperature semiconductor devices** — •Gadi Eisenstein
HL 60.2	Wed	15:30–16:00	H16	**Impact of coherent processes on the dynamics of quantum-dot lasers and amplifiers** — •Kathy Lüdge
HL 60.3	Wed	16:00–16:30	H16	**Ultrafast coherent exciton dynamics in individual quantum dots - phonons, coherent coupling, and CQED** — •Wolfgang Langbein
HL 60.4	Wed	16:45–17:15	H16	**Optical Properties of coupled InAs submonolayer depositions in GaAs** — •Udo W. Pohl, Thomas Switaiski, Ulrike Woggon, Jan-Hindrik Schulze, Tim D. Germann, André Strittmatter
HL 60.5	Wed	17:15–17:45	H16	**Coherent optical control of quantum dot spins and spin-photon entanglement** — •Sven Höfling, Kristiaan De Greve, Peter L. McMahon, David Press, Leo Yu, Jason S. Pelc, Chandra M. Natarajan, Na Young Kim, Thaddeus Ladd, Eisuke Abe, Sebastian Maier, Dirk Bisping, Christian Schneider, Martin Kamp, Robert H. Hadfield, Alfred Forchel, M. M. Fejer, Yoshihisa Yamamoto
HL 72.1	Thu	9:30–10:00	H13	**Defect reduction methods for GaN heteroepitaxial films grown along semipolar orientations** — •Philippe Vennéguès
HL 72.2	Thu	10:00–10:30	H13	**Identification of defects in semipolar GaN and (Al,Ga,In)N by cathodoluminescence spectroscopy** — •Klaus Thonke, Ingo Tischer, Matthias Hocker, Manuel Frey, Ferdinand Scholz
HL 72.3	Thu	10:30–11:00	H13	**Stacking fault elimination in heteroepitaxial semi-polar GaN** — •Armin Dadgar
HL 72.5	Thu	11:30–12:00	H13	**Strain and Relaxation in Nonpolar and Semipolar GaN-based LEDs and Laser Diodes** — •Kathryn Kelchner, Shuji Nakamura, Steven DenBaars, James Speck
HL 72.6	Thu	12:00–12:30	H13	**Semipolar GaN substrate grown on patterned sapphire substrate by hydride vapor phase epitaxy** — •Kazuyuki Tadatomo, Keisuke Yamane, Narihito Okada, Hiroshi Furuya, Yasuhiro Hashimoto

Sessions

HL 1.1–1.4	Sun	16:00–18:30	H2	**Tutorial: Coherent Control**
HL 2.1–2.5	Mon	9:30–10:45	H2	**Ultrafast phenomena**
HL 3.1–3.9	Mon	9:30–14:00	H13	**Focus Session: Electron-phonon interaction and ultrafast processes in semiconductors**
HL 4.1–4.11	Mon	9:30–12:30	H15	**III-V semiconductors: mainly wells and surfaces**
HL 5.1–5.9	Mon	9:30–11:45	H16	**Spintronics: mainly interfaces and heterostructures**
HL 6.1–6.7	Mon	9:30–11:15	H17	**Graphene: Magnetic fields (HL, jointly with O, TT)**
HL 7.1–7.4	Mon	9:30–10:45	H10	**Topological insulators 1 (MA, jointly with HL, O, TT)**
HL 8.1–8.13	Mon	9:30–13:00	H20	**Transport: Quantum dots, wires, point contacts 1 (TT, jointly with HL, O)**
HL 9.1–9.10	Mon	10:30–13:15	H36	**Focus Session: Frontiers of electronic structure theory I (O, jointly with HL, TT)**
HL 10.1–10.9	Mon	11:30–13:45	H17	**Graphene: Spin-orbit interaction (HL, jointly with O, TT)**
HL 11.1–11.7	Mon	12:00–13:45	H16	**Quantum information systems: mostly quantum dots**
HL 12.1–12.5	Mon	12:15–13:30	H1	**Charge transfer effects in molecular materials I (CPP, jointly with BP, DS, HL)**
HL 13.1–13.5	Mon	12:45–14:00	H15	**Preparation and characterization**
HL 14.1–14.1	Mon	13:30–14:00	H2	**Invited Talk: Chris van de Walle**
HL 15.1–15.11	Mon	15:00–19:20	H2	**Focus Session: Crystalline n-type semiconducting oxides - SnO_2, Ga_2O_3, and In_2O_3 for novel devices (HL, jointly with O)**
HL 16.1–16.9	Mon	15:30–18:00	H13	**Theory: Metal-insulator transitions / Electronic structure calculations**
HL 17.1–17.8	Mon	15:00–17:00	H15	**Interfaces and surfaces**
HL 18.1–18.6	Mon	15:00–16:30	H16	**Lasers and LEDs I**
HL 19.1–19.1	Mon	15:00–15:30	H17	**Invited Talk: Stephan Winnerl**
HL 20.1–20.10	Mon	15:00–18:00	H10	**Topological insulators 2 (MA, jointly with HL, O, TT)**
HL 21.1–21.9	Mon	15:00–17:30	H18	**Transport: Quantum dots, wires, point contacts 2 (TT, jointly with HL)**
HL 22.1–22.5	Mon	15:00–17:45	H20	**Focused Session: Correlations in topological bands (TT, jointly with HL, MA, O)**
HL 23.1–23.7	Mon	15:00–17:30	H40	**Charge transfer effects in molecular materials II (CPP, jointly with BP, DS, HL)**
HL 24.1–24.12	Mon	16:00–19:00	H17	**Graphene: Electronic properties and transport (O, jointly with HL, TT)**
HL 25.1–25.13	Mon	16:00–19:15	H36	**Focus Session: Frontiers of electronic structure theory II (O, jointly with HL, TT)**
HL 26.1–26.7	Mon	16:45–18:30	H16	**Lasers and LEDs II**
HL 27.1–27.24	Mon	17:00–20:00	Poster B1	**Joint Poster Session: Functionalized semiconductor nanowires (DS, jointly with HL); Resistive switching (DS, jointly with DF, KR, HL)**
HL 28.1–28.27	Mon	16:00–20:00	Poster A	**Poster Session: Graphen; Transport properties; Transport in high magnetic fields / Quantum Hall effect; Metal-semiconductor hybrid systems**
HL 29.1–29.28	Mon	16:00–20:00	Poster A	**Poster Session: Spintronics; Spin-controled transport; Topological insulators; Interfaces / Surfaces; Magnetic semiconductors**
HL 30.1–30.6	Mon	17:15–18:45	H32	**Organic electronics and photovoltaics I (DS, jointly with CPP, HL, O)**
HL 31.1–31.5	Tue	9:30–12:15	H2	**Focus Session: Dirac fermions in solid-state systems (HL, jointly with TT)**
HL 32.1–32.10	Tue	9:30–12:00	H3	**Spintronics and magnetic semiconductors (MA, jointly with HL)**
HL 33.1–33.1	Tue	9:30–10:00	H13	**Invited Talk: Hubert Krenner**
HL 34.1–34.5	Tue	9:30–10:45	H15	**Quantum dots and wires: Theory**
HL 35.1–35.12	Tue	9:30–12:45	H17	**Graphene: Transport (TT, jointly with HL, MA, O)**
HL 36.1–36.6	Tue	9:30–12:45	H8	**Focus Session: Functionalized semiconductor nanowires I (DS, jointly with HL)**
HL 37.1–37.10	Tue	9:30–12:30	H20	**Transport: Quantum dots, wires, point contacts 3 (TT, jointly with HL)**

HL 38.1–38.12	Tue	9:30–12:45	H32	**Organic electronics and photovoltaics II (DS, jointly with CPP, HL, O)**
HL 39.1–39.9	Tue	10:15–12:45	H13	**Optical properties**
HL 40.1–40.10	Tue	10:30–13:15	H36	**Focus Session: Frontiers of electronic structure theory III (O, jointly with HL, TT)**
HL 41.1–41.6	Tue	11:15–12:45	H15	**Quantum dots and wires: Preparation and characterization**
HL 42.1–42.1	Tue	12:30–13:00	H2	**Invited Talk: Gregor Mussler**
HL 43.1–43.1	Tue	15:00–15:30	H2	**Invited Talk: Stefan Ludwig**
HL 44.1–44.5	Tue	15:00–16:15	H3	**Photonic crystals**
HL 45.1–45.5	Tue	15:00–16:15	H13	**Transport in high magnetic fields / Quantum Hall effect**
HL 46.1–46.5	Tue	15:00–16:15	H15	**III-V semiconductors: mainly wires and dots**
HL 47.1–47.1	Tue	15:30–16:00	H2	**Invited Talk: Mitiko Miura-Mattausch**
HL 48.1–48.14	Wed	9:15–13:00	H16	**Topological insulators (HL, jointly with O, TT)**
HL 49.1–49.12	Wed	9:30–12:45	H2	**Molecular electronics (TT, jointly with CPP, HL, MA)**
HL 50.1–50.11	Wed	9:30–12:30	H13	**Organic semiconductors**
HL 51.1–51.1	Wed	9:30–10:00	H15	**Invited Talk: Jürgen Christen**
HL 52.1–52.13	Wed	9:30–13:00	H17	**Graphene: Characterization and devices (HL, jointly with MA, O, TT)**
HL 53.1–53.7	Wed	10:00–11:45	H15	**GaN: Devices**
HL 54.1–54.11	Wed	10:30–13:30	H36	**Focus Session: Frontiers of electronic structure theory IV (O, jointly with HL, TT)**
HL 55.1–55.4	Wed	11:45–12:45	H8	**Focus Session: Functionalized semiconductor nanowires II (DS, jointly with HL)**
HL 56.1–56.4	Wed	12:00–13:00	H15	**GaN: Optical characterization**
HL 57.1–57.14	Wed	15:00–18:45	H2	**Spintronics/Quantum information: Materials and methods (HL, jointly with TT)**
HL 58.1–58.6	Wed	15:00–18:00	H13	**Focus Session: Copper oxide semiconductors – An attractive material for photovoltaics?**
HL 59.1–59.7	Wed	15:00–16:45	H15	**Goup IV elements and their compounds I**
HL 60.1–60.8	Wed	15:00–18:30	H16	**Focus Session: Coherent dynamics in semiconductor nanostructures and coupled devices**
HL 61.1–61.6	Wed	15:00–18:00	H20	**Focused Session: Majorana fermions in condensed matter (TT, jointly with HL, MA, O)**
HL 62.1–62.13	Wed	16:00–19:15	H17	**Graphene: SiC substrates and intercalation (O, jointly with HL, TT)**
HL 63.1–63.12	Wed	16:00–19:00	H33	**Organic electronics and photovoltaics III (O, jointly with CPP, DS, HL)**
HL 64.1–64.13	Wed	16:00–19:30	H36	**Focus Session: Frontiers of electronic structure theory V (O, joinly with HL, TT)**
HL 65.1–65.22	Wed	16:30–18:30	Poster C	**Poster: Organic electronics and photovoltaics (CPP; jointly with HL, O)**
HL 66.1–66.10	Wed	17:00–19:30	H15	**GaN: Preparation and characterization of rods and wires**
HL 67.1–67.10	Wed	16:00–20:00	Poster A	**Focus Session (Posters): Crystalline n-type semiconducting oxides - SnO_2, Ga_2O_3, and In_2O_3 for novel devices**
HL 68.1–68.26	Wed	16:00–20:00	Poster A	**Poster Session: GaN: devices & preparation & characterization; III-V semiconductors; Photonic crystals; Semiconductor lasers**
HL 69.1–69.23	Wed	16:00–20:00	Poster A	**Poster Session: II-VI semiconductors; Organic semiconductors; Heterostructures**
HL 70.1–70.22	Wed	16:00–20:00	Poster A	**Poster Session: Devices; Preparation and characterization; C/diamond; Si/Ge**
HL 71.1–71.10	Thu	9:30–12:15	H2	**Exciton polaritons and their condensates (HL, jointly with TT)**
HL 72.1–72.9	Thu	9:30–13:15	H13	**Focus Session: Extended defects in semi- and nonpolar GaN I**
HL 73.1–73.7	Thu	9:30–11:15	H15	**Devices**
HL 74.1–74.10	Thu	9:30–12:15	H16	**Quantum dots: Optical properties**
HL 75.1–75.13	Thu	9:30–13:00	H18	**Transport: Spintronics and magnetotransport 1 (TT, jointly with HL, MA)**
HL 76.1–76.9	Thu	9:30–13:30	H32	**Focus Session: Organic materials for spintronics – From spinterface to devices (DS, jointly with HL, MA, O)**

HL 77.1–77.12	Thu	9:30–13:00	H34	**Organic electronics and photovoltaics IV (CPP, jointly with DS, HL, O)**
HL 78.1–78.11	Thu	10:30–13:15	H17	**Graphene: Preparation and characterization I (O, jointly with HL, TT)**
HL 79.1–79.10	Thu	10:30–13:15	H36	**Focus Session: Frontiers of electronic structure theory VI (O, jointly with HL, TT)**
HL 80.1–80.5	Thu	11:45–13:00	H15	**II-VI-compounds other than ZnO**
HL 81.1–81.12	Thu	14:45–18:15	H13	**Focus Session: Extended defects in semi- and nonpolar GaN II**
HL 82.1–82.10	Thu	15:00–17:45	H2	**Quantum dots and wires: Cavities and photons**
HL 83.1–83.6	Thu	15:00–16:30	H16	**Transport I**
HL 84.1–84.9	Thu	15:00–17:30	H17	**Graphene: Theory (HL, jointly with O, TT)**
HL 85.1–85.10	Thu	15:00–18:00	H18	**Topological insulators (TT, jointly with DS, HL, MA)**
HL 86.1–86.13	Thu	15:00–18:45	H34	**Organic electronics and photovoltaics V (CPP, jointly with HL, O)**
HL 87.1–87.7	Thu	15:45–17:30	H15	**Goup IV elements and their compounds II**
HL 88.1–88.12	Thu	16:00–19:00	H36	**Focus Session: Frontiers of electronic structure theory VII (O, jointly with HL, TT)**
HL 89.1–89.5	Thu	16:45–18:00	H16	**Transport II**
HL 90.1–90.18	Thu	16:00–20:00	Poster A	**Poster Session: Quantum information systems; Optical properties; Ultrafast phenomena**
HL 91.1–91.32	Thu	16:00–20:00	Poster A	**Poster Session: Quantum dots and wires: preparation & characterization & optical properties & transport properties**
HL 92.1–92.20	Thu	16:00–20:00	Poster A	**Poster Session: Structure and transport in organic photovoltaics; Photovoltaics; Impurities/Amorphous semiconductors; New materials**
HL 93.1–93.17	Fri	9:15–13:45	H2	**Photovoltaics (HL, jointly with CPP, O)**
HL 94.1–94.6	Fri	9:30–11:00	H13	**Quantum wires and nanocrystals: Optical properties**
HL 95.1–95.12	Fri	9:30–12:45	H14	**Spintronics/Quantum information: Vacancies in diamond and SiC (HL, jointly with TT)**
HL 96.1–96.10	Fri	9:30–12:15	H15	**GaN: Growth and doping**
HL 97.1–97.11	Fri	9:30–12:30	H16	**ZnO**
HL 98.1–98.13	Fri	9:30–13:00	H18	**Topological insulators (TT, jointly with DS, HL, MA, O)**
HL 99.1–99.4	Fri	9:30–10:30	H20	**Transport: Spintronics and magnetotransport 2 (TT, jointly with HL, MA)**
HL 100.1–100.12	Fri	9:30–12:45	H32	**Resistive switching (DS, jointly with DF, HL, KR)**
HL 101.1–101.10	Fri	10:30–13:00	H17	**Graphene: Preparation and characterization II (O, jointly with HL, TT)**
HL 102.1–102.8	Fri	11:15–13:15	H13	**Quantum dots and wires: Transport**

Symposium Charge Transfer Effects in Molecular Materials (SYCT)

SYCT 1.1	Mon	9:30–10:00	H1	**A coarse grained QM/MM approach for the description of charge transfer in complex systems** — •Marcus Elstner
SYCT 1.2	Mon	10:00–10:30	H1	**Identifying and resolving charge separation in organic solar cells** — •Eberhard Riedle
SYCT 1.3	Mon	10:30–11:00	H1	**Quantifying the energy of charge transfer states: From molecular crystals to donor-acceptor blends** — •Reinhard Scholz
SYCT 1.4	Mon	11:00–11:30	H1	**Efficient Exciton Generation and Collection in Organic Solar Cells** — •Mark Thompson, Cong Trinh, Steve Forrest, Jeramy Zimmerman
SYCT 1.5	Mon	11:30–12:00	H1	**Electron transport in organic single-crystal transistors and Schottky-gated heterostructures** — •Alberto Morpurgo

Symposium Strong Coupling in Solid State Quantum Systems (SYSC)

SYSC 1.1	Tue	9:30–10:00	H1	**Exploring the Physics of Superconducting Qubits Strongly Coupled to Microwave Frequency Photons** — •Andreas Wallraff

SYSC 1.2	Tue	10:00–10:30	H1	**Hybrid Quantum Circuit with a Superconducting Qubit Coupled to an Electron Spin Ensemble** — •Yuimaru Kubo, Cecile Grezes, Igor Diniz, Jun-ichi Isoya, Vincent Jacques, Anais Dreau, Jean-François Roch, Alexia Auffeves, Denis Vion, Daniel Esteve, Patrice Bertet
SYSC 1.3	Tue	10:30–11:00	H1	**Hybrid Quantum Systems with Rare-Earth Ion Spin Ensemble** — •Pavel Bushev
SYSC 1.4	Tue	11:00–11:30	H1	**Quantum Coherent Coupling between a Mechanical Oscillator and an Optical Mode** — Ewold Verhagen, Dalziel Wilson, Vivishek Sudhir, Nicolas Piro, Albert Schliesser, •Tobias Kippenberg
SYSC 1.5	Tue	11:30–12:00	H1	**Exploring Quantum Light-Matter Interactions of Quantum Dots in Photonic Crystal Nanostructures** — •Jonathan Finley, Arne Laucht, Michael Kaniber, Stefan Lichtmannecker, Thorsten Reichert, Guenther Reithmaier, Fabrice Laussy, Ulrich Hoheneester

Symposium Thermoelectric and Spincaloric Transport in Nanostructures (SYTS)

SYTS 1.1	Wed	9:30–10:00	H1	**Transport in Old and New Thermoelectric Materials** — •David Singh
SYTS 1.2	Wed	10:00–10:30	H1	**Binary oxide structures as model systems for thermoelectric transport** — •Peter J. Klar, Christian Heiliger
SYTS 1.3	Wed	10:30–11:00	H1	**Functional oxides films: from single crystals to polycrystalline substrates** — •Wilfrid Prellier
SYTS 1.4	Wed	11:00–11:30	H1	**The Planar Nernst Effect and the Search for Thermal Spin Currents in Ferromagnetic Metals** — •Barry Zink
SYTS 1.5	Wed	11:30–12:00	H1	**Tunneling magneto thermopower in magnetic tunnel junction nanopillars** — Niklas Liebing, Santiago Serrano-Guisan, Patryk Krzysteczko, Karsten Rott, Günter Reiss, Jürgen Langer, Berthold Ocker, •Hans Werner Schumacher

Symposium Quantum Plasmonics (SYQP)

SYQP 1.1	Wed	15:00–15:30	H1	**Quantum plasmonics and applications in light harvesting** — •Peter Nordlander
SYQP 1.2	Wed	15:30–16:00	H1	**Deterministic quantum plasmonics with single nanodiamonds** — •Serge Huant, Oriane Mollet, Aurelien Cuche, Aurelien Drezet
SYQP 1.3	Wed	16:00–16:30	H1	**Optically-active hybrid nanostructures: Exciton-plasmon interaction, Fano effect, and plasmonic chirality** — •Alexander Govorov
SYQP 1.4	Wed	17:00–17:30	H1	**Quantum nano-optics: Interaction of metallic nano-particles with quantum emitters** — •Salvatore Savasta
SYQP 1.5	Wed	17:30–18:00	H1	**Non-dipolar & magnetic interactions with optical antennas** — Alberto Curto, Martin Kuttge, Marta Castro-López, Ion Hancu, Tim Taminiau, •Niek van Hulst

Symposium Photons for Magnetism (SYPM)

SYPM 1.1	Thu	15:00–15:30	H1	**Ultrafast emergence of nanoscale ferromagnetism far from equilibrium** — •Hermann Dürr
SYPM 1.2	Thu	15:30–16:00	H1	**Free-Electron Laser for Ultrafast Measurements in Material Science** — •Sven Reiche
SYPM 1.3	Thu	16:00–16:30	H1	**Nanomagnetism seen by Femtosecond X-rays** — •Stefan Eisebitt
SYPM 1.4	Thu	16:30–17:00	H1	**Ultrashort Radiation Pulses at Storage Rings** — •Holger Huck
SYPM 1.5	Thu	17:00–17:30	H1	**Every atom counts - Magnetic properties of supported metal atoms and small alloy clusters** — Torben Beeck, Ivan Baev, Steffen Palutke, Kai Chen, Sören Meyer, Kari Jänkälä, Michael Martins, •Wilfried Wurth

Symposium Frontiers of Electronic Structure Theory: Discovery of Novel Functional Materials (SYES)

SYES 1.1	Fri	9:30–10:00	H1	**Molecular dynamics simulation of nucleation and growth of crystals from solution** — •Michele Parrinello
SYES 1.2	Fri	10:00–10:30	H1	**Describing, understanding, and discovering hybrid materials from first principles** — •Claudia Draxl
SYES 1.3	Fri	10:30–11:00	H1	**Mapping the Electronic Structure Landscape for Materials Discovery** — •Krishna Rajan
SYES 1.4	Fri	11:00–11:30	H1	**New ferroelectrics and antiferroelectrics by design** — •Karin Rabe
SYES 1.5	Fri	11:30–12:00	H1	**The Materials Project: The design of materials using high-throughput ab initio computations** — •Gerbrand Ceder

Annual General Meeting of the Semiconductor Physics Division

Thursday 18:00 H14

HL 1: Tutorial: Coherent Control

The term 'Coherent Control of Quantum Systems' comprises a variety of closely related ideas from different branches of physics. They all have the common goal of exploiting coherence properties of laser light or long-wavelength radiation to create quantum mechanical interferences of matter waves that can steer a quantum system into a certain pre-defined target channel. Coherent control techniques are very general and can be applied to virtually any quantum system. This Tutorial provides an introduction to coherent control concepts and discusses recent applications of such ideas in solid state physics and nanooptics as well as chemical physics and chemistry. Theoretical challenges posed by the many-body nature of all real systems are highlighted as well. (Organized by the Semiconductor Physics Division)

Time: Sunday 16:00–18:30 Location: H2

Tutorial HL 1.1 Sun 16:00 H2

Optimal Control Theory — •E.K.U. Gross — Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

An overview of quantum optimal control theory will be given. Usually in quantum mechanics we prescribe an external field, say a laser or a magnetic field, and then solve the time-dependent Schroedinger equation to calculate from the wave function the observables of interest. Optimal control deals with an inverse problem: One first defines a goal that the laser pulse should achieve, the so-called "control target", and then one calculates, with certain algorithms, an optimally shaped laser field that achieves the prescribed goal. Examples of control targets are (i) to switch the chirality of the current in a quantum ring [1], (ii) to keep electrons localized in a given region of space [2], (iii) to minimize or maximize ionization of a molecule with the total fluence of the laser kept fixed [3], or (iv) to drag a wave packet along a given path through a nanostructure. We shall describe in detail how a given goal can be formulated in terms of a target functional which is to be maximized by the optimized pulse. Together with the underlying equation of motion, i.e. the time-dependent Schroedinger equation or the time-dependent Kohn-Sham equation [4], this maximization leads to a set of variational equations whose numerical solution yields the desired optimal pulses. [1] E. Rasanen, A. Castro, J. Werschnik, A. Rubio, E.K.U. Gross, PRL 98, 157404 (2007). [2] E. Rasanen, A. Castro, J. Werschnik, A. Rubio, E.K.U. Gross, PRB 77, 085324 (2008). [3] A. Castro, E. Rasanen, A. Rubio, E.K.U. Gross, EPL 87, 53001 (2009). [4] A. Castro, J. Werschnik, E.K.U. Gross, PRL 109, 153603 (2012).

Tutorial HL 1.2 Sun 16:35 H2

Coherent control in ultrafast nano-optics — •Tobias Brixner[1], Martin Aeschlimann[2], and Walter Pfeiffer[3] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg — [2]Fachbereich Physik and Research Center OPTIMAS, Technische Universität Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern — [3]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld

Coherent control in general exploits the phase properties of light fields to manipulate coherent processes. While these concepts have initially been developed for molecular systems, it has recently become possible also to control nano-optical phenomena, i.e., the properties of electromagnetic fields below the diffraction limit of light. In this talk it will be shown how shaped femtosecond laser pulses can be used to achieve spatial and spatiotemporal control, and fundamental mechanisms will be illustrated [1]. Apart from closed-loop implementations using iterative learning algorithms, analytic schemes have been developed and realized experimentally. Applications of ultrafast nano-control also make possible novel nonlinear spectroscopy techniques.

[1] W. Pfeiffer, M. Aeschlimann, and T. Brixner, "Coherent control of nano-optical excitations," in "Optical Antennas," M. Agio and A. Alù, eds. (Cambridge University Press, 2013), Chapter 9.

Coffee break

Tutorial HL 1.3 Sun 17:20 H2

Coherent control of ultrafast electron dynamics — •Matthias Wollenhaupt — Universität Kassel

Exploiting the coherence properties of laser light along with quantum mechanical interferences of matter waves in order to steer a quantum system into a pre-defined target channel is at the heart of coherent control [1]. The increasing availability of laser sources operating on the time scale of molecular dynamics, i.e. the femtosecond regime, and the increasing capabilities of shaping light in terms of amplitude, phase and polarization (down to zeptosecond precision [2]) brought the temporal aspect of this field to the fore. In this tutorial on coherent control we will shortly review some of the physical principles of coherent control, present some pertinent examples and perspectives of current experimental efforts in controlling electronic excitations with tailored light fields such as the creation of designer electron wave packets [3,4] and charge oscillation driven chemistry [5,6]. [1] M. Wollenhaupt and T. Baumert, Faraday Discuss 153, 9 (2011). [2] J. Köhler et al., Opt Express 19, 11638 (2011). [3] M. Wollenhaupt et al., Appl Phys B 95, 245 (2009). [4] M. Wollenhaupt, M. Krug, and T. Baumert, Phys Journ 11, 37 (2012). [5] M. Wollenhaupt et al., Chem Phys Lett 419, 184 (2006). [6] T. Bayer, M. Wollenhaupt, and T. Baumert, J Phys B 41, 074007-13 (2008).

Tutorial HL 1.4 Sun 17:55 H2

Ultrafast coherent control of electrical currents in semiconductors and nanostructures — •Markus Betz — Experimentelle Physik 2, TU Dortmund

Current flow through semiconductor devices is usually achieved by applying potential differences to contacts. Over the last 15 years, however, also purely optical approaches to induce currents on the femtosecond timescale have been developed. Ultrabroadband light pulses - synthesized from a fundamental and its second harmonic - have proven particularly useful for such coherent control techniques. Current injection thereby relies on a quantum interference of one- and two-photon absorption pathways. The vectorial direction of the lateral current is dictated by the phase structure of the light field and its polarization. In my talk I will review the concept of coherent control of electrical currents in semiconductors. Starting from current injection in the prototypical direct semiconductor GaAs, we have extended the technique to the indirect bandgap materials silicon and germanium. Currents are also induced in single semiconductor nanostructures. In particular, we analyze optically induced currents in electrically contacted GaAs nanowires as well as hybrid structures functionalized with optical antennas. More recent experiments show up spectroscopic applications which conveniently combine the time resolution of ultrafast optics with amplitude- and phase-resolution of interferometric techniques.

HL 2: Ultrafast phenomena

Time: Monday 9:30–10:45 Location: H2

HL 2.1 Mon 9:30 H2

Ultrafast electron diffraction: Visualization of atomic motion in 4D — •Peter Baum — Max-Planck-Institute of Quantum Optics, and Ludwig-Maximilians-Universität München, Germany

The pathways of transitions in materials and molecules are determined by the motions of atoms and electron densities, on Angstrom scales and in femtosecond or attosecond times. We provide here an account of how ultrashort electron pulses can be used to obtain a four-dimensional visualization in space and time. At two examples, the

insulator-metal phase transformation in VO_2 [1] and the interlayer dynamics of graphite [2], we demonstrate the resolution of coherent and incoherent atomic displacements with picometer and femtosecond resolution, indicating the sequential nature of atomic motion in condensed matter transitions. Electron densities can move in times as short as attoseconds. Single-electron pulses [3] afford some promise to reach into this novel regime [4]; we will discuss our approaches and what discoveries we may expect to see [5-6].

[1] Baum, Yang, Zewail, Science 318, 788 (2007)
[2] Carbone, Baum, Rudolf, Zewail, PRL 100, 035501 (2008)
[3] Aidelsburger, Kirchner, Krausz, Baum, PNAS 107, 19714 (2010)
[4] Baum and Zewail, PNAS 104, 18409 (2007)
[5] Baum and Zewail, Chem. Phys. 366, 2-8 (2009)
[6] Baum, Manz, Schild, Sci. China 53, 987 (2010)

HL 2.2 Mon 9:45 H2

Femtosecond point-projection imaging of nanostructures with coherent low-energy electron pulses — •Melanie Müller, Alexander Paarmann, and Ralph Ernstorfer — Fritz-Haber-Institut der MPG, Berlin, Germany

We report on the development of a novel approach for time-resolved imaging of nanostructures based on a metal nanotip used as laser-triggered low-energy electron point source (LEEPS) delivering highly coherent ultrashort electron pulses. Due to their high sensitivity to weak fields, low-energy electron pulses are particularly well-suited for mapping transient electric fields and charge distributions in photoexcited nanostructures. We present first experimental data on LEEPS projection imaging of semiconductor nanowires with femtosecond electron pulses, demonstrating spatial resolution of several 10 nm. For the upcoming implementation of pump-probe measurements we expect 100 femtosecond temporal resolution, supported by numerical simulations of the electron pulse propagation.

HL 2.3 Mon 10:00 H2

Towards Terahertz Pulse Shaping — •Jan-Martin Rämer[1,2] and Georg von Freymann[1,2] — [1]Fraunhofer-Institut für Physikalische Messtechnik IPM, 67663 Kaiserslautern, Germany — [2]Technische Universität Kaiserslautern, 67663 Kaiserslautern, Germany

We present a system capable of manipulation of phase and amplitude of pulsed terahertz radiation. A grating stretcher is used to spatially disperse the spectra of frequency doubled laser pulses generated by a $1.56\,\mu m$ femtosecond fiber laser. A spatial light modulator is placed within the fourier plane of the grating stretcher, allowing the application of phase changes on spectral components of the femtosecond pulse. Phase masks for shaping of the optical pulses are retrieved using the Gercherg-Saxton algorithm, allowing a fast retrieval time. Light temporally shaped by this setup is focussed onto a LTG-GaAs photoconductive antenna generating terahertz radiation which is measured using a second photoconductive antenna. We demonstrate temporal shifts of terahertz pulses as well as generation of terahertz pulse trains.

HL 2.4 Mon 10:15 H2

Longitudinal fields in focused terahertz beams — •Stephan Winnerl[1], Ralf Hubrich[1], Martin Mittendorff[1,2], Harald Schneider[1], and Manfred Helm[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany

In textbooks electromagnetic waves are often described as infinitely extended plane waves, which are of purely transverse character. For beams of finite size, however, also longitudinal fields are expected. In case of focused radially polarized beams, the longitudinal fields can actually be stronger as compared to the transverse components. This has been found in experiments recording the intensity of near-infrared beams. In our study we directly record the electric field of single cycle terahertz pulses of radial and linear polarization. This enables us to reveal the phase relation between longitudinal and transverse fields. The obtained value of $\pi/2$ is of universal nature as it does not depend on the type of mode, frequency or focusing condition. Additionally we demonstrate that the longitudinal components of radially polarized beams exhibit superior focusing properties.

HL 2.5 Mon 10:30 H2

Manipulating intraexcitonic transitions in quantum wells — •Sangam Chatterjee[1], William D. Rice[2,3], Junichiro Kono[2,3], Sabine Zybell[4,5], Stephan Winnerl[4], Jayeeta Bhattacharyya[4], Harald Schneider[4], Manfred Helm[4,5], Benjamin Ewers[1], Alexey Chernikov[1], Martin Koch[1], Hyatt M. Gibbs[6], Galina Khitrova[6], Lukas Schneebeli[1], Benjamin Breddermann[1], Mackillo Kira[1], and Stephan W. Koch[1] — [1]Faculty of Physics, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]Department of Electrical and Computer Engineering, Rice University, Houston, Texas 77005, USA — [3]Department of Physics and Astronomy, Rice University, Houston, Texas 77005, USA — [4]Helmholtz-Zentrum Dresden-Rossendorf, P.O. Box 510119, D-01314 Dresden, Germany — [5]Technische Universität Dresden, 01062 Dresden, Germany — [6]College of Optical Science, University of Arizona, Tucson, Arizona 85721-0094, USA

We manipulate a 1s excitonic population in (GaIn)As quantum wells at cryogenic temperatures with free-electron laser (FEL) pulses tuned to the 1s-2p transition energy of the sample. The FEL induces strong emission at the 2s exciton seemingly invoking a transition which is forbidden in atomic systems due to selection rules. A microscopic many-body theory explains the experimental observations as a Coulomb-induced mixing of the 2s and 2p states, yielding an effective transition between the 1s and 2s populations making this observation a manifestation of the many-body nature of the excitonic system.

HL 3: Focus Session: Electron-phonon interaction and ultrafast processes in semiconductors

Femtosecond pulsed lasers have recently emerged as powerful tools to probe the vibrational properties of bulk as well as nanostuctured semiconductors. The results of such experiments require an accurate theoretical modeling for their interpretation. While the tools for conducting such calculations start to emerge, their application to real systems remains challenging. At the ab-initio level the methods are computationally extremely demanding; while at the mesoscopic level, the electron (excitonic) - vibronic interaction requires careful parametrization. This focus session will give an overview of the present state of the art ab-initio and mesoscopic descriptions, with connection to modern experiments. (Organizers: Gabriel Bester, MPI Stuttgart, and Michael Oestreich, University of Hannover)

Time: Monday 9:30–14:00 Location: H13

Topical Talk HL 3.1 Mon 9:30 H13

Ultrafast processes in carbon nanotubes and quantum dots — •Ulrike Woggon — Institute of Optics and Atomic Physics, TU Berlin, Germany

Phonon-assisted ultrafast relaxation determines the femtosecond and picosecond dynamics of a great variety of semiconductor nanostructures. Famous examples are quantum dots, colloidal nanocrystals and semiconducting carbon nanotubes. Devices based on these nanostrcutures are thus ideally suited for high-speed telecommunication applications. In particular, QD-SOAs feature a great potential for ultrafast nonlinear signal processing. The understanding of the ultrafast scattering processes in nanotubes is the key for exploiting the huge application potential which nanotubes offer, e.g. for light-emitting and detecting nanoscale electronic devices. We investigate population and phase dynamics in In(Ga)As QDs by heterodyne ultrafast two-color pump-probe spectroscopy which yields complementary information on amplitude and phase dynamics. In a joint study of two-color pump-probe experiments and microscopic calculations based on the density matrix formalism, we extract, both experimentally and theoretically, picosecond carrier relaxation dynamics in single-walled carbon nantubes and ascribe it to the intraband scattering of excited carriers with acoustic phonons. The calculated picosecond relaxation times show a

decrease for smaller tube diameters. Theoretical results of phonon-assisted scattering processes are in good agreement with the observed scattering and relaxation times.

HL 3.2 Mon 10:00 H13

Zero-point motion and temperature effects on the band gap renormalization of semiconductor nanoclusters — Peng Han and •Gabriel Bester — Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany.

Using the frozen-phonon approach based on *ab initio* density functional theory (DFT), we calculate the zero-point motion band gap renormalization and the temperature dependent of the band gap in semiconductor nanoclusters. Our method avoids the large computational costs (especially the slow convergence with respect to the number of unoccupied bands) associated with the calculation of the Fan- (self-energy-) and the Debye-Waller terms. A band gap reduction in silicon clusters with a magnitude of hundreds of meV induced by the quantum zero-point atomic motion is obtained; this quantum effect is found to increase with decreasing cluster size. Based on the Bose-Einstein distribution, we further study the temperature dependence of the band gap in semiconductor nanoclusters and find a reduction of 580 meV and 270 meV at room temperature for silicon clusters with radius of 9.6 and 11.9 Å, respectively. Furthermore, we find that the Si-H rotation and shear modes play an important role on the zero-point band gap renormalization of hydrogen passivated silicon clusters. By analyzing the mode dependence of the band gap reduction, we also see that the zero-point renormalization of the band gap is dominated by the optic-like vibrations with Γ_4 point group symmetry.

Topical Talk HL 3.3 Mon 10:15 H13

Quantum dots - artificial atoms, molecules or small pieces of bulk? Nonadiabatic molecular dynamics in the Kohn-Sham representation. — •Oleg Prezhdo[1], Heather Jaeger[1], Long Run[1], Amanda Neukirch[1], and Kim Hyeon-Deuk[2] — [1]University of Rochester, Rochester, NY, USA — [2]Kyoto University, Kyoto, Japan

Quantum dots (QD) are quasi-zero dimensional structures with a unique combination of solid-state and atom-like properties. Unlike bulk or atomic materials, QD properties can be modified continuously by changing QD shape and size. Often, the bulk and atomic viewpoints contradict each other. The atomic view suggests strong electron-hole and charge-phonon interactions, and slow energy relaxation due to mismatch between electronic energy gaps and phonon frequencies. The bulk view advocates that the kinetic energy of quantum confinement is greater than electron-hole interaction, charge-phonon coupling is weak, and relaxation through quasi-continuous bands is rapid. QDs exhibit new physical phenomena: The phonon bottleneck to electron energy relaxation and generation of multiple excitons can improve efficiencies of photovoltaic devices. Our state-of-the-art nonadiabatic molecular dynamics techniques, implemented within time-dependent density functional theory, allow us to model QDs at atomistic level and in time-domain, providing a unifying description of quantum dynamics on the nanoscale.

HL 3.4 Mon 10:45 H13

Ab initio molecular dynamics simulations of ultrafast melting of Si — •Tobias Zier, Eeuwe S. Zijlstra, and Martin E. Garcia — Theoretical Physics, University of Kassel, Germany

After an intense ultrashort-laser excitation of Si the crystalline structure disorders within several 100's of femtoseconds. This phenomenon is known as ultrafast melting. The underlying effect is the bond softening as a consequence of the laser-induced highly nonthermal state in which the electrons have a temperature of several 10 000 K, while the ions remain close to room temperature. Performing MD-Simulations for supercells with up to 640 atoms allowed us to follow the ionic motion after its excitation. Our results provide new insights in the first steps of nonthermal melting by showing that the ionic motion is dominated by different physical effects, dependent on the timescale, namely, acceleration, deceleration, and diffusion.

Topical Talk HL 3.5 Mon 11:00 H13

Out-of-equilibrium carrier dynamics in semiconductors: a novel approach — •Andrea Marini — Istituto di Struttura della Materia of the National Research Council, Via Salaria Km 29.3, I-00016 Monterotondo Stazione, Italy — European Theoretical Spectroscopy Facilities (ETSF)

In this talk I will present a novel approach based on the merging of Non-Equilibrium Green's function theory and Density Functional Theory to investigate the carrier dynamics following a pump excitation.

The case of bulk Silicon, a paradigmatic indirect gap semiconductor, is studied by using the Baym–Kadanoff equations. Both the electron–electron (e–e) and electron–phonon (e–p) self–energies are calculated fully *Ab–Initio* by using a semi–static *GW* approximation in the e–e case and a Fan self–energy in the e–p case. By using the generalized Baym–Kadanoff ansatz the two–time evolution is replaced by the only dynamics on the macroscopic time axis.

The enormous numerical difficulties connected with a real–time simulation of realistic systems is overcomed by using a completed collision approximation that further simplifies the memory effects connected to the time evolution. The carrier dynamics is shown to reduce in such a way to have stringent connections to the well–known equilibrium electron–electron and electron–phonon self–energies.

Lunch break

Topical Talk HL 3.6 Mon 12:30 H13

The role of phonons for exciton and biexciton generation in a quantum dot driven by adiabatic rapid passage — •Tilmann Kuhn — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

The excitation of a quantum dot with chirped laser pulses provides a powerful tool for a robust preparation of quantum states. This process, known as adiabatic rapid passage, can be well understood using the concept of dressed states. Compared to an ideal few-level system interacting with a chirped light pulse, however, the dynamics in a quantum dot is strongly modified by the influence of acoustic phonons which may lead to dephasing and transitions between the dressed states and therefore deteriorate the adiabatic passage.

In this talk I will present a theoretical analysis of the role of phonons for the preparation of either exciton or biexciton states in a quantum dot. At low temperatures phonon emission leads to pronounced asymmetries in the exciton state preparation when changing the sign of the chirp. When using linearly polarized light, the fidelity of the exciton preparation may be additionally reduced by phonon-assisted biexciton generation. On the other hand, by suitably tailoring the pulse parameters the biexciton state can be selectively prepared by using either a two-photon resonance excitation or a two-color scheme.

HL 3.7 Mon 13:00 H13

Electron-phonon coupling in colloidal CdSe/CdS core-shell quantum dots — •Steffen Westerkamp, Andrei Schliwa, Amelie Biermann, and Christian Thomsen — Institut für Festkörperphysik, Technische Universität Berlin, Germany

Phonon frequencies and eigenvectors, and their coupling to excited electronic states are calculated for approximately spherical, CdSe/CdS core-shell quantum dots (QD).

The equilibrium atomic positions and phonon modes are obtained using an empirical force model. Electron and hole wavefunctions are calculated using the 8-band-kp envelope function method, thus taking into account band coupling, strain, and piezo/pyroelectric effects. These results are combined to determine the Huang-Rhys-factors thus reflecting the electron-phonon coupling for each phonon mode.

We vary size, core-shell thickness ratio, and the sharpness of the interface of the quantum dots and discuss the impact of interface- and surface-phonons.

Topical Talk HL 3.8 Mon 13:15 H13

Spin lifetime and electron-phonon interaction in graphene — •Guido Burkard — University of Konstanz, Germany

Graphene and carbon nanotubes represent interesting platforms for exploring the quantum coherence of localized electron spins in suitably tailored nanostructures [1]. Due to the low density of nuclear spins in graphene, one can expect long spin coherence times. However, as in semiconductor quantum dots, the spin lifetime in graphene quantum dots at low temperatures will be limited by the spin-orbit coupling and phonon emission processes. We present a theoretical study of the spin lifetime of single electrons as a function of the magnetic field in quantum dots formed by electrostatic confinement in gapped graphene [2] and in armchair graphene nanoribbons [3]. We show that spin relaxation processes can be suppressed in a phonon cavity such as in suspended carbon nanotubes, and instead a coherent strong coupling of a single spin and a single phonon mode becomes possible [4]. This coupling opens new possibilities for spin readout [5] and manipulation.

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HL 3.9 Mon 13:45 H13

Theory of optical emission in semiconductor nanostructures - selforganized, colloidal quantum dots and quantum wells — •Marten Richter, Uyen-Khanh Dang, Julia Kabuss, Alexander Carmele, Mario Schoth, Matthias-Rene Dachner, and Andreas Knorr — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany

The coupling of electrons and phonons in semiconductor nanostructures shows a strong impact on their quantum dynamics. In this talk, we discuss the electron–phonon assisted optical emission of quantum dots and quantum wells. We start with an analysis of the influence of acoustical and optical phonons on the fluorescence and Raman signals of selforganized quantum dots. In particular, frequency and time resolved spectra are analyzed. For quantum well intersubband transitions, longitudinal phonons cause inter- and intrasubband relaxation. We discuss these processes and their visibility in 2D coherent spectra. At the end, we give an outlook to the electron–phonon interaction in colloidal quantum dots compared to selforganized quantum dots, with a focus on the process of carrier multiplication.

HL 4: III-V semiconductors: mainly wells and surfaces

Time: Monday 9:30–12:30 Location: H15

HL 4.1 Mon 9:30 H15

Modulating plasmons in two-dimensional hole gas systems by spin-orbit interactions — •Andreas Scholz, Tobias Dollinger, Paul Wenk, Klaus Richter, and John Schliemann — Institute for Theoretical Physics, University of Regensburg, Germany

We study the dynamical dielectric function of a two-dimensional hole gas, exemplified on [001]-GaAs and InAs quantum wells, within the four band Luttinger model including bulk and structure inversion asymmetric terms. The plasmon dispersion shows a pronounced anisotropy for GaAs and InAs based systems. In GaAs this leads to a suppression of plasmons due to Landau damping in some orientations while others are virtually undamped. Due to the large Rashba contribution in InAs based heterostructures, the lifetime of long-wavelength plasmons can be controlled efficiently by changing the electric field. This effect might be useful in plasmon field effect transistors as already proposed for electron gases.

HL 4.2 Mon 9:45 H15

Spin dynamics in high-mobility (110) GaAs-based quantum wells — •Roland Völkl[1], Tobias Korn[1], Markus Schwemmer[1], Michael Griesbeck[1], Sergey Tarasenko[2], Dieter Schuh[1], Werner Wegscheider[3], and Christian Schüller[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg — [2]A. F. Ioffe Physical-Technical Institute, Russian Academy of Sciences, St. Petersburg, Russia — [3]ETH Zurich, Switzerland

Here, we present a study of electron spin dynamics in symmetrical, high mobility (110)-grown, GaAs-based quantum wells. The Hanle-MOKE method is used to determine the spin lifetime and the spin polarization of electrons. These properties are studied regarding to changing parameters like temperature or pump power. Additionally the electron density can be tuned using the optical gating technique. Samples with a quantum well width of 20 nm and 30 nm are investigated. In the 30 nm quantum well the Bir-Aronov-Pikus mechanism is dominating, in the investigated temperature range between 4 and 60 K therefore high excitation intensity leads to a faster decay of electron spins. In the 20 nm quantum well this behavior is found at temperatures above 30 K. Below this temperature the Dyakonov-Perel mechanismus dominates. This results in an increase of the spin lifetime for increasing excitation intensities. Financial support by the DFG via SFB 689 and SPP 1285 is gratefully acknowledged.

HL 4.3 Mon 10:00 H15

Coherence measurements of dipolar, indirect excitons — J. Repp[1,2], •S. Dietl[1], G.J. Schinner[2], E. Schubert[2], A.K. Rai[3], D. Reuter[3], A.D. Wieck[3], A.O. Govorov[4], A. Högele[2], J.P. Kotthaus[2], and A.W. Holleitner[1] — [1]Walter Schottky Institut and Physik Department, Technische Universität München — [2]Fakultät für Physik and Center for Nanoscience, Ludwig-Maximilians-Universität München — [3]Angewandte Festkörperphysik, Ruhr-Universität Bochum — [4]Department for Physics and Astronomy, Ohio University, Athens, Ohio 45701, USA

We report on electrostatically widely tunable trapping devices for dipolar indirect excitons in InGaAs-based double quantum wells. Resonantly excited direct excitons transform into such indirect excitons which are then collected in electrostatically shaped energy landscapes. With their electron and hole confined to two different quantum wells, these indirect excitons exhibit a large dipole moment and long lifetimes. Employing a 3He-cooled confocal microscope at temperatures below 250 mK, we generate indirect excitons at a location outside the traps and measure their photoluminescence from the trap center after they have been cooled to lattice temperatures. Since the thermal de Broglie wavelength exceeds the excitonic separation in this temperature regime, many-body correlations between trapped indirect excitons are expected. We report on measurements of the temporal and spatial coherence of the emitted photoluminescence and discuss the coherence of the exciton ensemble.

HL 4.4 Mon 10:15 H15

MOVPE-growth and characterisation of GaPN/Si(100) for photoelectrolysis — •Helena Stange[1,2], Oliver Supplie[1,2], Matthias M. May[1,2], Christian Höhn[1], Wolf-Dietrich Zabka[1,2], Christian Koppka[3], Katja Tonisch[3], Henning Döscher[1,3,4], and Thomas Hannappel[1,3,5] — [1]Helmholtz-Zentrum Berlin, Institute of Solar Fuels — [2]Humboldt-Universität zu Berlin — [3]TU Ilmenau, Institut für Physik, Fachgebiet Photovoltaik — [4]NREL, Golden, USA — [5]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, Erfurt

Among III-V semiconductors, the dilute nitride GaPN offers a bandgap close to the optimum for the top cell of a photoelectrochemical tandem device with Si as bottom cell [1,2]. Bandgap engineering permits to adjust the bandgap of GaP to a suitable value by the incorporation of N, while simultanouesly converting it to a direct semiconductor [3] and achieving lattice match to Si. We used reflection anisotropy spectroscopy (RAS) and mass spectrometry to monitor GaP and GaPN growth on Si(100) in situ during metalorganic vapour phase epitaxy. Via a contamination-free transfer system, we related RAS results with UHV surface science techniques, such as low-energy electron diffraction and photoelectron spectroscopy. We applied high-resolution X-ray diffraction and AFM ex situ to analyse the dependence of crystal quality and surface morphology on MOVPE-parameters such as growth temperature, growth rate, P/N ratio and annealing conditions.
[1] Döscher et al., *ChemPhysChem* **13** (2012) 2899. [2] Geisz et al., *EUPVSEC* **19** (2004). [3] Wu et al., *PRB* **65** (2002) 241303.

HL 4.5 Mon 10:30 H15

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 the studies to clarify the impact of the Bi content on disorder effects in Ga(As1-xBix)/GaAs SQWs. The experimental techniques employed are continuous-wave and time-resolved photoluminescence. Two theoretical models are used to quantify the disorder parameters: Firstly, a simple model with a single energy scale based on the carrier dynamics at very low temperatures. Secondly, a model of hopping excitons with two energy scales based on the features of the PL spectra.

HL 4.6 Mon 10:45 H15

Temperature-dependent external quantum efficiency of Ga(NAsP) quantum wells — •Robin Döring[1], Nils Rosemann[1], Bernardette Kunert[2], Wolfgang Stolz[1,2], Kerstin Volz[1], and Sangam Chatterjee[1] — [1]Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]NAsP III/V GmbH, Am Kechtacker 19, D-35041 Marburg, Germany

Silicon is the basis for today's microelectronics and even some optoelectronic components such as waveguides; however, it is not considered useful as an active medium for lasers due to the nature of its indirect bandgap. Various approaches have been pursued to add this functionality to Si microelectronics such as Raman-or nanocrystal-based concepts both native to silicon or hybrid integration. An alternative concept is the quasi-lattice matched integration of direct-gap GaP based quaternary alloys. Here, electrically pumped lasing has already been demonstrated[1]. Nevertheless, many challenges such as low-temperature operation and comparatively large laser thresholds remain. To help tackle these, we investigated a series of Ga(NAsP)/GaP multiple quantum well (MQW) samples by temperature-dependent absolute photoluminescence spectroscopy using an integrating sphere mounted inside a cryostate. The results are compared to a standard laser material, a high-quality (GaIn)As/GaAs MQW. At low temperatures, the reference sample outperforms the Ga(NAsP) structures. While the EQEs of both materials are comparable at room temperature for our experimental conditions. [1]Appl. Phys. Lett. 99, 071109, (2011)

Coffee break

HL 4.7 Mon 11:15 H15

Bandgap modification of GaP and GaAs achieved by N-implantation and ultra-short thermal treatment — •Kun Gao, Slawomir Prucnal, Wolfgang Skorupa, Manfred Helm, and Shengqiang Zhou — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), P.O. Box 510119, 01314 Dresden, Germany

The giant band gap bowing effect observed in III-V dilute nitride alloys is promising for modification of III-V semiconductors to increase their flexibility in virtue of the strong electronegativity and small size of nitrogen atoms.

In this contribution we present the bandgap modification of GaAs and GaP by N-implantation followed by flash lamp annealing (FLA) and pulsed laser melting (PLM). In both GaAs and GaP wafers, N was implanted to form a 100 nm thick layer on top with an atomic concentration of about 1 %. After implantation, within the as-implanted range, both GaAs and GaP become amorphous. Post-implantation thermal treatment (FLA for GaAs:N and PLM for GaP:N) leads to the recrystallization of GaAs and GaP, as well as the incorporation of the N atoms into the lattice effectively, which is confirmed by micro-Raman and photoluminescence studies. The results show that about 40 % of the implanted N atoms are successfully incorporated into the lattice. According to our investigation, ion-implantation followed by ultrashort thermal treatment, which is quite efficient and low-cost, exhibits a promising prospect on bandgap engineering of semiconductors.

HL 4.8 Mon 11:30 H15

Indirect Excitons transport and manipulation in 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 of a double quantum well structure. Due to their long lifetimes and strong non-linear properties arising from dipole-dipole interactions IXs are particularly interesting for applications in optoelectronic devices [1]. In this contribution, we demonstrate that a high degree of control of IX fluids can be obtained by combining their manipulation via electrostatic gates with the long - range IX transport achieved by Surface Acoustic Waves (SAW). The moving type-I band-gap modulation induced by the SAW strain field traps and transports the long-living IXs [2]. The spatial and energetic distributions of IXs are investigated using spatially and spectrally resolved photoluminescence. In addition, time resolved techniques are used to study the space and temporal dynamics of the IXs packets transported by SAW.

[1] A. A. High et al., Science 321, 229-231 (2008)
[2] J. Rudolph, R. Hey and P. V Santos, Phys. Rev. Lett. 99, 047602[4] (2007)

HL 4.9 Mon 11:45 H15

Interaction of potassium with InN(0001)-(2×2)-surfaces — •Stephanie Reiss, Anja Eisenhardt, Stefan Krischok, and Marcel Himmerlich — Institut für Physik and Institut für Mikro- und Nanotechnologien, TU Ilmenau, PF 100565, 98684 Ilmenau, Germany

In this work we investigate the interaction of potassium with InN(0001)-(2×2)-surfaces. The 2×2 reconstructed InN-films were grown by plasma assisted molecular beam epitaxy (PAMBE) on GaN/Sapphire-templates. Immediately after epitaxy the samples were in-situ characterised by photoelectron spectroscopy (PES). Potassium was offered via an alkali metal dispenser while performing PES-measurements. The potassium adsorption leads to a strong reduction of the work function of the InN indicating the formation of a positive potassium-induced surface dipole acting as an electron donator. In parallel, the core levels and valence band (VB) maximum shift by 0.2 eV towards lower binding energies. Thus potassium adsorption leads to a reduction of the surface downward band bending from originally 0.6 eV to 0.4 eV. Furthermore, complex changes in the valence band region are observed and will be discussed with particular emphasis on the occupied states close to E_F. Here, the potassium adsorption leads to the appearance of new states at 1.2 eV and 0.6 eV whereas a depletion of the surface state at the Fermi edge caused by the 2×2-surface reconstruction is observed.

HL 4.10 Mon 12:00 H15

Influence of adsorbates on the surface electronic properties of polar InN — •Anja Eisenhardt, Stephanie Reiss, Stefan Krischok, and Marcel Himmerlich — Institut für Physik and Institut für Mikro- und Nanotechnologien, TU Ilmenau, PF 100565, 98684 Ilmenau, Germany

Thin stoichiometric InN(0001)-2×2 (In-polar) and InN(000-1) (N-polar) samples were grown by plasma-assisted molecular beam epitaxy and in-situ characterized by photoelectron spectroscopy (XPS, UPS). While the InN(0001)-2×2 surface shows a valence band maximum (VBM) to Fermi-level distance (E_F - VBM) of 1.4 eV, indicating a strong surface electron accumulation, the band bending at the InN(000-1) surfaces is reduced (E_F - VBM $\sim$1.0 eV). This difference can be microscopically explained by surface states that influence the position of the surface Fermi level. For InN(0001)-2×2 they are located above the conduction band minimum while at InN(000-1) an occupied surface state is located at the VBM. We will show how the interaction with adsorbates (especially oxygen and water) and the corresponding dipole formation change the surface electronic properties and the band alignment at InN surfaces. At In-polar InN surfaces, oxygen adsorbates as electron acceptors strongly reduce the electron accumulation due to the interaction with the free dangling bonds of the In-adatoms. At N-polar InN surfaces, oxygen has no further impact on the already reduced band bending. Water instead tends to increase the downward band bending at N-polar InN surfaces, while it has minor effect on the initial band alignment at In-polar InN surfaces.

HL 4.11 Mon 12:15 H15

Si–doping of AlGaN with high aluminum mole fractions by MOVPE — •F. Mehnke[1], T. Wernicke[1], C. Kuhn[1], C. Reich[1], J. Stellmach[1], F. Brunner[2], V. Kueller[2], A. Knauer[2], M. Weyers[2], and M. 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

Currently one of the main challenges of III–nitride growth is the doping of AlGaN layers with high aluminum mole fraction. Only very few

reports exist that show conductive AlGaN:Si layers with an aluminum content of more than 80 %. In this contribution we will present a study on the influence of the aluminum content and the SiH_4 supply on the resistivity and the optical properties of silicon doped $Al_xGa_{1-x}N$ layers ($0.8 < x < 1$) grown pseudomorphically on defect reduced AlN–sapphire templates. With increasing aluminum content the resistivity increases exponentially but even for $Al_{0.95}Ga_{0.05}N$ n–conductivity is observable with a resistivity of 4.3 Ω cm. Defect luminescence at 4.4 eV was observed by photoluminescence measurements (PL) becoming more dominant with increasing aluminum content and shifting towards higher energy. By increasing the SiH_4 supply during the growth of $Al_{0.82}Ga_{0.18}N$ layers a minimum resistivity of 0.026 Ω cm was obtained. By further increasing the SiH_4 supply the resistivity increased strongly. PL show dominant defect luminescence at 3 eV hinting to a compensation by point defect formation e.g. group–III vacancies or vacancy–oxygen–complexes.

HL 5: Spintronics: mainly interfaces and heterostructures

Time: Monday 9:30–11:45 Location: H16

HL 5.1 Mon 9:30 H16

Spin Transport and Spin Dephasing in ZnO — Matthias Althammer[1,2], Eva-Maria Karrer-Müller[1], Sebastian T. B. Goennenwein[1], •Matthias Opel[1], and Rudolf Gross[1,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]University of Alabama, Center for Materials for Information Technology MINT, Tuscaloosa, AL 35487 USA — [3]Physik-Department, TU München, 85748 Garching, Germany

The wide bandgap semiconductor ZnO is interesting for spintronic applications because of its small spin-orbit coupling implying a large spin coherence length. Utilizing vertical spin valve devices with ferromagnetic electrodes (TiN/Co/ZnO/Ni/Au), we create and detect a spin-polarized ensemble of electrons and demonstrate the transport of this spin information across several nanometers in ZnO [1]. The measured magnetoresistance of up to 8.4% at 2 K agrees well with the prediction of a two spin channel model with spin-dependent interface resistance [2]. Fitting the data yields spin diffusion lengths of 10.8 nm (2 K), 10.7 nm (10 K), and 6.2 nm (200 K) in ZnO, corresponding to spin lifetimes of 2.6 ns (2 K), 2.0 ns (10 K), and 31 ps (200 K) [1]. The evolution of the measured spin relaxation rates with temperature is consistent with the D'yakonov-Perel' mechanism above 30 K. For future semiconductor spintronic devices, such all-electrical experiments will be mandatory to extract the relevant spin transport parameters.

This work was supported by the DFG via SPP 1285 (GR 1132/14).

[1] M. Althammer *et al.*, Appl. Phys. Lett. **101**, 082404 (2012).
[2] A. Fert and H. Jaffrès, Phys. Rev. B **64**, 184420 (2001).

HL 5.2 Mon 9:45 H16

Anisotropy at the Fe/GaAs(001) interface - resistance and AMR-effect — •Thomas Hupfauer[1], Alex Matos-Abiague[2], Bernhard Endres[1], Matthias Sperl[1], Georg Woltersdorf[1], Martin Utz[1], Dieter Schuh[1], Dominique Bougeard[1], Christian Back[1], Jaroslav Fabian[2], and Dieter Weiss[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute of Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

We investigate transport anisotropies at Fe/GaAs interfaces. These experiments were motivated by theoretical calculations derived from a spin-orbit-field model for the TAMR-effect [1,2] which was applied to the case of lateral transport. Samples with an epitaxially grown Fe-layer consisting of six monolayers were investigated. The measurements show an anisotropy of the conductance dependent on the crystallographic axes of the GaAs, featuring a maximum along the [110]-direction and a minimum in $[1\bar{1}0]$. Additionally the strength of the AMR-effect is also dependent on the crystallographic axes, showing maxima in both [110]- and $[1\bar{1}0]$-directions, with the maximum in [110] being somewhat larger. This behavior could be reproduced by the theoretical model. Financial support by DFG via SFB 689 is gratefully acknowledged.

[1] M. Wimmer, *et al.*, Phys. Rev. B **80**, 121301(R) (2009)
[2] J. Moser, *et al.*, Phys. Rev. Lett. **99**, 056601 (2007)

HL 5.3 Mon 10:00 H16

Anisotropic Thermal Transport Through Magnetic Tunnel Junctions — •Carlos López-Monís, Alex Matos-Abiague, and Jaroslav Fabian — Institute für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

Tunneling anisotropic magnetoresistance (TAMR) has been observed in Fe/GaAs/Au tunneling heterostructures [1]. Theoretically, the twofold symmetry observed in the TAMR was shown to be originated by the C_{2v} symmetry of the tunneling probability, resulting from the interference between Bychkov-Rashba and Dresselhaus spin-orbit interactions [2]. In this talk I shall discuss further extensions to this model in order to account for thermal spin transport phenomena in magnetic tunnel junctions in the presence of spin-orbit interaction. We acknowledge financial support from the DFG via No. SPP 1538.

[1] J. Moser, A. Matos-Abiague, D. Schuh, W. Wegscheider, J. Fabian and D. Weiss, Phys. Rev. Lett. **99**, 056601 (2007).
[2] A. Matos-Abiague and J. Fabian, Phys. Rev. B **79**, 155303 (2009).

HL 5.4 Mon 10:15 H16

Spin storage and readout in charge-tunable structures with InGaAs quantum dots — •Andreas Merz, Helge Wurst, Franziska Reiter, Arne Ludwig, Andreas Wieck, Michael Hetterich, and Heinz Kalt — KIT, Karlsruhe, Germany

To enable electron spin manipulation in semiconductor quantum dots (QDs), the control over the lifetime of the created excitonic species in the QD is indispensable. For Schottky diode-like structures this can be obtained with charge tuning via top and back contact. The applied voltage controls electron and hole tunneling rates, enabling carrier separation and subsequent storage of spin-polarized carriers in the microsecond regime [1]. This is a promising scenario for coherent microwave spin manipulation with optically detected magnetic resonance experiments to enable spin manipulation in QDs. Since the optical injection and readout of the spin states in these devices is well-controlled, this would enable the last but most important step towards an application of single QDs as spin memory devices. [1] Carrier storage and capture dynamics on quantum-dot heterostructures. J.M. Smith, P. A. Dalgarno, R.J. Warburton et al., Appl. Phys. Lett. 82, 21 (2003).

HL 5.5 Mon 10:30 H16

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

We perform time-resolved Kerr rotation, as well as resonant spin amplification measurements, on an undoped, [100]-grown GaAs/AlAs double quantum well (QW) structure to resolve the spin dynamics of hole ensembles at low temperatures. The 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 build up a hole spin polarization with a spin lifetime of several nanoseconds in the narrower QW. On the other hand, we observe a tunable behaviour in the broader QW, where the spin dynamics are dominated either by holes or by electrons, depending on the gate voltage.

A system like this might expand the recent, very successful investigations on hole spins in [100]-grown, p-doped GaAs/AlGaAs QWs to different growth directions or other materials like InGaAs, where the difficulty of proper p-type doping has limited detailed observations, so far.

HL 5.6 Mon 10:45 H16

Electric suppression of spin dephasing in GaAs (111) quantum wells — •Alberto Hernandez-Minguez, Klaus Biermann, Rudolph Hey, and Paulo V. Santos — Paul-Drude-Institut für Festkörperelektronik

Diakonov-Perel spin dephasing is a major mechanism limiting the electron spin lifetime in III-V zincblende quantum wells: electrons with different wavevector experience different effective magnetic fields associated to spin-orbit interaction (SOI). Their spins will then precess at different frequencies, thus leading to a reduction of the initial spin

polarization of an electron ensemble. In this contribution, we demonstrate that this dephasing can be effectively suppressed in GaAs (111) quantum wells by applying an electric field. The suppression has been attributed to the compensation, for all electron wavevectors simultaneously, of the intrinsic SOI associated to the bulk inversion asymmetry (BIA) of the GaAs lattice by a structural induced asymmetry (SIA) SOI term induced by the electric field [1]. We provide direct experimental evidence for this mechanism by demonstrating the transition between the BIA-dominated to a SIA-dominated regime via photoluminescence measurements carried out over a wide range of applied fields in quantum wells embedded in a n-i-p structure. Spin lifetimes exceeding 100 ns are obtained near the compensating electric field [2], thus making GaAs (111) quantum wells excellent candidates for spin-based quantum information processing.

[1] X. Cartoixà *et al.*, Phys. Rev. B **71**, 045313 (2005).
[2] A. Hernández-Mínguez *et al.*, Phys. Rev. Lett., accepted.

HL 5.7 Mon 11:00 H16

Spin injection into semiconductor 2D systems — •Martin Oltscher, Mariusz Ciorga, Josef Loher, Dieter Schuh, Dominique Bougeard, and Dieter Weiss — Institute for Experimental and Applied Physics, University of Regensburg, Regensburg, Germany

Electrical generation and control of electron spins in semiconductor material is the central theme in semiconductor spintronics and of a big importance for device prospects. In particular spin injection into two-dimensional (2D) electron systems would allow for many new functionalities in future devices, with a Datta-Das Spin Field Effect Transistor [1] being a primary example. Building on successful realization of spin injection into bulk GaAs employing the diluted magnetic semiconductor (Ga,Mn)As as a ferromagnetic material [2] we extended our work into heterostructures containing 2D electron gases. We investigate two types of systems: an electron gas confined in an inverted AlGaAs/GaAs heterojunction and an InGaAs quantum well structure. We observe clear nonlocal spin-valve signals in both systems, however the origin of the high signal amplitude and its strong bias dependence for the high mobility AlGaAs/GaAs structure is still an open issue.

[1] S. Datta and B. Das, Appl. Phys. Lett. 56, 665 (1990)
[2] M . Ciorga et al., Phys. Rev. B 79, 165321 (2009)

HL 5.8 Mon 11:15 H16

Spin injection and spin relaxation: Magnetic field effects — •Henning Höpfner[1], Carola Fritsche[1], Arne Ludwig[2], Astrid Ludwig[2], Frank Stromberg[3], Heiko Wende[3], Werner Keune[3], Dirk Reuter[2], Andreas D. Wieck[2], Nils C. Gerhardt[1], and Martin R. Hofmann[1] — [1]Photonik und Terahertztechnologie, Ruhr-Universität Bochum, D-44780 Bochum — [2]Angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum — [3]Fakultät für Physik und CENIDE, Universität Duisburg-Essen, D-47048 Duisburg

In the last two decades, intensive research in the field of spintronics has led to remarkable progress of spintronic devices. Particularly electrical spin injection into semiconductors has provided a challenge to researchers around the world.

In magnetic remanence spin polarization of up to 3% could be achieved in spin-LEDs, while using external fields values up to 32% have been reached. We show experimentally that external magnetic fields strongly suppress spin relaxation during transport from the injector to the active region (APL 101, 112402 (2012)). Consequently, results obtained for spin injection with and without magnetic fields can hardly be compared and the efficiency of spin-induced effects will be overestimated as long as magnetic fields are applied. Since strong magnetic fields are not acceptable in application settings, this leads to wrong conclusions and potentially impairs proper device development.

Nevertheless, our results show that spin injection in magnetic remanence is possible and may provide a viable path to overcome the challenges at hand.

HL 5.9 Mon 11:30 H16

Low Temperature Spin Relaxation Rate Anisotropy in (001) GaAs/AlGaAs Quantum Wells — •David English[1], Peter Eldridge[1], Richard Harley[2], Roland Winkler[3], Jens Hübner[1], and Michael Oestreich[1] — [1]Institute for Solid State Physics, Leibniz University Hannover, Appelstr. 2, 30167 Hannover, Germany — [2]School of Physics and Astronomy, University of Southampton, Southampton, SO17 1BJ, UK — [3]Department of Physics, Northern Illinois University, DeKalb, IL 60115, USA

We present measurements of the appearance of an unexpected spin relaxation rate anisotropy below a temperature of 80K in (001) GaAs/AlGaAs quantum wells with asymmetric barriers. We develop a theoretical model that reveals the origin of this anisotropy.

In general, in-plane anisotropy of the spin relaxation rate is produced by interference of the bulk inversion asymmetry (BIA) term in the spin-orbit field with the structural inversion asymmetry (SIA) term [1]. Quantum wells with asymmetric barrier growth lack an SIA term due to the isomorphous nature of the bands [2]. The new theoretical model accounts for the temperature dependent filling of k-space by the conduction electrons away from k = 0. By considering higher order k states we demonstrate that the relaxation rate can be anisotropic at low temperatures, requiring only a BIA term and an asymmetric conduction electron wavefunction.

[1] N. Averkiev and L. Golub, Physical Review B 60, 15582 (1999).
[2] P. Eldridge, et al. Physical Review B 82, 045317 (2010).

HL 6: Graphene: Magnetic fields (HL, jointly with O, TT)

Time: Monday 9:30–11:15 Location: H17

HL 6.1 Mon 9:30 H17

Quantum interference in an electron-hole graphene ring system — •Dmitri Smirnov, Hennrik Schmidt, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2 30167 Hannover, Germany

We analyze the electronic properties of a topgated monolayer graphene ring. Micro-mechanical cleavage was used to place a flake on a Si/SiO2 substrate. The structuring and contacting was done via plasma etching and electron beam lithography. An additional gate was placed on top of one arm of the ring which allows us to control the charge carrier concentration locally and additionally to create a pnp- (npn-) junction inside the ring. The sample was measured in a He3 cryostat and is identified as single layer graphene via magnetotransport measurements.

We observe Aharonov Bohm (AB) effect by sweeping the magnetic field around 0 T. The period of the oscillations is approx. 16 mT which fits the size of the ring well. The AB-oscillations are measured for different temperatures and the amplitude shows a saturation for lower temperatures. We also observe the AB-oscillations when a pnp-junction is created inside the ring. The period is independent of the existence of a pnp-junction and stays constant in all situations. We analyze the amplitude in dependence of the charge carrier concentration. The absolute amplitude is constant in the bipolar and unipolar region [1].

[1] D.Smirnov. et. al, Appl. Phys. Lett. 100, 203114 (2012).

HL 6.2 Mon 9:45 H17

Experiments on Superlattice Graphene Structures with Patterned Top Gates — •Franz-Xaver Schrettenbrunner, Martin Drienovsky, Bastian Birkner, Sebastian Ringer, Dominik Koch, Dieter Weiss, and Jonathan Eroms — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D-93040 Regensburg

We report on fabrication, finite element modelling (FEM), and the measurements of single- and bilayer graphene with structured top gates. By using micromechanically exfoliated graphene on SiO_2 surface, a Al_2O_3 dielectric was fabricated on top of the structure by either atomic layer deposition (ALD), evaporating thin aluminum films, or by combination of both methods. A digitated, patterned top gate electrode out of an AuPd alloy was fabricated by electron beam lithography (EBL). FEM yields that form and strength of the modulation strongly depend on thickness of the top gate dielectric, periodicity of the gate fingers, and applied voltage. Using both, the planar SiO_2 back gate and the patterned Al_2O_3 top gate the electric field effect creates variable modulations of the charge carrier concentration like pnp, nn'n, n0n, etc. along the whole underlying graphene. Measurements on these structures show typical behaviour for Klein-Tunneling resulting in an asymmetric curve of the Dirac Point. At high magnetic

fields up to 14T unusual plateaus were observed when filling factors are mixing up in the top gated and the non top gated areas of the graphene samples.

HL 6.3 Mon 10:00 H17

Weak Localization and Raman Study of Graphene Antidot Lattices Obtained by Crystallographically Anisotropic Etching — •Florian Oberhuber, Stefan Blien, Stefanie Heydrich, Tobias Korn, Christian Schüller, Dieter Weiss, and Jonathan Eroms — Experimentelle und Angewandte Physik, Universität Regensburg, D-93040 Regensburg

We report the crystallographically anisotropic etching of exfoliated graphene on SiO_2 substrates by applying an etching mechanism that was demonstrated to eliminate carbon atoms located on armchair sites thus leading to zigzag edges [1]. Before exposing samples to this carbothermal reaction, they were patterned with circular antidots (diameter ≈40nm) by EBL and RIE. In the subsequent carbothermal etching step the predefined holes evolved into hexagonal antidots (≈100nm).

We investigated a set of samples patterned with square lattices of hexagonal antidots and compare them to graphene patterned with lattices of circular holes investigated previously [2]. First, we compare samples by analyzing the weak localization peak in electron transport from which we obtain the phase coherence length and lengths for inter- and intravalley scattering. Second, samples were characterized by Raman spectroscopy focusing on G, D and D* peaks. In addition to the above mentioned comparison we demonstrate the influence of the etching reaction on graphene's properties by showing a series of Raman maps acquired between consecutive sample preparation steps.

[1] Nemes-Incze et al., Nano Res. (2010)
[2] Eroms et al., New J. Phys. (2009), Heydrich et al., APL (2010)

HL 6.4 Mon 10:15 H17

Electronic structure of graphene twist flakes — •Wolfgang Landgraf, Sam Shallcross, Karla Türschmann, Dominik Weckbecker, and Oleg Pankratov — Lehrstuhl für Theoretische Festkörperphysik, Staudtstraße 7, D-91058 Erlangen

We study the electronic structure of bilayer graphene flakes with mutually rotated layers. The twist induces a large scale superstructure, a so called moiré pattern, which is a regular array of AA and AB stacked regions. We find that at low energies the electrons are trapped in the AA regions. This feature is visible even for a flake hosting a single AA moiré spot, which is thus acting as a quantum well. The electron density fluctuations induced by the moiré lattice are significant, being an order of magnitude greater than those generated by the rippling of a suspended graphene sheet. Finally, we determine the electronic properties of the twisted graphene flakes in the presence of an external magnetic field. We find a novel "zero-mode" structure, as well as Landau states that exhibit an electron current circulating between two graphene layers of the flake. The current distribution can be visualized as an electron flow on a torus circumventing the AA spot of the moiré lattice.

HL 6.5 Mon 10:30 H17

Functionalized Graphene in Quantizing Magnetic Field: The case of bunched impurities — •Peter Silvestrov — Dahlem Center for Complex Quantum Systems, Freie Universitaet Berlin, 14195 Berlin, Germany

Covalent bonding of impurity atoms to graphene, in many cases leads to creation of unusual (singular) zero energy localized electron states. Existence of such states would lead to interesting phenomena, actively discussed recently.

In this talk I consider the behavior of localized impurity levels in graphene in quantizing magnetic field. In the magnetic field the impurity level effectively hybridizes with one of the n=0 Landau level states and splits into two close opposite-energy states. In turn, mixing of localized and Landau levels changes a spin content of a quantum Hall ferromagnet and modifies, via the exchange interaction, the spectrum of electrons surrounding the impurity.

Existing theories investigate graphene uniformly covered by adatoms, though some experiments indicate the tendency towards their clusterization. To address this "unpleasant" possibility, I consider the case of a dense bunch of the impurity atoms, and show how such bunch changes dynamics and spin polarization of a large dense electron droplet surrounding it.

HL 6.6 Mon 10:45 H17

Quantum Hall measurements on epitaxial graphene with oxygen adsorption — •Emiliano Pallecchi[1], Mohamed Ridene[1], Dimitris Kazazis[1], Felicien Schopfer[2], Wilfrid Poirier[2], Mark Goergig[3], and Abdelkarim Ouerghi[1] — [1]Laboratoire de Photonique et de Nanostructures (LPN-CNRS), 91460 Marcoussis, France — [2]Laboratoire National de Métrologie et d'Essais, 78197 Trappes — [3]Laboratoire des Physique de Solides, F-91505, Orsay

In this contribution we present quantum transport, ARPES, and LEED investigations of molecular oxygen-adsorbed epitaxial graphene grown on SiC. We show that the carrier concentration can be significantly reduced by exposing the sample to molecular oxygen. From Hall measurements we obtain a carrier concentration on the order of 1.2 x 10^{12} cm^{-2}, about one order of magnitude smaller than typical values of intrinsic epitaxial graphene. The reduction of electron doping is consistent with estimates from ARPES measurements. At high magnetic field, we find a fully developed quantum Hall effect, with a plateau at filling factor around 2, and a vanishing longitudinal resistance. Such a plateau is the hallmark of single layer graphene and suggests that the buffer layer is not fully decoupled from the substrate. This is further confirmed by LEED study. We then discuss the intermediate field regime, where we analyze the transition between a localized state observed at low fields and the quantum Hall regime at high fields. Finally, we compare these findings to the results obtained on epitaxial graphene exposed to atomic oxygen. We find that atomic oxygen is a more violent process that can damage significantly the graphene flake.

HL 6.7 Mon 11:00 H17

Splitting of the Zero-Energy Landau Level and Universal Dissipative Conductivity at Critical Points in Graphene — •Frank Ortmann[1] and Stephan Roche[1,2] — [1]Catalan Institute of Nanotechnology, Barcelona (Spain) — [2]ICREA, Barcelona (Spain)

In graphene, the interaction of electrons with disorder impacts on their transport signature in a variety of experiments. Magnetotransport experiments can serve as an additional tool to probe this interaction with magnetic fields ranging from the low-field limit of weak antilocalization (∼mT) [1,2] to high fields defining the quantum Hall regime (∼10T). Being under study ever since the discovery of graphene, magnetic fields may unveil some interesting physics hidden otherwise or may generate new effects [3]. We are calculating the Kubo conductivity of graphene σ_{xx} and σ_{xy} in the presence of both weak and strong disorder and magnetic fields using a linear scaling method. This allows us to model realistic graphene samples up to micrometer size. Here we present our recent work on charge transport in the quantum-Hall regime and discuss our findings of universal conductivities. Particular emphasize is put on the non-trivial interference of disorder and magnetic-field and results from our novel order-N Hall-transport code.

[1] F.V. Tikhonenko et al. Phys. Rev. Lett. 103, 226801 (2009)
[2] F. Ortmann et al. EPL 94, 47006 (2011)
[3] D.A. Abanin et al. Science 332, 328 (2011)

HL 7: Topological insulators 1 (MA, jointly with HL, O, TT)

Time: Monday 9:30–10:45 Location: H10

Invited Talk HL 7.1 Mon 9:30 H10

Breaking time reversal symmetry in topological insulators — •Jagadeesh Moodera — Massachusetts Institute of Technology, Cambridge, MA 02139, USA

Breaking time reversal symmetry in a topological insulator (TI) can lead to many exotic properties, such as image magnetic monopole, topological magneto-electric effects as well as Majorana Fermions in superconducting TIs (STI). Recently Gedik*s group in MIT demonstrated that manipulating the magnetic properties via ultrashort light pulses, selectively exciting the spin states of the surface state by exploiting its spin texture to induce a transient magnetic state. Using linearly polarized light in a pump-probe experiment unusual behavior was seen by Muenzenberg group in Gottingen University. The

TI surface state can be magnetically manipulated by proximity effect. The proximity-induced ferromagnetism in a TI/ferromagnetic insulator heterostructure breaks the time reversal symmetry in the TI: a large uniformly induced surface exchange gap appears on the TI without introducing scattering centers, thus keeping intact the transport of spin-momentum locked surface electrons as well as the superconducting pairing in an STI. This TI/ferromagnetic insulator bilayer system showed an induced interface magnetic moment accompanied by an unusual planar hysteresis magnetoresistance demonstrating the magnetic manipulation of the surface channel. This research is supported by ONR, NSF.

HL 7.2 Mon 10:00 H10

Magnetic properties of the Mn doped topological insulator Bi_2Te_3 probed by ESR — •S. Zimmermann[1], V. Kataev[1], Huiwen Ji[2], R.J. Cava[2], and B. Büchner[1] — [1]IFW Dresden, 01171 Dresden, Germany — [2]Dept. Chem., Princeton Univ., NJ 08544, USA

Doping of a topological insulator (TI) with magnetic elements can break the time reversal symmetry and thus open a gap in the protected spin polarized conducting surface states, driving the system into a quantum spin Hall regime [1]. Understanding of the interactions between localized magnetic moments of dopants via delocalized electrons that give rise to ferromagnetism in TIs is therefore of significant interest. Such interactions can be of a long-range character and can also be mediated by surface conducting states [2]. Electron Spin Resonance (ESR) spectroscopy is a sensitive local technique that can probe interactions of localized spins with conduction electrons as well as spin-spin interactions in semiconductors and metals. In this contribution we report an ESR study of the Mn spin dynamics and magnetic interactions in high-quality single crystals of the Mn doped 3-dimensional TI Bi_2Te_3 [3]. We have observed a well-defined ESR signal from Mn spins and have studied the temperature dependences of the ESR parameters for a set of Bi_2Te_3 crystals with different Mn doping levels. The experimental ESR data will be presented in detail and the doping dependence of the Mn spin relaxation via conducting states and the establishment of ferromagnetic order as seen by ESR will be discussed. [1] R. Yu et al., Science **369**, 61 (2010); [2] L.A. Wray et al., Nature Physics **7**, 32 (2011); [3] Y.S. Hor et al., PRB **81**, 195203 (2010)

HL 7.3 Mon 10:15 H10

Investigation of the relation between surface band gaps and magnetism in the magnetic topological insulator $(Bi_{1-x}Mn_x)_2Se_3$ — •Jaime Sánchez-Barriga[1], Andrei Varykhalov[1], Gunther Springholz[2], Hubert Steiner[2], Raimund Kirchschlager[2], Günther Bauer[2], Ondrei Caha[3], Enrico Schierle[1], Eugen Weschke[1], Akin Ünal[1], Sergio Valencia[1], Florian Kronast[1], and Oliver Rader[1] — [1]Helmholtz-Zentrum Berlin — [2]Johannes Kepler Universität Linz — [3]Masaryk University, Brno

The Dirac cone at the surface of a magnetic topological insulator is expected to open a band gap when ferromagnetically magnetized perpendicularly to the surface plane. Angle-resolved photoemission from epitaxial films of $(Bi_{1-x}Mn_x)_2Se_3$ shows for $x > 0.02$ a band gap at the Dirac point of a size that varies with Mn concentration, is much larger than theoretically predicted (~ 100 meV), and does not change with temperature from 7 to 300 K. Based on our measurements with x-ray magnetic circular dichroism (XMCD) we can exclude that the surface band gap is due to ferromagnetic order in the bulk or at the surface. In addition, we investigate by XMCD in photoemission microscopy the reported proximity magnetization induced by a ferromagnetic overlayer.

HL 7.4 Mon 10:30 H10

Mapping the influence of cobalt atoms on the topological states of Bi2Te3 — •Paolo Sessi, Thomas Bathon, Lydia El-Kareh, and Matthias Bode — Institute of Experimental Physics II, University Würzburg, Am Hubland, 97074 Würzburg

Topological insulators are characterized by linearly dispersing gapless topological surface states protected by time-reversal symmetry. For these states, spin is perpendicularly locked to its momentum by spin-orbit interaction resulting in a chiral spin structure that forbids backscattering. However, this is predicted to not be the case when magnetic impurities are introduced into the system. Here, by means of scanning tunneling microscopy we investigate the robustness of the surface states of Bi2Te3 when single Co atoms are deposited on the surface. By analyzing the energy dependence of the quasi particle interference pattern produced by coherent scattering of surface states, we will examine the influence of Co atoms on scattering channels and energy dispersion relation.

HL 8: Transport: Quantum dots, wires, point contacts 1 (TT, jointly with HL, O)

Time: Monday 9:30–13:00 Location: H20

HL 8.1 Mon 9:30 H20

Tunneling-induced renormalization in interacting quantum dots — •Janine Splettstoesser[1], Michele Governale[2], and Jürgen König[3] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University — [2]School of Physical and Chemical Sciences, Victoria University of Wellington, New Zealand — [3]Theoretische Physik, Universität Duisburg-Essen, Germany

A single-level quantum dot with arbitrarily strong onsite Coulomb interaction weakly coupled to electronic reservoirs is studied. We here present an analysis of tunneling-induced quantum fluctuations, generating cotunneling processes and renormalizing system parameters. For a perturbative treatment of these quantum fluctuations in the limit of weak tunnel coupling, we remove off-shell parts of the Hamiltonian via a canonical transformation. We find that the tunnel couplings for the transitions connecting empty and single occupation respectively single and double occupation of the dot renormalize with the same magnitude but with *opposite* signs [1]. This has an important impact on the shape of the renormalization extracted for example from the conductance. Finally, we verify the compatibility of our results with a systematic second-order perturbation expansion of the linear conductance performed within a diagrammatic real-time approach.

[1] J. Splettstoesser, M. Governale, J. König, Phys. Rev. B **86**, 035432 (2012).

HL 8.2 Mon 9:45 H20

Interaction-induced charge and spin pumping through a quantum dot at finite bias — Hernan L. Calvo[1], •Laura Classen[1], Janine Splettstoesser[1], and Maarten R. Wegewijs[1,2] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University, Germany and JARA - Fundamentals of Future Information Technology — [2]Peter Grünberg Institut, Forschungszentrum Jülich, Germany

We discuss charge and spin transport through an adiabatically driven, strongly interacting quantum dot weakly coupled to two metallic contacts with finite bias voltage. We identify coefficients of response to the time-dependent external driving and relate these to the concept of emissivity [1]. These coefficients allow for a straightforward analysis of the predicted interaction-induced pumping under periodic modulation of the gate and bias voltage [2]. We extend this adiabatic Coulomb blockade spectroscopy to spin pumping. In the absence of a magnetic field, we show a striking, simple relation between the pumped charge at zero bias and at bias equal to the Coulomb charging energy. At finite magnetic field, we discuss the possibility to have interaction-induced pure spin pumping. For large-amplitude driving, the magnitude of both the pumped charge and spin saturates at values which are independent of the specific shape of the pumping cycle. Each of these values provides an independent, quantitative measurement of the junction asymmetry.

[1] M. Büttiker, H. Thomas, and A. Prêtre, Z. Phys. B 94, 133 (1994). [2] F. Reckermann, J. Splettstoesser, and M. R. Wegewijs, Phys. Rev. Lett. 104, 226803 (2010).

HL 8.3 Mon 10:00 H20

Structure and conductance analysis of atomic-sized contacts — •Manuel Matt[1], Fabian Pauly[1], Juan Carlos Cuevas[2], and Peter Nielaba[1] — [1]University of Konstanz, Department of Physics, 78457 Konstanz, Germany — [2]Departamento de Física Teórica de

la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

We study the conductance histograms of different metals such as Au and Al. Our theoretical approach combines molecular dynamics simulations of the stretching of atomic-sized wires with the non-equilibrium Green's function formalism based on the tight-binding modelling of the electronic system. As compared to pervious work [1,2], we consider substantially larger wires and explore different lattice orientations. The results show good agreement with experiments.

[1] M. Dreher, F. Pauly, J. Heurich, J. C. Cuevas, E. Scheer, and P. Nielaba, Phys. Rev. B 72, 075435 (2005)
[2] F. Pauly, M. Dreher, J. K. Viljas, M. Häfner, J. C. Cuevas, and P. Nielaba Phys. Rev. B 74, 235106 (2006)

HL 8.4 Mon 10:15 H20

Transport through two interacting resonant levels connected by a Fermi sea — •Elena Canovi, Alexander Moreno, and Alejandro Muramatsu — Institut für Theoretische Physik III, Universität Stuttgart

We study transport at finite bias, i.e. beyond the linear regime, through two interacting resonant levels connected by a Fermi sea. Our results are obtained by means of time-dependent density matrix renormalization group. We find that at finite size both the current and the occupations of the interacting levels oscillate as a function of time. We determine the amplitude and period of such oscillations as a function of bias and extension of the Fermi sea. In particular, the occupations on the two dots oscillate with a relative phase which depends on the distance between the impurities and on the Fermi momentum of the Fermi sea, as expected for RKKY interactions. The approximant to the steady-state current displays oscillations as a function of the distance between the impurities. In the free case we find that it is affected by resonances. The latter can be understood by considering the transmission coefficient of one particle propagating freely in the system. We discuss finally the incidence of interaction on such a behavior.

HL 8.5 Mon 10:30 H20

Magnon-driven quantum-dot heat engine — •Björn Sothmann and Markus Büttiker — Département de Physique Théorique, Université de Genève, CH-1211 Genève 4, Switzerland

Recently, thermoelectric effects have generated a lot of interest. In Ref. [1], transport through two capacitively coupled quantum dots in a three-terminal setup was investigated in the Coulomb-blockade regime. It was shown how such a device can convert a heat current into a directed charge current. This converter is optimal in the sense that it transfers one electron for every quantum of energy delivered by the hot dot and thus allows to reach Carnot efficiency. A generalization to systems with many transport channels was analyzed in Ref. [2].

Here, we discuss a new class of devices where a single-level quantum dot is coupled to two ferromagnetic electrodes as well as to a ferromagnetic insulator at different temperatures [3]. We demonstrate that the system can convert a magnon current into a pure electron spin current or a spin-polarized electron current depending on the magnetic configuration. We analyze the maximal output power as well as the efficiency and show that the tight-coupling limit where heat and charge currents are proportional to each other can be reached.

[1] R. Sánchez and M. Büttiker, Phys. Rev. B **83**, 085428 (2011).
[2] B. Sothmann, R. Sánchez, A. N. Jordan and M. Büttiker, Phys. Rev. B **85**, 205301 (2012).
[3] B. Sothmann and M. Büttiker, EPL **99**, 27001 (2012).

HL 8.6 Mon 10:45 H20

Iterative summation of path integrals for nonequilibrium molecular quantum transport — Roland Huetzen[1], •Stephan Weiss[1,2], Michael Thorwart[3], and Reinhold Egger[1] — [1]Heinrich-Heine Universität Düsseldorf, Universitätsstr.1, 40225 Düsseldorf — [2]Universität Duisburg-Essen and CENIDE, 47048 Duisburg — [3]Universität Hamburg, Jungiusstr. 9, 20355 Hamburg

We formulate and apply a nonperturbative numerical approach to the nonequilibrium current, $I(V)$, through a voltage-biased molecular conductor. We focus on a single electronic level coupled to an unequilibrated vibration mode (Anderson-Holstein model), which can be mapped to an effective three-state problem. Performing an iterative summation of real-time path integral (ISPI) expressions, we accurately reproduce known analytical results in three different limits. We then study the crossover regime between those limits and show that the Franck-Condon blockade persists in the quantum-coherent low-temperature limit, with a nonequilibrium smearing of step features in the IV curve.

[1] S. Weiss, J. Eckel, M. Thorwart, and R. Egger, Phys. Rev. B **77**, 195316 (2008).
[2] R. Hützen, S. Weiss, M. Thorwart, and R. Egger, Phys. Rev. B **85**, 121408 (2012).

15 min. break

HL 8.7 Mon 11:15 H20

Spin dynamics in nanoparticles near Stoner instability — •Philipp Stegmann[1], Björn Sothmann[2], Jürgen König[1], and Yuval Gefen[3] — [1]Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany — [2]Département de Physique Théorique, Université de Genève, CH-1211 Genève 4, Switzerland — [3]Dept. of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 76100, Israel

We analyse the spin dynamics of a nanoparticle close to the Stoner instability. The nanoparticle is weakly tunnel coupled to two ferromagnetic leads. By mapping to an effective Fokker-Planck description we identify two different types of dynamic behaviour (diffusion vs. drift), which are revealed by characteristic relaxation times and a Fano factor that oscillates as a function of an applied bias voltage. Finally, we propose biasing schemes to generate states with magnetic quadrupole moments that dominate over a negligible dipole moment.

HL 8.8 Mon 11:30 H20

Nonlinear transport through interacting quantum dots with superconducting leads in the weak coupling regime — •Sascha Ratz and Milena Grifoni — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

We present a nonequilibrium real-time diagrammatic transport theory for the systematic investigation of the quasiparticle and Josephson currents through a hybrid superconductor-quantum dot system in the weak coupling regime. In details, our device consists of an interacting quantum dot coupled to two biased spin-singlet superconducting leads. To describe the transport dynamics, we derive a completely general equation of motion for the reduced density matrix including all the contributions of a perturbation expansion in the tunneling Hamiltonian. Within these investigations, already in fourth order we can identify the contributions of the nonlocal time evolution kernel to the quasiparticle and DC Josephson transport. To clarify the difference between quasiparticle cotunneling and phase-coherent two-particle Andreev tunneling in fourth order, we first choose a single-level Anderson impurity model for the interacting quantum dot. In particular, one can give a clear explanation for subgap features due to proximity effects, which are also important when we finally compare our theoretical results for a carbon nanotube quantum dot with experimental observations.

HL 8.9 Mon 11:45 H20

Spindephasing and Coherent Control of an Ensemble of Quantum Dots — •Andre Jovchev and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund, Germany

We present a numerical treatment of pump-and-probe experiments with an ensemble of singly charged quantum dots in a magnetic field. We examine the excitation of trions, which is part of an effective polarization mechanism for the spin of the residual electrons, precessing around the magnetic field vector. Inhomogeneities in the magnetic g-factor of different electrons lead to dephasing. The effect of the short pump pulses is described by a unitary operator in the subspace of a spin degenerated electron and trion. For the dynamics between the pulses we apply a Lindblad theory to describe the decoherence due to environmental effects and the hyperfine interaction of the electrons with surrounding nuclei. We study the polarization of the whole ensemble after the application of different pulse protocols, and give an explanation for the polarization of the nuclear spins, which can lead to a remarkably increase of dephasing times which were already seen in experiments.

HL 8.10 Mon 12:00 H20

Adiabatic pumping in the quasi-one-dimensional triangle lattice — Michael Schulze[1], •Dario Bercioux[1], and Daniel F. Urban[2,3] — [1]Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität, 79104 Freiburg, Germany — [2]Physikalisches

Institut, Albert-Ludwigs-Universität, 79104 Freiburg, Germany — [3]Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstraße 11, 79108 Freiburg, Germany

We analyze the properties of the quasi-one-dimensional triangle lattice emphasizing the occurrence of flat bands and band touching via the tuning of the lattice hopping parameters and on-site energies [1]. The spectral properties of the infinite system will be compared with the transmission through a finite piece of the lattice with attached semi-infinite leads. Furthermore, we investigate the adiabatic pumping [2] properties of such a system: depending on the transmission through the lattice, this results in nonzero integer charge transfers or transfers that increase linearly with the lattice size.

[1] M. Schulze, D. Bercioux, D. F. Urban, arXiv:1208.6113.
[2] P. W. Brouwer, Phys. Rev. B **58**, 10135(R) (1998).

HL 8.11 Mon 12:15 H20

Thermoelectric efficiency of a driven double quantum dot — •Federica Haupt[1], Stefan Juergens[1], Michael Moskalets[2], and Janine Splettstoesser[1] — [1]RWTH Aachen University, Aachen, Germany — [2]Kharkiv Polytechnical Institute, Kharkiv, Ukraine

By applying phase-shifted AC signals to the gates of two quantum dots connected in series, it is possible to transfer charge from one lead to another in a quantized way [1,2], even in the presence of an applied bias voltage or a temperature gradient. In this work we investigate the thermoelectric properties of such a double quantum dot device. We show that not only charge but also heat can be pumped in a quantized way. If the modulation frequency Ω is sufficiently small, we find regimes in which the unit of heat $2\pi k_B T \ln 2$ is transported during each period, where T is the temperature of the considered lead and the factor $\ln 2$ stems from spin degeneracy. This would open the possibility of using the pumping cycle to transfer heat against a temperature gradient or to extract work from a hot reservoir with Carnot efficiency. However, the performance of a real device is limited by dissipative effects due to leakage currents and finite time operation, which we rigorously take into account by means of a real-time diagrammatic approach in the regime of weak coupling to the leads. We show that despite these dissipative effects, efficiencies up to 70% of the maximal theoretical value can be reached.

[1] H. Pothier, *et al.*, Europhys. Lett **17**, 249 (1992)
[2] S. J. Chorley, *et al.* App. Phys. Lett. **100**, 143104 (2012).

HL 8.12 Mon 12:30 H20

Controlling entanglement and spin-correlations in double quantum dots in the non-equilibrium regime — •Carlos Alberto Büsser[1] and Fabian Heidrich-Meisner[2] — [1]Ludwig-Maximilians-Universität, München, München — [2]FAU Erlangen-Nuremberg and LMU München

We study the non-equilibrium dynamics in a parallel double-quantum dot structure induced by a large bias voltage. By applying both a magnetic flux and a voltage, it is possible to generate spin-spin-correlations between the two quantum dots. The sign and absolute value of these correlations can be controlled by changing the bias voltage. Using a canonical transformation we argue that the mechanism that drives the spin-spin correlations can be understood in terms of an effective Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction that is mediated by the current. Our study is based on the Anderson-impurity model and we use time-dependent density matrix renormalization group (tDMRG) simulations to obtain currents and spin-correlations in the steady state of the non-equilibrium regime. We also perform quench in the Hamiltonian to prove the stability of the entangled state.

HL 8.13 Mon 12:45 H20

Role of coherent state superpositions in the bipolar spin blockade of a triple quantum dot — Maria Busl[1], Ghislain Granger[2], Louis Gaudreau[2], •Rafael Sánchez[1], Alicia Kam[2], Michel Pioro-Ladrière[3], Sergei Studenikin[2], Piotr Zawadzki[2], Zbigniew Wasilewski[2], Andrew Sachrajda[2], and Gloria Platero[1] — [1]Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Madrid, Spain — [2]National Research Council Canada, Ottawa, Canada — [3]Université de Sherbrooke, Sherbrooke, Canada

In double quantum dots, Pauli spin blockade manifests as a rectified current: charge flows or is blocked depending on the sign of the applied voltage[1]. We present experimental and theoretical investigations of the equivalent process in triple quantum dots in series. We focus on a configuration where (2,0,2) (2,1,1), (1,1,2) and (2,1,2) states are degenerate. When a bias is applied in a magnetic field beyond 10mT, bipolar spin blockade is observed where current is suppressed independent of the applied bias direction. As the field is reduced to zero, leakage resonances are observed. Of special interest are two very sharp resonances which correspond to triple dot conditions when states in the left and right dot but not the center dot align. One of these resonances is found itself to involve bipolar spin blockade and is found to result from a purely quantum coherent effect: electrons occupy states that involve their transference from one extreme to the other of the triple quantum dot without ever visiting the center[2].

[1] K. Ono et al., Science 297, 1313 (2002).
[2] M. Busl et al., unpublished.

HL 9: Focus Session: Frontiers of electronic structure theory I (O, jointly with HL, TT)

Organizers: R. Drautz (Ruhr-Universität Bochum), N. Marzari (EPFL, Lausanne), Matthias Scheffler (FHI, Berlin)

Time: Monday 10:30–13:15 Location: H36

Topical Talk HL 9.1 Mon 10:30 H36

Fully ab initio determination of free energies: Basis for high-throughput approaches in materials design — •Joerg Neugebauer, Fritz Kormann, Martin Friak, Blazej Grabowski, and Timann Hickel — MPI für Eisenforschung, Düsseldorf, Germany

A key requirement in developing systematic tools to design novel materials on the computer is the availability of accurate computational tools determining energies not only at T = 0 K but also under realistic conditions, i.e., at finite temperature. Combining accurate first principles calculations with mesoscopic/macroscopic thermodynamic and/or kinetic concepts allows now to address this issue and to determine free energies and derived thermodynamic quantities such as heat capacity, thermal expansion coefficients, and elastic constants with an accuracy that often rivals available experimental data.

In the talk we will show how novel sampling strategies in configuration space together with highly converged density-functional theory calculations allow an unbiased and accurate determination of all relevant temperature dependent free energy contributions. The flexibility and the predictive power of these approaches and the impact they can have in developing new strategies in materials design will be discussed for modern high strength steels and light weight metallic alloys.

HL 9.2 Mon 11:00 H36

Fast screening of perovskites' phase stability using AIDA, a materials' informatics platform for materials design and discovery — •Giovanni Pizzi[1], Andrea Cepellotti[1], Boris Kozinsky[2], Marco Fornari[3], and Nicola Marzari[1] — [1]Theory and Simulation of Materials, EPFL (CH) — [2]Robert Bosch LCC Research and Technology Center, Cambridge (USA) — [3]Dept. of Physics, Central Michigan University (USA)

Many perovskite systems display a high-temperature cubic phase with zero net polarization, whose microscopic nature is still debated. We perform a systematic study of this phase for representative ABO_3 perovskites, showing that there is not a unique microscopic model for it. Some systems are consistent with a displacive or an order/disorder model; others can sustain a stable displacement pattern of B-site cations in supercells, preserving zero net polarization. In such high-throughput searches, a key challenge is the need of a "materials' informatics" infrastructure to automatically prepare, execute and monitor workflows of calculations for large classes of materials, and then retrieve, store and analyze the results. To this aim, we are developing an open-source platform for high–throughput (AIDA–"Automated Infrastructure and Database for Ab-initio design"). Using AIDA free-energy workflows, we studied the phase stability of $BaTiO_3$, evaluating

the critical temperatures between the cubic, tetragonal, orthorhombic, and rhombohedral phases.

HL 9.3 Mon 11:15 H36

Fast ab-initio screening of magnetic properties applied to the design of new hard magnetic materials — •Nedko Drebov[1], Christian Elsässer[1], Lothar Kunz[2], Alberto Martinez[2], Takashi Shigematsu[3], and Thomas Eckl[2] — [1]Fraunhofer IWM, Freiburg, Germany — [2]Robert Bosch GmbH, Stuttgart, Germany — [3]Bosch Corporation, Tokyo, Japan

We present a fast computational ab-initio screening method which we use for the identification of new permanent magnetic materials based on rare-earth (RE) and transition-metal (TM) elements.

The candidates for new hard magnetic phases with specific structures and compositions are selected from ab-initio screening of their magnetic properties by using the TB-LMTO-ASA method. This procedure considers a large variety of possible combinations of RE and TM elements. At rather low computational costs one can get sufficiently accurate magnetic moments and exchange coupling parameters to be subsequently used in the process of virtual material design.

The results for selected candidate phases are further refined with a more accurate ab-initio method without potential-shape approximation. The Curie temperatures of the phases can be estimated from the calculated magnetic moments and exchange coupling by means of Monte Carlo simulations.

Acknowledgement: This work was supported by the Co-Operative Project 'Suche nach neuen hartmagnetischen Phasen mit hoher Energiedichte (REleaMag)' funded by the BMBF.

HL 9.4 Mon 11:30 H36

Designer Single-Band Hubbard Materials — •Sinead Griffin and Nicola Spaldin — ETH Zurich, Switzerland

The low-energy physics of the High-Tc superconducting cuprates is believed to be encompassed in a single-band Hubbard model. Much work focuses on the computational solutions of the Hubbard model with a view to understanding the complex nature of metal-insulator transitions, superconductivity and strong-correlations physics in general.

Here we take the opposite approach of designing a real material which has the Hamiltonian of a 'single-band Hubbard model' material using first-principles electronic structure theory. By combining crystal field splitting with chemistry, we engineer a class of candidate materials with a single d-electron band at the Fermi level. We report the results of ab initio calculations of the electronic and magnetic structure of these new designer materials and discuss the possibilities for experimental synthesis.

HL 9.5 Mon 11:45 H36

The stability of Bi-Sb-Te layered structures: a first-principles study — •Kirsten Govaerts[1], Marcel H.F. Sluiter[2], Bart Partoens[3], and Dirk Lamoen[1] — [1]EMAT, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerpen, Belgium — [2]Department of Materials Science and Engineering, 3mE, Delft University of Technology, Mekelweg 2, 2628 CD, Delft, The Netherlands — [3]CMT group, Department of Physics, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerpen, Belgium

Using an effective one-dimensional cluster expansion in combination with first-principles electronic structure calculations we have studied the energetics and electronic properties of Bi-Sb-Te layered systems. Our modified, quintuple based cluster expansion explicitly accounts for the Bi and Sb bilayer formation which is due to a Peierls instability. With this new method, groundstates of Bi-Sb-Te can be found without making the dataset of ab initio calculated structures unreasonably large. Groundstates are found within the binary alloys X-Te, with X corresponding to Bi or Sb, for a Te concentration between 0 and 60 at.%. They form an almost continuous series of (meta)stable structures consisting of consecutive X bilayers next to consecutive X_2Te_3 units. Another binary groundstate is the BiSb structure, consisting of alternating Bi and Sb layers, again forming pairs. Groundstates of ternary compounds all consist of consecutive units of Bi_2Te_3, Sb_2Te_3 and TeSbTeBiTe.

HL 9.6 Mon 12:00 H36

RPA Correlation Potential in the Adiabatic Connection Fluctuation-Dissipation formalism — •Stefano de Gironcoli[1], Nicola Colonna[1], and Ngoc Linh Nguyen[1,2] — [1]Scuola Internazionale Superiore di Studi Avanzati (SISSA), via Bonomea 265, I-34136 Trieste, Italy — [2]Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne (CH)

Calculations of correlation energies within the formally exact Adiabatic Connection Fluctuation-Dissipation (ACFD) formalism, within the Random Phase Approximation (RPA) for the exchange-correlation kernel, have been recently carried out for a number of isolated and condensed systems. The efficiency of such calculations has been greatly improved by exploiting iterative algorithms to diagonalize RPA dielectric matrices [1]. However for several systems correlation energies may significantly depend about the choice of input single particle wavefunctions [2]. We derive an expression for the RPA self-consistent potential based on Density Functional Perturbation theory and we present self-consistent RPA calculations for weakly bound molecular dimers, including the controversial case of Beryllium dimer. In this case the self-consistent determination of RPA potential is crucial to determine the stability of the system which however results to be unstable toward dissociation in separated fragments.

[1] H.-V. Nguyen and S. de Gironcoli, Phys. Rev. B 79, 205114 (2009); H. F. Wilson, F. Gygi, and G. Galli, Phys. Rev. B 78, 113303 (2008).

[2] Huy-Viet Nguyen and G.Galli, J. Chem.Phys. 132, 044109 (2010).

HL 9.7 Mon 12:15 H36

The bond-breaking and bond-making puzzle: many-body perturbation versus density-functional theory — •F. Caruso[1], D. Rohr[2], M. Hellgren[3], X. Ren[1], P. Rinke[1], A. Rubio[4,1], and M. Scheffler[1] — [1]Fritz-Haber-Institut, Berlin, Germany — [2]Rice University, Houston, USA — [3]SISSA, Trieste, Italy — [4]Universidad del Pais Vasco, Donostia, Spain

Diatomic molecules at dissociation provide a prototypical situation in which the ground-state cannot be described by a single Slater determinant. For the paradigmatic case of H_2-dissociation we compare state-of-the-art many-body perturbation theory in the *GW* approximation and density-functional theory (DFT) in the exact-exchange plus random-phase approximation for the correlation energy (RPA). Results from the recently developed renormalized second-order perturbation theory (rPT2) are also reported. For an unbiased comparison and to prevent spurious starting point effects both RPA and *GW* are iterated to *full* self-consistency (i.e. sc-RPA and sc-*GW*). Both include topologically identical diagrams for the exchange and correlation energy but are evaluated with a non-interacting Kohn-Sham and an interacting *GW* Green function, respectively. This has profound consequences for the kinetic and the correlation energy. *GW* and rPT2 are both accurate at equilibrium, but fail at dissociation, in contrast to sc-RPA. This failure demonstrates the need of including higher order correlation diagrams in sc-*GW*. Our results indicate that RPA-based DFT is a strong contender for a universally applicable electronic-structure theory. F. Caruso *et al.* arxiv.org/abs/1210.8300.

HL 9.8 Mon 12:30 H36

Density-Functional Theory Applied to Rare Earth Metals: Approaches Based on the Random-Phase Approximation — •Marco Casadei[1], Xinguo Ren[1], Patrick Rinke[1], Angel Rubio[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]University of the Basque Country UPV/EHU, Donostia, Spain

The description of the volume collapse exhibited by some *rare earth* metals poses a great challenge to density-functional theory (DFT) since local/semilocal functionals (LDA/GGA) fail to produce the associated phase transitions. We approach this problem by treating all electrons at the same quantum mechanical level, using both hybrid functionals (e.g. PBE0 and HSE06) and exact-exchange plus correlation in the random-phase approximation (EX+cRPA). We also assess the performance of recently developed beyond RPA schemes (e.g. rPT2 [1]). The calculations are performed for cerium and praseodymium, that display a volume collapse, and neodymium, in which the volume collapse is absent. The isostructural α-γ phase transition in cerium is the most studied. The exact exchange contribution in PBE0 and HSE06 is crucial to produce two distinct solutions that can be associated with the α and γ phases, but quantitative agreement with the extrapolated phase diagram requires EX+cRPA [2]. [1] Ren *et al.*, J. Mater. Sci. **47**, 7447 (2012). [2] M. Casadei *et al.*, Phys. Rev. Lett. **109**, 14642 (2012).

HL 9.9 Mon 12:45 H36

Thermodynamics of the $\alpha \rightleftharpoons \gamma$ transition in cerium from first principles — •Jordan Bieder and Bernard Amadon — CEA, DAM, DIF, F-91297 Arpajon, France

The Dynamical Mean Field Theory (DMFT) combined with density functional theory has been successful to describe strongly correlated materials [1]. However, the computation of the ground state properties requires a good accuracy from both the DFT and the DMFT side. We use thus a strong coupling Continuous Time Quantum Monte Carlo (CT-QMC) solver, which is fast and able to reach low temperatures, in combination with a projector augmented wave (PAW) DMFT implementation.

Extensive calculations using this implementation allows us to carefully reassess the ground state properties and thermodynamics of the $\alpha \rightleftharpoons \gamma$ phase transition in Cerium at low temperatures. In particular, stochastic noise is small enough to avoid any ambiguity on the interpretation of energy versus volume curves. The DMFT picture is put in perspective with recent DFT calculations [2] and recent experimental investigations [3,4].

[1] G. Kotliar *et al.* Rev. Mod. Phys. 78, 865(2006)
[2] M. Casadei *et al.* Phys. Rev. Lett. 109, 146402(2012)
[3] F. Decremps *et al.* Phys. Rev. Lett. 106, 065701(2011)
[4] M. J. Lipp *et al.* Phys. Rev. Lett. 109, 195705 (2012)

HL 9.10 Mon 13:00 H36

Exciton dispersion in wide-gap insulators: there and back again — •Francesco Sottile[1,2] and Matteo Gatti[1,2] — [1]LSI, Ecole Polytechnique, Palaiseau, France — [2]European Theoretical Spectroscopy Facility

We present ab initio calculations of exciton dispersion of wide-gap insulators, like LiF and solid Argon. With the help of the Bethe-Salpeter equation (recently extended to describe full coupling finite momentum excitonic effects) we calculate the momentum dispersion of the first low-lying excitons, both visible and dark. Their particular behaviour (the exciton shows up, lower down, shows up again, to finally disapper) is analized with respect to: direction of the momentum dispersion, the coupling effect, real space exciton distribution and many-body interference effects. The results [1] are finally compared with recent inelastic X-ray scattering experiments [2,3] for what concerns LiF, while they constitutes a completely ab initio prediction for solid Ar.

[1] The Bethe-Salpeter calculation are carried out with the EXC code (http://www.bethe-salpeter.org/) [2] P.Abbamonte et al., PNAS 105, 12159 (2008) [3] C.-C. Lee et al. arXiv:1205.4106v1

HL 10: Graphene: Spin-orbit interaction (HL, jointly with O, TT)

Time: Monday 11:30–13:45 Location: H17

HL 10.1 Mon 11:30 H17

Impurity-induced spin relaxation time in graphene from first principles — •Dmitry Fedorov[1], Martin Gradhand[2], Sergey Ostanin[1], Igor Maznichenko[3], Arthur Ernst[1], Jaroslav Fabian[4], and Ingrid Mertig[3,1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany — [2]H. H. Wills Physics Laboratory, University of Bristol, Bristol BS8 1TL, United Kingdom — [3]Martin-Luther-Universität Halle, Institut für Physik, 06099 Halle, Germany — [4]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

The spin relaxation time of conduction electrons in graphene caused by carbon and silicon impurities is studied by means of our *ab initio* approach, which was recently developed for bulk systems [1] and adapted now for the film geometry. It is found that both the momentum and spin relaxation times are extremely sensitive to the position of the impurities. We show that adatoms provide spin-flip rates 4 to 5 orders of magnitude larger than in-plane impurities. Our results strongly support the adatom-induced extrinsic mechanism of the experimentally observed spin relaxation in graphene [2].

[1] M. Gradhand et al., PRB 81, 020403(R) (2010)
[2] N. Tombros et al., Nature 448, 571 (2007)

HL 10.2 Mon 11:45 H17

D'yakonov-Perel' spin dephasing in single and bilayer graphene and the role of contact resistance on the spin dephasing time — Frank Volmer[1,2], Marc Drögeler[1,2], Eva Maynicke[1,2], •Nils von den Driesch[1,2], Tsung-Yeh Yang[1,2], Gernot Güntherodt[1,2], and Bernd Beschoten[1,2] — [1]II. Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — [2]JARA: Fundamentals of Future Information Technology, 52074 Aachen, Germany

We investigate spin transport in both single and bilayer graphene nonlocal spin-valve devices. Similar to our previous studies on bilayer graphene [1], we observe an inverse dependence of the spin dephasing time on the carrier mobility in our single layer devices indicating the importance of D'yakonov-Perel' like spin dephasing in exfoliated single and bilayer samples.

This general trend is only observed in devices with large contact resistances (>1 kΩ). In contrast, the spin dephasing time is significantly reduced in samples with low ohmic contacts for both single and bilayer graphene indicating that an additional spin dephasing occurs underneath the spin injection and detection electrodes.

This work has been supported by DFG through FOR 912.

[1] T.-Y. Yang *et al.* Phys. Rev. Lett. **107**, 047206 (2011)

HL 10.3 Mon 12:00 H17

Intrinsic and substrate induced spin-orbit interaction in chirally stacked trilayer graphene — •Andor Kormanyos and Guido Burkard — University of Konstanz

We present a combined group-theoretical and tight-binding approach to calculate the intrinsic spin-orbit coupling (SOC) in ABC stacked trilayer graphene. We find that compared to monolayer graphene, a larger set of d orbitals (in particular the d_{z^2} orbital) needs to be taken into account. We also consider the intrinsic SOC in bilayer graphene, because the comparison between our tight-binding bilayer results and the density functional computations allows us to estimate the values of the trilayer SOC parameters as well. We also discuss the situation when a substrate or adatoms induce strong SOC in only one of the layers of bilayer or ABC trilayer graphene. Both for the case of intrinsic and externally induced SOC we derive effective Hamiltonians which describe the low-energy spin-orbit physics. We find that at the K point of the Brillouin zone the effect of Bychkov-Rashba type SOC is suppressed in bilayer and ABC trilayer graphene compared to monolayer graphene.

The the combination of group-theoretical and tight-binding approaches can be used to study the spin-orbit interaction in other quasi-two dimensional materials, such as MoS_2, as well.

HL 10.4 Mon 12:15 H17

Long Electron Spin Lifetimes in Armchair Graphene Nanoribbons — •Matthias Droth and Guido Burkard — University of Konstanz, 78457 Konstanz

Armchair graphene nanoribbons (aGNR) are promising as a host material for electron spin qubits because of their potential for scalability and long coherence times [1]. The spin lifetime T_1 is limited by spin relaxation, where the Zeeman energy is absorbed by lattice vibrations [2], mediated by spin-orbit and electron-phonon coupling. We have calculated T_1 by treating all couplings analytically and find that T_1 can be in the range of seconds for several reasons: (i) Van Vleck cancellation; (ii) weak spin-orbit coupling; (iii) low phonon density; (iv) vanishing coupling to out-of-plane modes due to the electronic structure of the aGNR. Owing to the vanishing nuclear spin of ^{12}C , T_1 is a good measure for overall coherence. These results and recent advances in the controlled production of graphene nanoribbons [3] make this system interesting for classical and quantum spintronics applications.

[1] B. Trauzettel *et al.*, Nature Phys. **3**, 192-196 (2007).
[2] M. Droth and G. Burkard, Phys. Rev. B **84**, 155404 (2011).
[3] X. Zhang *et al.*, arXiv:1205.3516 (2012).

HL 10.5 Mon 12:30 H17

Tunneling-induced Spin Anisotropy Barrier in Quantum Dot Spin-Valves — •Michael Hell[1,2], Maciej Misiorny[1,2], and Maarten Wegewijs[1,2,3] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich — [2]JARA - Fundamentals of Future Information Technology — [3]Institut für die Theorie der Statistischen Physik, RWTH Aachen, 52056 Aachen

Spintronics employs the two fundamental properties of a each electron: its charge and its spin-dipole moment. However, recent studies indicate that the interplay of these two degrees of freedom does not exhaust the

potential of spintronics when approaching the nano-scale: spin correlations between electrons, partly characterized by the spin-anisotropy, provide an independent resource of spin information, which is stored even in a simple ferromagnet and couples to the spin-dipole moment in quantum dots. The interest in spin anisotropy also emerges from the research on single-molecule magnets (SMMs) and magnetic adatoms, in which the transport is controlled by a large spin anisotropy barrier intrinsically generated by strong spin-orbit coupling. In this talk we show that such a spin-anisotropy barrier can be externally induced by the transport of spin-correlations from ferromagnets into a a spin-isotropic interacting quantum dot with large spin S>1/2 and negligible spin-orbit interaction. This proximity-induced spin-anisotropy has the hallmarks of a spintronic exchange-field of a quadrupolar nature, a generalization of the well-established dipolar exchange field. The barrier increases with the tunnel coupling, achieving values comparable to that of SMMs, but with the flexibility of electric and magnetic tuneability.

HL 10.6 Mon 12:45 H17

First-principles study of the spin-orbit interaction in graphene induced by hydrogen adatoms — •Martin Gmitra, Denis Kochan, and Jaroslav Fabian — University of Regensburg

We have performed first principles calculations of the spin-orbit coupling effects in hydrogenated graphene structures, for varying hydrogen coverage densities, using the linearized augmented plane wave method as implemented in the FLEUR code. The covalent bonding between the hydrogen and carbon atoms leads to a local structural puckering of graphene sheets, giving rise to an overlap between the Dirac and sigma electrons and a giant enhancement (from roughly 0.01 to 1 meV) of the local spin-orbit interaction. The calculated effects on the band structure and the emerging spin patterns of the electronic states can be well explained by effective Hamiltonian models derived from group theoretical principles.

This work is supported by the DFG SPP 1285, SFB 689, and GRK 1570.

HL 10.7 Mon 13:00 H17

Theory of the hydrogen adatoms induced spin-orbit coupling in graphene — •Denis Kochan, Martin Gmitra, and Jaroslav Fabian — University Regensburg

We have analyzed the first-principles data of the electronic structure of hydrogenation in graphene by means of group theory derived effective Hamiltonians. We propose effective models for semihydrogenated graphene as well as for graphene with a single hydrogen adatom. The chemisorption of hydrogen modifies the structural symmetry of the plane graphene in two essential ways—it breaks the pseudospin (sublattice) symmetry and induces rippling. We show that in addition to the Rashba spin-orbit interaction there emerges another spin-orbit field which is induced by the pseudospin inversion asymmetry due to the adatoms. Our realistic effective Hamiltonians should be useful for spin transport and spin relaxation investigations.

This work is supported by DFG SFB689

HL 10.8 Mon 13:15 H17

Optical properties of hydrogenated graphene from first principles — •Sebastian Putz, Martin Gmitra, and Jaroslav Fabian — Universität Regensburg, Universitätsstraße 31, 93053 Regensburg

We investigate the effect of hydrogen coverage on the optical properties of single-side hydrogenated graphene from first principles. To account for different degrees of uniform hydrogen coverage we calculate the complex dielectric function for graphene supercells of various size, each containing a single additional H atom. We use the Linearized Augmented Planewave (LAPW) method, as implemented in WIEN2k, to show that the hydrogen coverage strongly influences the complex dielectric function and thus the optical properties of hydrogenated graphene. The absorption coefficient in the visible range, for example, has different characteristic features depending on the hydrogen coverage. This opens up new possibilities of determining the hydrogen coverage of hydrogenated graphene samples in the experiment by contact-free optical absorption measurements.

This work is supported by the DFG GRK 1570.

HL 10.9 Mon 13:30 H17

Electron scattering and spin polarization at the graphene/Ni(111) interface — Aran Garcia-Lekue[1], Timofey Balashov[2], Marc Ollé[2], Gustavo Ceballos[2], Andrés Arnau[1,3], Pietro Gambardella[2], Daniel Sánchez-Portal[1,3], and •Aitor Mugarza[2] — [1]Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal 4, E-20018 San Sebastian, Spain — [2]Catalan Institute of Nanotecnology (ICN), UAB Campus, E-08193 Bellaterra, Spain — [3]Centro de Fisica de Materiales CFM - MPC, Centro Mixto CSIC-UPV, Apdo. 1072, San Sebastian, Spain

The interaction of graphene with a metal often perturbs the unique electronic properties of Dirac electrons in graphene. This interaction can be positively exploited to engineer the Dirac bands and obtained graphene interfaces with different functionalities. In this work we study the electronic properties of graphene nanoislands grown on Ni(111) [1] by combining scanning tunnelling microscopy and ab-initio calculations. We show that the interaction with the Ni surface opens a gap and spin-polarizes the Dirac bands, which results in a spin filtering effect in the transport across the interface [2]. On the other hand, the standing wave pattern created around the nanoislands reveal an asymmetric potential that depends both on the spin and edge type, suggesting a lateral 2D spin-filter effect similar to that occurring across the interface.

[1] M. Olle et al. Nano Lett. 12, 4431 (2012). [2] V. M. Karpan et al. Phys. Rev. Lett. 99, 176602 (2007).

HL 11: Quantum information systems: mostly quantum dots

Time: Monday 12:00–13:45 Location: H16

HL 11.1 Mon 12:00 H16

Phase-locked indistinguishable photons from a solid-state source — •Clemens Matthiesen, Martin Geller, Carsten H. H. Schulte, Claire Le Gall, Jack Hansom, Zhenyong Li, and Mete Atature — Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom

Recent years have seen significant progress in the control of solid-state quantum bits, such as spins in self-assembled InAs quantum dots (QDs). Entangling individual spins through quantum interference of flying qubits has been identified as a promising approach to realising a quantum network of distant spins. Hoever, generating indistinguishable photons (as flying qubits) from separate QDs has proved challenging, due to fast and slow dephasing of the optical QD transitions.

Resonance fluorescence in the Heitler regime [1] provides access to single photons with coherence well beyond the Fourier transform limit of the transition, and holds the promise to circumvent environment-induced dephasing. We first demonstrate that the coherently generated single photons from a single QD display mutual coherence with the excitation laser on a timescale exceeding 3 seconds. Exploiting this degree of mutual coherence we shape single photons pulses. Separate photons generated phase-locked to the excitation laser field are shown to be fundamentally indistinguishable [2], lending themselves to creation of distant entanglement through quantum interference.

[1]Matthiesen et al. Phys. Rev. Lett. 108, 093602 (2012). [2]Matthiesen et al. arXiv:1208.1689 [quant-ph] (2012).

HL 11.2 Mon 12:15 H16

Post-selective Entanglement Generation with solid state single photon sources — •Alexander Pawlis[1,2], Klaus Lischka[1], and Yoshihisa Yamamoto[2] — [1]Universität Paderborn, Paderborn, Deutschland — [2]Stanford University, Palo Alto, California

The ability to isolate single fluorine donors in nano-structures fabricated from fluorine doped ZnMgSe/ZnSe QWs allows for direct access to the atom-like transitions of the donors. Such nano-structures are particularly applicable as solid-state single photon sources (SPS) and electron spin qubits. The quantum interference of single photons emitted from two independent ZnSe:F SPS revealed sufficient indistinguishability [1] for the realisation of all-optical concepts [2] of quantum-computation and -communication in a solid-state material. Furthermore the electron spin of the neutral donor can be used as a long-lived matter qubit [3]. Here we report on the post-selection of polarization entangled photon pairs emitted from two independent ZnSe:F SPS. The density matrix of the state was reconstructed by quantum state

tomography and it yields a fidelity of 0.58 [4]. The results constitutes the first realization of two indistinguishable ZnSe:F SPS that can be used to generate substantial entanglement over macroscopic distances.

[1] K. Sanaka et al., Phys. Rev. Lett. 103(5), 053601 (2009). [2] J.L. O'Brien et al., Science 318(5856), 1567{1570 (2007). [3] A. Greilich et al., Phys. Rev. B 85(12), 121303R (2012). [4] K. Sanaka et al., Nano Letters 12, 4611 82012).

HL 11.3 Mon 12:30 H16

Tomography scheme for two spin qubits in a double quantum dot — •Niklas Rohling and Guido Burkard — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

We present a set of measurements which allows the reconstruction of the density matrix for the full two-qubit space of two electron spins in a double quantum dot. Our scheme employs non-local quantum gates induced by the exchange interaction between the spins and selective single-spin rotations by electron spin resonance (ESR). Recently, both kinds of gates have been realized experimentally in the same quantum dot [1]. Projection on specific states can be achieved by an adiabatic spin-to-charge conversion after applying the quantum gate. State tomography for a singlet-triplet qubit, i.e. a subspace of the full two-qubit space, has been demonstrated [2]. It turns out that ESR is harder to realize than exchange interaction. Whereas ESR is unnecessary to gain full information of the state of a single singlet-triplet qubit, it is needed for state tomography of the full four-dimensional space of two single-spin qubits. For each of the measurements we suggest, no more than one $\pi/2$-rotation of one of the spins needs to be done by ESR. We estimate the precision of our tomography scheme in dependence of the fidelity of the quantum gates.

[1] N. Brunner, Y.-S. Shin, T. Obata, M. Pioro-Ladrière, T. Kubo, T. Taniyama, Y. Tokura, and S. Tarucha, Phys. Rev. Lett. **107**, 146801 (2011).

[2] S. Foletti, H. Bluhm, D. Mahalu, V. Umansky, and A. Yacoby, Nature Phys. **5**, 903 (2009).

HL 11.4 Mon 12:45 H16

Characterization of S-$T+$ qubit dynamics via correlation functions — •Christian Dickel[1,2] and Hendrik Bluhm[1,2] — [1]2nd Institute of Physics C, RWTH Aachen University, Aachen, Germany — [2]JARA - Fundamentals of Future Information Technology

Semiconductor spin qubits encoded in the singlet state S and the $m = 0$ triplet state T_0 of two electrons in a double quantum dot (DQD) have been pursued very successfully. GaAs is the most advanced material in this context, but it suffers from dephasing due to the hyperfine interaction. Recently the alternative encoding in S-T_+ has been explored. For the control of such an S-T_+ qubit, the dynamics at the S-T_+ transition are crucial. They are driven by hyperfine coupling and spin-orbit interaction.

Here we show, through experiment and theory, that these dynamics can be probed by measuring temporal correlations of the flip probabilities during Landau-Zener-Stückelberg transitions. Those correlation functions reveal oscillations originating from the relative Lamor precession of the different nuclear species present in GaAs. Incoherent nuclear spin evolution results in a loss of correlations. In the presence of spin-orbit coupling, oscillations with the absolute Lamor frequencies are expected in addition. Observations of the latter could be useful to quantify the spin-orbit coupling in DQDs.

HL 11.5 Mon 13:00 H16

A Landau-Zener-Stückelberg charge qubit — •Florian Forster[1], Gunnar Petersen[1], Dieter Schuh[2], Werner Wegscheider[3], Sigmund Kohler[4], and Stefan Ludwig[1] — [1]CeNS, Universität München — [2]Universität Regensburg — [3]ETH Zürich — [4]Inst. Ciencia Materiales, CSIC, Madrid

Quantum dots in the few electron regime in GaAs/AlGaAs heterostructures are a powerful system for observing fundamental quantum effects. For instance, it is possible to prepare arbitrary charge superposition states of a double quantum dot (DQD) by driving it through avoided crossings. Multiple Landau-Zener transitions can give rise to quantum interference in time, in analogy to the interference in space in Mach-Zehnder interferometers. Here, we perform Landau-Zener-Stückelberg (LZS) interferometry [1] by periodically driving a DQD between two-electron singlet states. We analyze the decoherence of this strongly driven charge qubit as a function of temperature and external noise. Our goal is to use LZS interferometry as a tool to probe the solid state environment interacting with the qubit. To reach this goal we compare our experimental data with numerical calculations based on the Floquet transport theory [2] augmented by dissipative terms. This approach allows an accurate determination of qubit coherence times and its bath properties. Our fundamental studies lay the basis for possible applications in quantum information based on qubits at the interface between adiabatic and non-adiabatic quantum dynamics.

[1] S. N. Shevchenko et. al., Phys. Rep. 492, 1-30 (2010)

[2] S. Kohler et al., Phys. Rep. 406, 397 (2005)

HL 11.6 Mon 13:15 H16

Undoped Si/SiGe heterostructures for field-effect devices — •Simon Pfaehler[1,2], Johannes Kierig[1], Andreas Wild[1,2], Christoph Buhlheller[1,2], Gerhard Abstreiter[2], Kentarou Sawano[3], and Dominique Bougeard[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]Walter Schottky Institut, Technische Universität München, Garching, Germany — [3]Advanced Research Laboratories, Tokyo City University, Japan

Two-dimensional electron systems (2DES) in modulation doped heterostructures represent a promising building block for the development of electrostatically defined spin qubits. The hyperfine interaction with the nuclear spin bath being a dominant qubit decoherence mechanism, Si/SiGe heterostructures have been receiving steadily increasing attention for building devices almost free of nuclear spin carrying isotopes. However, such modulation doped heterostructures still suffer from fluctuating charges due to the presence of ionized dopants which can also in the end limit the spin decoherence time.

One possible way to reduce fluctuating charges is to avoid doping in Si/SiGe heterostructures and induce a 2DES capacitively. In this contribution, we report on the realization and experimental characterization of undoped Si/SiGe heterostructures designed for the implementation of electrostatically defined double quantum dots. A global top gate is used to operate this device via field effect to induce a 2DES in the undoped Si quantum well. The electronic behavior is additionally studied in band structure simulations.

HL 11.7 Mon 13:30 H16

Controllable spin environments in carbon based systems — •Moritz Fuchs[1], John Schliemann[2], and Björn Trauzettel[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg — [2]Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg

Carbon based quantum dots are promising candidates for the investigation of electron spin dynamics in a nuclear spin environment. While isotopic purification offers a way to control the number of involved nuclear spins, the coupling between these spins and the electron spin changes with the shape of the quantum dot. We analyze the time evolution of a single electron spin bound to a graphene quantum dot for exemplary models using both analytical and numerical methods.

HL 12: Charge transfer effects in molecular materials I (CPP, jointly with BP, DS, HL)

Related to SYCT organized by Frank Schreiber (Tübingen) and Wolfgang Brütting (Augsburg).

Time: Monday 12:15–13:30 Location: H1

HL 12.1 Mon 12:15 H1

Thermally Activated Intermixing in Pentacene - Perfluoropentacene Heterostructures — •Tobias Breuer and Gregor Witte — Molekulare Festkörperphysik, Philipps-Universität Marburg, Renthof 7, 35032 Marburg

We report on the thermal stability of pentacene (PEN, $C_{22}H_{14}$) and perfluoropentacene (PFP, $C_{22}F_{14}$) heterostructures. We show that the thermal stability of the heterostructure compared to the single compounds is significantly enhanced by about 20 K. By varying preparation methods and stochiometric ratios of the heterostructures we show

that the stabilization is restricted to heterostructures with stochiometric ratio of 1:1. Moreover, the thermal stabilization strongly depends on the preparation method, especially the deposition sequence of both materials in subsequent stacks. While PFP as bottom and PEN as top layer yield stabilized layers, no such effect is found for PEN as bottom layer and PFP on top. This asymmetry of intermixing and corresponding morphological information obtained by means of AFM measurements as well as optical absorption spectra as benchmark for hetero-interaction are discussed. The results are compared to additional preparation methods of heterostructures like co-evaporation and post-deposition-annealing.

HL 12.2 Mon 12:30 H1

Mixing-induced anisotropic correlations in molecular crystalline systems: Rationalizing the behavior of organic semiconductor blends — •Katharina Broch, Antje Aufderheide, Jiří Novák, Alexander Hinderhofer, Rupak Banerjee, Alexander Gerlach, and Frank Schreiber — Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen

Binary mixtures of organic semiconductors (OSCs) have recently become an important field of research, as they find applications in optoelectronic devices [1]. In these systems, the mixing (intermixing vs. phase separation) and ordering behavior is crucial, since it affects the optical and electronic properties including the degree of charge-transfer (CT). We present a comprehensive study of binary mixtures of the three prototypical OSCs pentacene (PEN), perfluoropentacene (PFP) and diindenoperlyene (DIP) in all possible combinations [1,2,3]. Using X-ray reflectivity and grazing incidence X-ray diffraction we investigate the structural properties of the mixed films as well as their impact on the optical spectra obtained by spectroscopic ellipsometry. For PEN:DIP we find an anisotropic ordering behavior, comparable to that observed in some liquid crystals, which is fundamentally new for OSCs [2]. The influence of sterical compatibility and the strength of the intermolecular interactions on the mixing and ordering behavior in the different blends will be discussed by extending a conventional mean-field model [1]. [1] A. Hinderhofer and F. Schreiber, Chem.Phys.Chem., **13**, 628 (2012); [2] A. Aufderheide et al., Phys.Rev.Lett., **109**, 156102 (2012); [3] J. Reinhardt et al., J.Phys.Chem. C, **116**, 10917 (2012)

HL 12.3 Mon 12:45 H1

Screening Effects on Excitation Energy Transfer in Supramolecular Complexes in a Mixed Quantum Classical Description — •Jörg Megow[1], Thomas Renger[2], and Volkhard May[1] — [1]Humboldt-Universität zu Berlin, Deutschland — [2]Johannes Kepler Universität Linz, Österreich

Excitation energy transfer (EET) within the supramolecular complex P16 (sixteen pheophorbide a molecules covalently linked to a DAB-dendrimer) is studied using a mixed quantum classical methodology [1,2] that takes the screening of excitonic coupling into acount. The excitonic coupling between two chromophores is calculated as Coulomb-coupling between transition partial charges. This treatment neglects the screening effects due to interaction with the solvent molecules. The Poisson-TrEsp (transition charges from electrostatic potentials) method [3], developed in the group of Renger, allows the calculation of screening factors that correct the excitonic coupling between two chromophores dependent on their distance, mutual orientation and conformation. A new method is proposed that allows to obtain the orientation and conformation dependence of the Poisson-TrEsp screening factors in a mixed quantum-classical description by introducing a novel fitting procedure. While all screening ansatzes result in a deceleration of the EET, the new approach results in a considerable acceleration of the EET compared to standard screening approaches.

[1] J. Megow et al., ChemPhysChem 12, 645 (2011) [2] J. Megow et al., Chem. Phys. 377, 10 (2010) [3] J. Adolphs et al., Photosynth. Res. 95 (2008)

HL 12.4 Mon 13:00 H1

In operando STXM investigations of charge carriers in SAMFET devices — •Andreas Späth[1], Thomas Schmaltz[2], Benjamin Watts[3], Marcus Halik[2], and Rainer H. Fink[1] — [1]FAU Erlangen-Nürnberg, Physical Chemistry II, Erlangen, Germany — [2]FAU Erlangen-Nürnberg, Polymer Sciences, Erlangen, Germany — [3]Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland

Based on previous work on pentacene based organic FETs [1], we present first results of zone plate scanning transmission soft x-ray microspectroscopy (STXM) on novel organic devices based on self assembled monolayers (SAMs). STXM combines high lateral resolution and spectroscopic sensitivity. Electron detection is used to achieve surface sensitivity, thus offering access to monolayer films. The SAMs implement all functionalities of the FET, i.e. gate dielectric and organic semiconductor [2]. STXM analysis within the active channel during operation of the SAMFET shows small variations in the electronic structure which are interpreted in terms of field induced shifts of the electronic levels and/or local charges. The unique combination of STXM and AFM provided by the NanoXAS beamline at the Swiss Light Source enables us to monitor both, the morphological homogeneity of the SAM film and modifications in the electronic structure. Thus, a more detailed insight into the correlation of morphological and electronic properties of these ultrathin devices can be achieved. The project is funded by the BMBF (contract 05K10WEA).

[1] C. Hub, et al., J. Mater. Chem. 20, 2010, 4884
[2] A. Rumpel, et al., Langmuir 27, 2011, 15016

HL 12.5 Mon 13:15 H1

Scanning Kelvin Probe Microscopy on FIB-milled Cross Sections of Organic Solar Cells — •Rebecca Saive[1,2,3], Christian Müller[1,2,3], Michael Scherer[1,2,3], Dominik Daume[1,2,3], Michael Kröger[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

Scanning Kelvin probe microscopy (SKPM) is a promising tool to analyze charge carrier transport paths in electronic devices. Conventional SKPM is limited to analysis of charge transport parallel to the device surface, e.g. within planar field-effect transistors, whereas the transport in vertical devices e.g. bulk heterojunction solar cells is not accessible to further characterization. Therefore we introduce a method to directly measure at the cross sections of organic devices by milling with a focused ion beam (FIB) and adjacent SKPM characterization. By this method we can reveal a spatially resolved potential distribution and therefore indentify charge injection and charge transport barriers. In this work, we could correlate microscopic measurement results like the work function difference between the contact materials to macroscopic device characteristics received by J-V measurements and impedance spectroscopy.

HL 13: Preparation and characterization

Time: Monday 12:45–14:00 Location: H15

HL 13.1 Mon 12:45 H15

Sortierung von einwandigen Kohlenstoffnanoröhren mittels Gel-Permeations-Chromatographie — •Frieder Ostermaier und Michael Mertig — TU Dresden, Professur für Physikalische Chemie, Mess- und Sensortechnik, 01062 Dresden, Germany

Einwandige Kohlenstoffnanoröhren (SWCNT) haben aufgrund ihrer elektronischen Eigenschaften großes Potenzial als Bausteine einer nanoskaligen Elektronik. Halbleitende scSWCNT können beispielsweise zur Herstellung von Feldeffekttransistoren verwendet werden. Dafür ist es erforderlich, SWCNT mit definierten elektronischen Eigenschaften zur Verfügung zu stellen. Bisher gibt es allerdings kein Syntheseverfahren, welches nur metallische mSWCNT oder nur scSWCNT produziert. Deshalb ist eine Sortierung der SWCNT für technische Anwendungen unbedingt erforderlich.

Wir haben die skalierbare Gel-Permeations-Chromatographie verwendet, um SWCNT aus verschiedenen Herstellungsverfahren nach ihren Eigenschaften zu sortieren. Es konnte gezeigt werden, dass der bekannte Ansatz für SWCNT aus dem HiPCO-Prozess sich auch auf kommerziell erhältliche SWCNT aus dem CVD-Verfahren anwenden lässt. Zur quantitativen Charakterisierung der Proben wurde UV/Vis Spektroskopie angewendet. Die Methode erlaubt, schnell den metallischen Anteil mit dem halbleitenden Anteil zu vergleichen. Mit den sortierten Proben wurden Feldeffekttransistoren mittels Dielektrophorese

assembliert. Die Messung der U-I-Kennlinien zeigte, dass sich mit sortierten scSWCNT unmittelbar Transistoren assemblieren lassen. Ein selektives "Wegbrennen" der mSWCNT entfällt damit.

HL 13.2 Mon 13:00 H15

Stability of AlOx Gate Dielectrics for High Temperature Field Effect Transistors — •Björn Christian[2], Volker Cimalla[1], Lutz Kirste[1], Martina Baeumler[1], Frank Bernhardt[1], Fouad Benkhelifa[1], and Oliver Ambacher[1,2] — [1]Fraunhofer Institute for Applied Solid State Physics Freiburg, Germany — [2]Laboratory for Compound Semiconductor Microsystems, Department of Microsystems Engineering - IMTEK, University of Freiburg, Germany

AlO_x is a promising high-k dielectric material to replace SiO_2 in field effect transistors scaled to smaller dimensions (< 100 nm) or operating at higher temperatures. High temperature operation, however, causes phase transitions such as crystallization of metal oxides, which has a negative impact on the properties of dielectric layers. Dielectric films can be stabilized in nanolaminates using stacks of different dielectric materials. In this work, the phase transitions and their impact on the electrical properties of aluminum oxide as a single layer as well as stacks of aluminum oxide, silicon oxide and differently prepared silicon nitride has been characterized. Basic film properties and crystallization were investigated by x-ray diffraction, spectral ellipsometry, and scanning microscopy techniques. Electrical properties have been analyzed by C/V and I/V measurements. In addition, device structures based on AlGaN/GaN HEMTs were prepared and the influence of the gate stacks on threshold voltage was analyzed.

HL 13.3 Mon 13:15 H15

Controlled Electrodeposition of ZnO — •Miriam Schwarz, Karolis Parfeniukas, Torsten Balster, and Veit Wagner — Jacobs University Bremen, Campusring 1, D-28759 Bremen, Germany.

Depending on the application of nano-structured ZnO, the dimensional demands, for instance crystal spacing, vary. In general, electrodeposition is an attractive method to deposit versatile nanostructures, since it bears significant influence on crystal shape and density. We present different ways to tailor electrodeposited ZnO in the context of requirements for light management and as n-type semiconductor for application in hybrid-organic solar cells. In general a strong dependence of the electrode material is observed. While dense structures growing perpendicular to the surface are obtained on sputtered gold, structures on sputtered ITO electrodes grow tilted and in wider spacing in the range of 1 um. With pulsed voltage deposition at different voltages (-0.775 V, -0.875 V, -0.975 V), the density of the structures on ITO can be adjusted from the micrometer range to below 200 nm with increasing applied potential. The impact on light scattering properties of the resulting ZnO nanostructures is shown. For highly ordered ZnO nano arrays, electrodeposition through an electron-beam structured template is performed enabling to control equidistant spacing of the ZnO crystals from 50 to 100 nm. Learning how to reliably control the growth of electrodeposited ZnO enables the design of a suitable ZnO structures for promising application.

HL 13.4 Mon 13:30 H15

Double-crystal-diffraction measurements of oxygen clusters in single-crystalline silicon — •Christoph Bergmann, Alexander Gröschel, Johannes Will, Matthias Weisser, and Andreas Magerl — Lehrstuhl für Kristallographie und Strukturphysik, Universität Erlangen-Nürnberg, Germany

Semiconductor-grade silicon being close to structural perfection is the basic material for nowadays integrated circuits with structural dimensions reaching the nano-regime. Nevertheless, oxygen clusters which lower the grade of perfection are deliberately introduced as they act as gettering centers for metallic impurities.

Recently, new approaches to the treatment of diffraction data of lattice distortions as arising from clusters were proposed by Molodkin et al. [1]. With this approach it is possible to describe the entire Bragg profile including coherent Bragg scattering and the defect-induced diffuse scattering within a dynamical formalism.

We present X-ray diffraction data obtained with synchrotron and laboratory sources of CZ-Si being distorted by small and medium size clusters (4 nm - 25 nm). By recording the Bragg peaks with a double crystal setup, it is possible to derive information about the oxygen cluster size, density and morphology. The data is compared with TEM measurements.

[1] V. B. Molodkin et al., Phys. Rev. B 78, 224109 (2008)

HL 13.5 Mon 13:45 H15

Epitaxial cubic and wurtzite ZnS thin films grown on GaP and ZnS substrates — •Gunther Haas, Melanie Pinnisch, Johannes Bieber, Yinmei Lu, Elisabeth Zolnowski, and Bruno Meyer — I. Physikalisches Institut, Justus-Liebig-Universität Giessen, Heinrich-Buff Ring 16, 35392 Giessen

Zinc sulfide is a wide band gap material with two stable solid structures. A cubic structured phase with a room temperature band gap of 3.6 eV and a wurtzite phase, which is known to form at temperatures above 1050 °C, with a band gap of approx. 3.9 eV. We have grown epitaxial zinc sulfide thin films and investigated the influence of different substrates (GaP (001), GaP (111), GaP (011) and ZnS (011)) on the resulting properties and orientations of the grown films. For a variation in growth temperatures (from 450 to 800 °C) our results show a structural transition from zinc blende to wurtzite structure at higher growth temperatures when using GaP (111) substrates. These observations are underlined by X-ray analysis and atomic force microscopy, which shows hexagonal structures at the surface for zinc sulfide grown at higher temperatures on GaP (111) substrates. Low temperature photoluminescence measurements at 4 K provide an insight into the optical properties of the two different zinc sulfide phases.

HL 14: Invited Talk: Chris van de Walle

Time: Monday 13:30–14:00 Location: H2

Invited Talk HL 14.1 Mon 13:30 H2

Complex oxides for next-generation electronics — •Chris G. Van de Walle — Materials Department, University of California, Santa Barbara, USA

The formation of a two-dimensional electron gas (2DEG) at the interface between two insulators, $SrTiO_3$ (STO) and $LaAlO_3$ (LAO), has sparked huge interest in oxide electronics. The mechanisms that determine the density of this 2DEG have not yet been unravelled. The polar discontinuity at the STO/LAO interface can in principle sustain an electron density of 3.3×10^{14} cm^{-2} (0.5 electrons per unit cell), but experimentally observed densities are more than an order of magnitude lower. We have used a combination of first-principles calculations and Schrödinger-Poisson simulations to investigate the origin of the electrons in the 2DEG at the STO/LAO interface. We find that the inability to form a symmetric set of interfaces limits the 2DEG density [1]. The effects of different terminations of the LAO surface are examined. Our results apply to oxide interfaces in general, and explain why the $SrTiO_3/GdTiO_3$ interface has been found to exhibit the full density of 0.5 electrons per unit cell [2].

Work performed in collaboration with L. Bjaalie, L. Gordon, and A. Janotti, and supported by the ARO and NSF.

[1] A. Janotti, L. Bjaalie, L. Gordon, and C. G. Van de Walle, Phys. Rev. B 86, 241108(R) (2012).

[2] P. Moetakef, T. A. Cain, D. G. Ouellette, J. Y. Zhang, D. O. Klenov, A. Janotti, C. G. Van de Walle, S. Rajan, S. J. Allen, and S. Stemmer, Appl. Phys. Lett. 99, 232116 (2011).

HL 15: Focus Session: Crystalline n-type semiconducting oxides - SnO_2, Ga_2O_3, and In_2O_3 for novel devices (HL, jointly with O)

Traditionally, wide band gap semiconducting oxides have been synthesized as thin polycrystalline films for mainly passive components such as transparent conducting electrodes or gas sensors. More recently, however, it has been recognized that — highly pure and single-crystalline — these oxides can become semiconductor materials for active devices. Development of high quality oxides allows to study their intrinsic physics and enables potential applications in transparent (opto)electronics, power electronics, photonics, and chemical and biological sensors. This session sets a focus on crystalline SnO_2, Ga_2O_3, and In_2O_3 as n-type semiconducting oxides and gives a state-of-the-art survey of their physics including the prospects of applications. (Organizers: Oliver Bierwagen, PDI Berlin, and Saskia Fischer, HU Berlin)

Time: Monday 15:00–19:20 Location: H2

Topical Talk HL 15.1 Mon 15:00 H2

Optical absorption and radiation damage in transparent conducting oxides — •Andre Schleife[1], Friedhelm Bechstedt[2], Alfredo Correa[1], and Yosuke Kanai[3] — [1]Lawrence Livermore National Laboratory — [2]Friedrich-Schiller-University Jena — [3]University of North Carolina at Chapel Hill

Transparent conducting oxides are promising semiconductors with important technological applications in various areas of optoelectronics and photovoltaics. An accurate description of *electronic excitations and their dynamics* is crucial for predictive materials design: Outer-space applications, for instance, not only require fundamental understanding of optical absorption but also of radiation damage.

This talk outlines how parameter-free computational electronic-structure techniques based on many-body perturbation theory accomplish the scientific challenge of describing the quantum-mechanical many-body nature of the electron-electron interaction. Insight will be provided into quasiparticle and excitonic effects affecting optical properties of magnesium-, cadmium, and tin-oxide compounds. The impact of free electrons on the optical band gap will be discussed as an important real-structure effect, e.g. in n-doped cadmium oxide.

In addition, this talk will outline high-performance first-principles computational schemes for accurately characterizing non-adiabatic dynamics of electrons and nuclei: Understanding the *electronic stopping* and defects, e.g. when fast hydrogen atoms penetrate magnesium oxide, is essential for developing materials with high radiation resistance. Partly prepared by LLNL under Contract DE-AC52-07NA27344.

HL 15.2 Mon 15:30 H2

Anisotropic dielectric function and carrier density of rutile SnO_2 — •Christian Lidig[1], Karsten Lange[1], Martin Feneberg[1], Maciej Neumann[2], Norbert Esser[2], Mark E. White[3], Min-Ying Tsai[3], Oliver Bierwagen[3,4], James S. Speck[3], and Rüdiger Goldhahn[1] — [1]Otto-von-Guericke-Universität Magdeburg, Institut für Experimentelle Physik, Abteilung für Materialphysik — [2]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V. , Berlin — [3]University of California, Santa Barbara, USA — [4]Paul-Drude-Institut, Berlin

The anisotropic dielectric function of rutile SnO_2 is presented from 0.04 eV up to 20 eV. The results were obtained on a sample grown on TiO_2 having the optical axis in plane. After modelling the layer stack and taking surface roughness into account, the full dielectric function is extracted wich is compared with theoretical calculations. It turns out that electron-hole interaction influences the dielectric function up to 20 eV resulting in a pronounced redshift and redistribution of oscillator strength of features related to van Hove singularities.
Additionally, infrared spectroscopic ellipsometry was performed on a series of SnO_2:Sb layers grown on r-plane sapphire. The plasmon-longitudinal optical phonon- coupling modes yield results for the free carrier concentrations which are discussed in detail.

Topical Talk HL 15.3 Mon 15:45 H2

Growth from the melt of high-quality In2O3 and Ga2O3 single crystals — •Roberto Fornari, Zbigniew Galazka, Reinhard Uecker, and Klaus Irmscher — Leibniz Institute for Crystal Growth, Max-Born-Str. 2, 12489 Berlin

Because of their interesting properties semiconducting oxides, in particular Ga2O3 and In2O3, have recently received much attention. However, as they were deposited as films on hetero-substrates their quality was quite poor. The growth of high-quality bulk Ga2O3 and In2O3 and manufacture of the corresponding substrates can allow the deposition of high-quality epilayers with lower residual carrier density and fewer extended defects. For this reason IKZ has undertaken an effort to grow large single crystals of these oxide compounds from the melt. Transparent semiconducting Ga2O3 single crystals with diameter of about 20 mm and 50-60 mm long were grown by the Czochralski method along the b-axis, using an Iridium crucible and a dynamic protective atmosphere to minimize the dissociation of Ga2O3 melt and ingot. In the case of In2O3 the Czochralski technique is not applicable and it was necessary to develop a novel melt growth method. This new method indeed supplied crystals from which oriented substrates could be prepared. In this presentation the melt growth of Ga2O3 and In2O3 single crystals will be reviewed. An important feature of both materials is given by their strong sensitivity to thermal processing: the free carrier concentration and the absorption spectra drastically vary as a function of annealing temperature, duration and ambient. The possible causes will be discussed.

Coffee break

HL 15.4 Mon 16:30 H2

Surface structure of metal oxides via Fast Atom Diffraction — •Marco Busch[1], Eric Meyer[1], Jan Seifert[1], Helmut Winter[1], Klaus Irmscher[2], Zbigniew Galazka[2], and Roberto Fornari[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 (H and ^{4}He) and molecules (H_2) with energies from 200 eV up to several keV are grazingly scattered from clean and flat surfaces. For scattering along low-indexed axial channels, we observe defined diffraction patterns in the angular distributions of scattered projectiles, which can be ascribed to Fast Atom Diffraction (FAD) with de Broglie wavelengths as low as about 10^{-3} Å. As example, we have investigated the quantum scattering from the cleaved (100) surface of a Ga_2O_3 single crystal, grown by the Czochralski method following by in situ annealing. 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 $Al_2O_3(11\bar{2}0)$ surface we found, that beside the *normal coherence* also the *longitudinal coherence* is preserved, so that *Laue circles* are observed. Then, quantum scattering from surfaces gives rise to interesting features and enhances the resolution of FAD by one order of magnitude. As example, we have resolved the (12x4) superstructure on the $Al_2O_3(11\bar{2}0)$ surface obtained after annealing to about 2000 K.

Topical Talk HL 15.5 Mon 16:45 H2

Development of gallium oxide power devices — •Masataka Higashiwaki[1,2], Kohei Sasaki[1,3], Akito Kuramata[3], Takekazu Masui[4], and Shigenobu Yamakoshi[3] — [1]National Institute of Information and Communications Technology, Koganei, Tokyo, Japan — [2]JST PREST, Chiyoda, Tokyo, Japan — [3]Tamura Corporation, Sayama, Saitama, Japan — [4]Koha Co., Ltd., Nerima, Tokyo, Japan

Gallium oxide (Ga_2O_3) has excellent material properties for power device applications represented by the extremely large breakdown field of 8 MV/cm due to a large band gap of 4.8–4.9 eV. Another important feature in industry is that large single-crystal β-Ga_2O_3 bulks can be fabricated with melt-growth methods. We recently succeeded in fabricating Ga_2O_3 metal-semiconductor field-effect transistors (MES-

FETs) and Schottky barrier diodes (SBDs) on single-crystal β-Ga_2O_3 substrates by using newly developed technologies for making single-crystal substrates, growing conductivity-controlled epitaxial films, and fabricating devices. The MESFETs exhibited excellent device characteristics including an off-state breakdown voltage (V_{br}) over 250 V, an extremely low leakage current (several μA/mm), and a high on/off drain current ratio of around 10,000. The SBDs also showed good characteristics such as an ideal factor very close to 1.0 and a high reverse V_{br}. These results indicate that Ga_2O_3 have comparable or even more potential than Si and typical widegap semiconductors SiC and GaN for power device applications.

HL 15.6 Mon 17:15 H2

Structural, optical and electrical properties of Si-doped β-β-Ga_2O_3 thin films — •Stefan Müller, Holger von Wenckstern, Florian Schmidt, Daniel Splith, and Marius Grundmann — Universität Leipzig, Semiconductor Physics Group, Institut für Experimentelle Physik II, Leipzig, Germany

The wide bandgap oxide semiconductor β-Ga_2O_3 (E_g = 4.9 eV at room temperature) is a promising material for realization of transparent optoelectronics like FETs [1] or solar-blind photodetectors.
In this contribution we present structural, optical and electrical properties of 1% SiO_2-doped β-Ga_2O_3 thin films grown by pulsed-laser deposition (PLD) on *c*-plane sapphire substrates. The oxygen partial pressure was set between 3×10^{-4} and 0.024 mbar and the substrate temperature between 570°C and 730°C. The thin films are $(\bar{2}01)$-oriented if grown at low oxygen partial pressures and high temperatures. At a growth temperature of 730°C and for oxygen partial pressures above 10^{-3} mbar additional orientations are visible in the XRD pattern. The transmissivity between 1100 nm and 280 nm is in the range of 80% for most investigated samples. However, the optical bandgap increases from 4.7 eV (0.04 mbar) to 4.9 eV (3×10^{-4} mbar) with decreasing oxygen partial pressure. The maximal conductivity and electron mobility of our thin films is in the range of 20 S/m and 0.15 cm^2/Vs, respectively.
[1] M. Higashiwaki *et al.*, Appl. Phys. Lett. **100**, 013504 (2012).

HL 15.7 Mon 17:30 H2

Schottky contacts on β-Ga_2O_3 thin films grown by pulsed laser deposition — •Daniel Splith, Stefan Müller, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Semiconductor Physics Group, Institut für Experimentelle Physik II, Leipzig, Germany

A promising oxide semiconductor for high power electronics and transparent optoelectronic devices is β-gallium oxide (Ga_2O_3) with a band gap of about 4.9 eV. We have investigated the preparation and the properties of Schottky contacts (SCs) on Ga_2O_3 thin films. The thin films were grown from a Ga_2O_3 target with 1% SiO_2 on c-sapphire substrates using pulsed-laser deposition at an oxygen pressure of 10^{-3} mbar. The ohmic contacts were fabricated by thermal evaporation of Ti and Al as reported in [1]. Subsequently, we prepared SCs by normal and reactive DC sputtering of metals like Nb, W or Cu. The $I-V$ characteristics of such SCs showed rectification ratios up to 8 orders of magnitude for some of the Nb contacts. The dominant current transport mechanism is thermionic emission. From fits we determined ideality factors n down to 1.15 for the best W contacts and barrier heights Φ_B up to 1.2 eV for the best Cu contacts. Temperature dependent $I-V$ measurements yielded a linear dependence of Φ_B and $\frac{1}{n}-1$ on the inverse temperature in accordance to the theory of thermionic emission in the presence of a laterally inhomogeneous barrier. E. g. the mean barrier height $\overline{\Phi}_B$ for the Cu contacts is determined to be 1.6 eV with a standard deviation σ_Φ of 0.17 eV.
[1] E. G. Villora *et al.*, Appl. Phys. Lett. 92, 202118 (2008)

Coffee break

HL 15.8 Mon 18:00 H2

Printed, high performance inorganic oxide transistors from halide precursors — •Suresh Kumar Garlapati[1,2], Nilesha Mishra[1], Ramona Hahn[1], Simone Dehm[1], Robert Kruk[1], Subho Dasgupta[1], and Horst Hahn[1,2,3] — [1]Institute for nanotechnology, Karlsruhe institute of technology(KIT) ,Eggenstein, Germany — [2]KIT-TUD Joint research laboratory nanomaterials, TU Darmstadt, Darmstadt, Germany — [3]Center for functional nanostructures, KIT, Germany

Ink-jet printed field-effect transistors (FETs) are recently of great interest for large area electronics; especially when they exhibit high field-effect mobility. The importance of such devices increases even further when they are operated with very low voltages and compatible to portable electronic applications. However, examples of low voltage driven, high mobility FETs that are scalable for high volume production is scarce in the literature. Here, we report ink-jet printed, halide precursor based extremely high mobility oxide (In2O3) FETs that are gated with composite solid polymer electrolytes to limit the operation voltage to 1 V. The printed precursors have been annealed at different temperatures (573-773 K) and as a result devices have shown little dissimilar performance depending on the degree of crystallization and size of crystallites. Nevertheless, the performance for the lowest temperature annealed devices (573 K) has also been quite outstanding; device mobility close to 50 cm^2V^-1s^-1 and On/Off ratio in excess of 10^5 is noted. The achieved field-effect mobility ensures high semiconductor quality and excellent semiconductor/dielectric interface.

Topical Talk HL 15.9 Mon 18:15 H2

Surface electron accumulation layers in oxide semiconductors — •Tim Veal — University of Liverpool, Liverpool, UK

In contrast to the electron depletion at the surface of almost all n-type semiconductors, electron accumulation has long been known to occur at ZnO surfaces. It has recently been found to be characteric of several other oxide semiconductors, including CdO [1,2], In_2O_3 [3] and SnO_2. They all have a significant size and electronegativity mismatch between their cation and anion. As a result, they have a particularly low Γ-point conduction band minimum which is ultimately responsible for the propensity for electron accumulation. As well as the existence of an electron-rich layer, it has been found, using angle-resolved photoemission spectroscopy (ARPES), to be quantized into 2D subbands [1]. Moreover, the conventional one-electron picture of surface space-charge in semiconductors is shown to be inconsistent with the electronic structure observed directly from ARPES, indicating that many-body interactions play a large role in the surface electronic properties of these oxides. Such interactions lead to a depth-dependent shrinkage of the semiconductor band gap, resulting in a surface band gap which differs from the bulk value [1]. The most recent studies have focussed on the influence of depositing alkali metals onto these surfaces. Many collaborators are acknowledged for samples and ARPES expertise.
[1] P. D. C. King, T. D. Veal *et al.*, PRL **104**, 256803 (2010); [2] P. D. C. King, T. D. Veal *et al.*, PRB **79**, 035203 (2009); [3] P. D. C. King, T. D. Veal *et al.*, PRL **101**, 116808 (2008)

HL 15.10 Mon 18:45 H2

Surface and bulk derived in-gap states of In_2O_3 single crystals — •Dorothee Braun[1], 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-Str. 2, 12489 Berlin, Germany

The influence of intrinsic point defects on the electronic structure of n-type In_2O_3 single crystals grown by two methods, namely chemical vapor transport (CVT) and melt growth, was examined by two different spectroscopic methods. First, with scanning tunneling spectroscopy (STS), a very surface sensitive technique for measuring the local density of states (LDOS). So far not resolved states within the fundamental band gap have been observed. The gap states have been studied for different crystals and after several temper treatments in oxygen. Second, low-energy angular-resolved photoemission spectroscopy (low-e ARPES) at $h\nu = 9$ eV photon energy has been used to investigate the gap states in the bulk. In contrast to conventional ARPES at typical VUV we were now able to resolve individual emissions of the gap states as well as their momentum dependence. The spectroscopic results will be compared to state of the art DFT-calculations revealing the origin of the gap states in In_2O_3 to be due to oxygen vacancies as well as indium and oxygen interstitials.

HL 15.11 Mon 19:00 H2

Electron transport in molecular-beam-epitaxy-grown SnO_2 and In_2O_3 films: Doping, defects, and the surface — •Oliver Bierwagen[1,2], Natalie Preissler[1], Takahiro Nagata[2,3], Mark E. White[2], Min-Ying Tsai[2], and James S. Speck[2] — [1]Paul-Drude-Institut, Berlin, Germany — [2]University of California, Santa Barbara, USA — [3]National Institute for Material Science, Tsukuba

Electron transport and its control are key issues for the application of semiconducting oxides in (opto)electronic devices. To this end, the

electron transport in unintentionally- and intentionally doped, high quality, molecular-beam-epitaxy-grown tin oxide (SnO_2) and indium oxide (In_2O_3) films is reviewed.[1] Comparably high mobilities indicate high purity and quality.[2] The resistivity was successfully varied over more than seven orders of magnitude from a transparent conducting oxide-like conductivity by donor doping up to the semi-insulating range (but no p-type conductivity) by acceptor doping.[3,4] Oxygen-related defects play a critical role in In_2O_3.[2, 4] A surface electron accumulation layer is present in both oxides.[5,6] While it strongly influences contact properties,[6,7] its conductance is negligible.[3,6]

[1] O. Bierwagen et al.*Chapter 15 - MBE of transparent semiconducting oxides* in *Molecular Beam Epitaxy*, Elsevier Oxford (2012).
[2] O. Bierwagen and J.S. Speck, Appl. Phys. Lett. 97, 072103 (2010).
[3] O. Bierwagen et al., J. Mater. Res. 27, 2232 (2012).
[4] O. Bierwagen and Speck, Appl. Phys. Lett. 101, 102107 (2012).
[5] T. Nagata et al., Appl. Phys. Lett. 98, 232107 (2011).
[6] O. Bierwagen et al., Appl. Phys. Lett. 98, 172101 (2011).
[7] O. Bierwagen et al., Appl. Phys. Express 2, 106502 (2009); T. Nagata et al. J. Appl. Phys. 107, 033707 (2010).

Concluding remarks

HL 16: Theory: Metal-insulator transitions / Electronic structure calculations

Time: Monday 15:30–18:00 Location: H13

HL 16.1 Mon 15:30 H13

Robust Nodal Structure of Landau Level Wave Functions Revealed by Fourier Transform Scanning Tunneling Spectroscopy — K Hashimoto[1,2], T Champel[3], S Florens[4], C Sohrmann[5], J Wiebe[6], Y Hirayama[1,2], •RA Römer[5], R Wiesendanger[6], and M Morgenstern[7] — [1]Tohoku University, Sendai, Japan — [2]JST, ERATO Nuclear Spin Electronics Project, Sendai 980-8578, Japan — [3]Universite Joseph Fourier Grenoble I / CNRS UMR 5493, Grenoble, France — [4]CNRS and Universite Joseph Fourier, Grenoble, France — [5]University of Warwick, Coventry, UK — [6]Institute of Applied Physics, Hamburg University, Hamburg, Germany — [7]RWTH Aachen University, Aachen, Germany

Scanning tunneling spectroscopy is used to study the real-space local density of states (LDOS) of a two-dimensional electron system in magnetic field, in particular within higher Landau levels (LL). By Fourier transforming the LDOS, we find a set of n radial minima at fixed momenta for the nth LL. The momenta of the minima depend only on the inverse magnetic length. By comparison with analytical theory and numerical simulations, we attribute the minima to the nodes of the quantum cyclotron orbits, which decouple in Fourier representation from the random guiding center motion due to the disorder. Adequate Fourier filtering reveals the nodal structure in real space in some areas of the sample with relatively smooth potential disorder.

HL 16.2 Mon 15:45 H13

A functional renormalization group approach for treating interactions in disordered electron systems — •Christian Seiler[1,2] and Ferdinand Evers[1,2] — [1]Institut für Nanotechnologie, Karlsruher Institut für Technologie, Karlsruhe, Germany — [2]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, Karlsruhe, Germany

We propose an approach to treat the effects of interactions in disordered electron systems on a numerical level. The idea is to solve the non-interacting disorder problem for a given disorder realization exactly. We then use the functional renormalization group method to introduce interactions on a perturbative level. In contrast to usual applications of the fRG, we formulate it in terms of the eigenfunctions of the disordered non-interacting Hamiltonian. Disorder averaging of physical quantities is performed as the final step. The main advantage of our approach is that we are able to treat disorder exactly from a numerical point of view. In fRG applications for clean systems the number of active degrees of freedom is reduced by projecting momenta near the Fermi surface to certain spots on this surface. Disordered systems do not lend themselves to such a treatment since momentum no longer is a good quantum number. Here, the challenge is to find another appropriate decimation technique. We devise, compare and discuss several candidates for such disorder-adapted decimation schemes.

HL 16.3 Mon 16:00 H13

Dependence Of Physical Properties Of Materials On The Approximations For The Exchange-Correlation Potential — •Arcesio Castaneda M., Aldo Humberto Romero C., Sangeeta Sharma, John Kay Dewhurst, and Eberhard Gross — Max-Planck-Institut für Mikrostrukturphysik Weinberg 2, D-06120 Halle, Germany

Density Functional Theory (DFT) is in principle exact, but the quality of the results obtained using it, critically depend upon the approximation employed for the exchange-correlation functional. There exist a plethora of exchange-correlation functionals with increasing complexity and computational cost. However, increasing complexity does not necessarily imply better description of material properties. With this in mind, in the present work we analyze the structural, electronic and optical properties of 14 different semiconductors with 16 different exchange-correlation functionals (LDA and GGA type) using the libxc library and the all electron Elk code [1,2]. We discuss different trends and try to understand the effects of the studied functionals on the measured properties. We further propose regimes of application for the considered functionals depending on the property of interest.

[1] M.A.L. Marques, M.J.T. Oliveira and T. Burnus, Libxc: a library of exchange and correlation functionals for density functional theory, Comput. Phys. Commun. 183, 2272 (2012).
[2] K. Dewhurst, S. Sharma, L. Nordström et. al., The Elk FP-LAPW Code, http://elk.sourceforge.net/.

HL 16.4 Mon 16:15 H13

Dynamical processes and temperature effects in semiconductor nanoclusters — Peng Han and •Gabriel Bester — Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany.

Electron-phonon interactions in colloidal semiconductor quantum dots consisting of thousands of atoms are calculated using first principles density functional theory (DFT) and the frozen-phonon approach. In the computation, the electronic states and the change of the potentials caused by a phonon induced distortion of the lattice are self-consistently calculated using DFT; the electron-phonon interaction matrix elements are then obtained using perturbation theory. Using the electron-phonon coupling matrix elements obtained from this approach, we study the electronic relaxation processes in colloidal semiconductor nanoclusters (NCs) via the Liouville-von Neumann equation including a phenomenological Lindblad decay term. We observe a decaying Rabi oscillation with a period of tens of fs, corresponding to emission/absorption of a phonon, and with a decay rate that is dominated by the phonon lifetime. To estimate the phonon lifetime in NCs, we perform *ab initio* molecular dynamics simulations of a $Si_{10}H_{16}$ cluster and extract the time evolution of the energy of selected vibrational modes from the energy auto-correlation functions. We find vibrational cooling times of are around 1 ps for pure Si modes, which are close to the phonon lifetimes in bulk Si.

HL 16.5 Mon 16:30 H13

Ab initio simulation of crystallization in phase change materials — •Ider Ronneberger[1], Yan Li[1], Wei Zhang[1], Sebastiano Caravati[2], Eshet Hagai[2], Michele Parrinello[2], and Riccardo Mazzarello[1] — [1]Institut für Theoretische Physik, RWTH Aachen — [2]Comp. Science, Dep. of Chem. and Appl. Biosciences, ETH Zürich

The microscopic understanding of the crystallization processes in the technologically relevant phase change materials (PCM) is desirable, in that it could eventually lead to improved properties for applications. Ab initio Molecular Dynamics (AIMD) simulations are very useful to investigate these processes and plenty of atomistic studies were conducted in the field of PCM research. However typical simulation times of AIMD are of the order of 1 ns or less, so that observation of long-time processes and rare events (such as crystallization at low temperature) is computationally not affordable. A new efficient sampling method, called metadynamics, was introduced a decade ago, which can accel-

erate the dynamics by biasing with history-dependent potentials and lead to an estimation of the free energy change during the process. In this study we employed the so called Well-Tempered version of metadynamics in combination with AIMD to study the crystallization of GeTe as a model representative of PCMs. Using a few selected reaction coordinates, models with up to 512 atoms were considered and the free energy change upon crystallization computed at 600 K. The results show that this method is a promising tool to determine nucleation barriers in PCMs. We plan to extend this study to different temperature ranges and other PCMs.

Coffee break

HL 16.6 Mon 17:00 H13

Metal-Insulator Transitions of Crystalline Phase-Change Materials — •Wei Zhang[1], Alexander Thiess[2], Peter Zalden[1], Rudolf Zeller[2], Peter Dederichs[2], Jean-yves Raty[3], Matthias Wuttig[1,4], Stefan Bluegel[2,4], and Riccardo Mazzarello[1,4] — [1]RWTH Aachen, Germany — [2]Forschungszentrum Jülich, Germany — [3]University of Liege, Belgium — [4]JARA, Germany

The study of metal-insulator transitions (MITs) in crystalline solids is a subject of paramount importance. Recently, a metal-insulator transition solely due to disorder has been observed experimentally in the crystalline phase-change material (PCMs) $Ge_1Sb_2Te_4$ (GST): upon annealing at temperatures T below 548K, the system shows insulating behavior due to Anderson localization; when annealing at higher T, it exhibits metallic properties. In this work, we present an ab initio Density Functional Theory study of this effect. By considering a set of very large models of GST containing one to several thousand atoms and different degree of disorder, we identify the microscopic mechanism which localizes the electron wavefunctions near the Fermi energy in the insulating phase as due to vacancy clustering. The ordering of these vacancy clusters upon annealing eventually drives the system to the metallic phase. Our results about crystalline PCMs could help to extend the capacity of current data storage devices based on PCMs, which only utilize the electrical contrast between the crystalline and the amorphous phase.

HL 16.7 Mon 17:15 H13

Large-Scale Electronic Structure calculations of Semiconductor Nanostructures using Atomic Effective Pseudopotentials — •Frank Zirkelbach, Jairo Ricardo Cardenas, Pierre-Yves Prodhomme, Peng Han, Roby Cherian, and Gabriel Bester — Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

In the presented scheme [1], the Schrödinger equation of an electronic system is solved within an effective single-particle approach utilizing atomic effective pseudopotentials [2], which are derived from screened local effective crystal potentials obtained from self-consistent density functional theory calculations on elongated and slightly deformed bulk structures. The use of these potentials allows to bypass a self-consistent procedure, which drastically reduces the computational effort. Furthermore, iterative solvers can be used to focus only on a few eigenstates of interest, e.g., states in the vicinity of the band gap of a semiconductor. Hence, this approach enables first-principles investigations of the electronic structure of semiconductor nanostructures consisting of ten thousands of atoms. In addition to the non-local contribution of the *ab initio* pseudopotential to reconstruct the full crystal potential, a real space treatment scaling linearly with the number of atoms is used to include spin-orbit effects.

[1] G. Bester et. al., unpublished (2012).
[2] J. R. Cárdenas and G. Bester, Phys. Rev. B **86** (2012).

HL 16.8 Mon 17:30 H13

Calculation of branch points and band offsets for cubic $Ga_xAl_{1-x}N$ — •Daniel Mourad — Insitut für Theoretische Physik, Universität Bremen

The anisotropic valence band offset (VBO) across the interface between two materials is an important material parameter and can approximately be calculated from the branch points (BPs, aka charge neutrality levels) of the constituent materials. $Ga_xAl_{1-x}N$ is a technologically important semiconductor alloy and often used as barrier material in optoelectronic devices. Nevertheless, most work and available data concentrates on the hexagonal modification, while there is considerably less data for the zincblende phase of the alloy. The latter also shows an interesting direct to indirect band gap transition on the Al-rich side, which makes it an interesting model system for the calculation of concentration-dependent properties.

We show how the concentration-dependent BP of the disordered $Ga_xAl_{1-x}N$ alloy can be calculated within a combination of a suitable tight-binding model and the coherent potential approximation (CPA). We then analyse the resulting VBOs for several material combinations and interface orientations and discuss the extension to the wurtzite phase and further nitride alloys like $In_xGa_{1-x}N$.

HL 16.9 Mon 17:45 H13

Density Functional Theory Investigation of inner-Surface Methylated Aluminosilicate Nanotubes — •Joshua Elliott — University of Liverpool, Liverpool United Kingdom

We present a linear-scaling Density Functional Theory (LS-DFT) investigation into the electronic structure and stability of organic/inorganic hybrid Methyl-Aluminosilicate nanotubes (me-AlSi) as prepared and characterized in [1]. Due to the size of the considered systems (with unit-cells in excess of 350 atoms), we make use of the LS-DFT code ONETEP [2]. Following investigation of the convergence of the results with respect to the ONETEP simulation setup (kinetic energy cutoff, number and radius of the in situ optimised basis-set [2]), the effect of inner methyl incorporation on the structure of aluminosilicate nanotubes has been studied. We find that the lowest-energy tube structure has 13 unit repeat units in its circumference and a periodicity along tube axis in good agreement with available experimental data (8.0 Å[1]). We find that the presence of methyl groups does not inhibit the real space localisation of the Conduction Band (CB) and Valence Band (VB) on different sides of the nanotube cavity, nor the accumulation of positive (negative) charge at the outer (inner) surface of the tube, typical of Aluminosilicate (AlSi) nanotubes [3]. The methyl-induced shift on the me-AlSi VB and CB edges is finally quantified and suggested as an effective strategy towards doping of aluminosilicate interfaces.

[1] Phys. Chem. Chem. Phys., 13, 2, 744, (2010). [2] J. Chem. Phys. 122, 084119 (2005). [3] J. Phys.: Cond. Mat., 21, 195301 (2009).

HL 17: Interfaces and surfaces

Time: Monday 15:00–17:00 Location: H15

HL 17.1 Mon 15:00 H15

Photoluminescence spectroscopy of singlelayer MoS_2 — •Gerd Plechinger, Stefanie Heydrich, Johannes Schmutzler, Jonathan Eroms, Dieter Weiss, Christian Schüller, and Tobias Korn — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany

Complementary to the gapless material graphene, the transition-metal dichalcogenide MoS_2 is a promising two-dimensional layered semiconductor for future ultrathin nanoelectronic and optoelectronic devices. Subnanometer thickness, large bandgap in the visible range and ultrafast carrier dynamics make it interesting for devices like transistors, ultrafast optical switches or photovoltaic applications.

Our monolayer MoS_2 flakes were prepared by the well-known mechanical cleavage method. With a μPL experimental setup, we can perform photoluminescence spectroscopy at temperatures from 4 K up to room temperature. Under different external influences like temperature, magnetic fields or circular polarisation of the exciting laser light, we investigated the behavior of the A and B excitons, arising from transitions from the spin-orbit split valence band to the conduction band at the K-point of the Brillouin zone. Thereby, we could gather information about charged and neutral excitons and a possible valley polarisation. Furthermore, we could produce monolayer regions out of few-layer flakes via intense focussed laser radiation.

Financial support by Deutsche Bundesstiftung Umwelt is gratefully acknowledged.

HL 17.2 Mon 15:15 H15

Optical properties of single-layer, double-layer, and bulk MoS2 — •Alejandro Molina-Sánchez[1], Ludger Wirtz[1], and Kerstin Hummer[2] — [1]University of Luxembourg, Luxembourg — [2]University of Vienna, Vienna, Austria

The rise of graphene has brought attention also to other layered materials that can complement graphene or that can be an alternative in applications as transistors. Single-layer MoS2 has shown interesting electronic and optical properties such as as high electron mobility at room temperature and an optical bandgap of 1.8 eV. This makes the material suitable for transistors or optoelectronic devices [1]. We present a theoretical study of the optical absorption and photoluminescence spectra of single-layer, double-layer and bulk MoS2. The excitonic states have been calculated in the framework of the Bethe-Salpeter equation, taking into account the electron-hole interaction via the screened Coulomb potential. In addition to the step-function like behaviour that is typical for the joint-density of states of 2D materials with parabolic band dispersion, we find a bound excitonic peak that is dominating the luminescence spectra. The peak is split due to spin-orbit coupling for the single-layer and split due to layer-layer interaction for few-layer and bulk MoS2. We discuss the changes of the optical bandgap and of the exciton binding energy with the number of layers, comparing our results with the reported experimental data.

[1] See recent review: Nature Nanotechnology 7, 699 (2012).

HL 17.3 Mon 15:30 H15

Time and spatially resolved measurement of interface and bulk recombination of low bandgap multijunction solar cell material — •Anja Dobrich[1], Klaus Schwarzburg[1], and Thomas Hannappel[1,2,3] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin — [2]Technische Universität Ilmenau, Institut für Physik, Fachgebiet Photovoltaik, Ilmenau — [3]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, Erfurt

Triple junction III-V compound semiconductor solar cells are today's most efficient photovoltaic devices with conversion efficiencies >41%. A next generation multijunction cell with four or more junctions and optimized bandgaps is expected to break the present record efficiency surpassing the 50% mark. For this purpose, we developed a GaInAsP/GaInAs tandem cell lattice-matched to InP, which could be utilized as a low bandgap part of a well-established high bandgap GaInP/GaAs tandem cell. Since one of the most important properties of solar cell absorber materials is the lifetime of minority carriers, double heterostructures with the low bandgap GaInAs absorber embedded between InP barriers were grown, for photoluminescence measurements. We investigated the effect of different preparation routes for the GaInAs/InP interface on the lifetime, interface recombination velocity and its lateral interface homogeneity. The preparation routines were varied in order to initiate a lateral homogenous layer growth and to form the interface as sharp as possible, which is of major importance for the performance of thin device structures such as quantum well structures or tunnel junctions in multijunction solar cells.

HL 17.4 Mon 15:45 H15

Surface characterization of MOVPE prepared Si(111) substrates for III-V nanowire solar cells — •Weihong Zhao[1,2], Agnieszka Paszuk[1,2], Matthias Steidl[1,2], Sebastian Brückner[1,2], Anja Dobrich[2], Johannes Luczak[2], Peter Kleinschmidt[1,3], Henning Döscher[1,2], and Thomas Hannappel[1,2,3] — [1]Technische Universität Ilmenau, Institut für Physik, Fachgebiet Photovoltaik, D-98684 Ilmenau — [2]Helmholtz-Zentrum Berlin, Institut für Solare Brennstoffe und Energiespeichermaterialien, D14109 Berlin — [3]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, D99099 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 enviroment. We used in situ RAS to monitor the Si (111) surface during preparation in MOVPE. A contamination-free transfer system enabled us to study the MOVPE prepared surfaces with numerous UHV based surface science tools. A dedicated wet-chemical pretreatment is crucial to obtain atomically flat Si(111) surfaces. It is shown that our preparation in a hydrogen ambient results in a monohydride terminated (1x1)-reconstructed Si(111) surface.

HL 17.5 Mon 16:00 H15

From surface dimers to Si—P bonds at the GaP/Si(100) heterointerface — •Oliver Supplie[1,2], Sebastian Brückner[1,3], Henning Döscher[1,3,4], Peter Kleinschmidt[1,5], and Thomas Hannappel[1,4,5] — [1]Helmholtz-Zentrum Berlin, Institut für Solare Brennstoffe — [2]Humboldt-Universität zu Berlin, Institut für Physik — [3]TU Ilmenau, Institut für Physik, Fachgebiet Photovoltaik — [4]NREL, Golden, CO, USA — [5]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, Erfurt

Dimerized (100) surfaces of cubic crystals often exhibit characteristic reflection anisotropy (RA) spectra, as reported for both monohydride [1] and As [2] terminated Si(100), as well as for P-rich GaP(100) [3]. This allows in situ control during metalorganic vapor phase epitaxy which is essential, in particular, directly before III-V nucleation since preparation routes strongly vary with offcut and desired surface termination. Given the polarity of the GaP film and the dimer orientation of the substrate prior to nucleation, a simplistic model [4] allows to conclude whether Si—III or Si—V bonds are preferred at the heterointerface. Since GaP polarity corresponds to orientation of P-dimers at the P-rich GaP/Si(100) surface, we can deduce the preferred bonding from in situ RA spectra only. We find that P-polar GaP was grown both on As-terminated Si(100) and H-terminated, B-type Si(100) while Ga-polar GaP grew on H-terminated A-type Si(100). In all three cases, Si—V bonds established preferentially.

[1] Brückner et al., *PRB* **86**:195310. [2] Kipp et al., *PRL* **76**:2810. [3] Töben et al., *Surf.Sci.* **494**:755. [4] Beyer et al., *JAP* **111**:083534.

HL 17.6 Mon 16:15 H15

Surface characteristics of polar InN layers grown by MOVPE, MBE and migration enhanced afterglow techniques. — •Daria Skuridina[1], Duc V. Dinh[1], Rolf Aidam[2], Michael Kneissl[1], and Patrick Vogt[1] — [1]Institute of Solid State Physics, Technische Universitaet Berlin, Hardenbergstr. 36, EW6-1, 10623 Berlin, Germany — [2]Department Epitaxy, Fraunhofer Institute IAF, Tullastr. 72, 79108 Freiburg, Germany

The surface morphology of an InN layer affects its optical and electrical properties and thus influences the efficiency of InN based devices. In this work we investigate the correlation between morphology, bonding configuration and preparation conditions for polar surfaces of InN layers grown by different growth techniques: metal-organic vapour phase epitaxy (MOVPE), molecular beam epitaxy (MBE), and migration enhanced afterglow (MEAglow) that results in a growth of N-rich InN layers [1]. Morphology, atomic structure and symmetry of the InN surfaces were measured by scanning tunneling microscopy (STM) and low energy electron diffraction (LEED). Auger and X-ray photoelectron spectroscopy (XPS) were used for chemical composition analysis of the layers. InN surfaces were prepared under ultra-high vacuum conditions by annealing, significantly reducing surface contaminations. We find that the surface oxide bonding configuration differs for InN grown by MEAglow and the observed $(\sqrt{3}\times\sqrt{3})\mathrm{R}\,30^\circ$ surface symmetry differs from the commonly observed (1×1) surfaces for InN grown by MBE and MOVPE. We will discuss the related atomic structure and bonding configuration.[1]K.S.A.Butcher, Phys.Stat.Sol. A 209, 41(2012)

HL 17.7 Mon 16:30 H15

AlGaN/GaN Enzyme-Modified Field-Effect Transistors for Analysis of Enzyme Functionality — •Gesche Mareike Müntze, Wladimir Schäfer, Kai Röth, Alexander Sasse, and Martin Eickhoff — I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Germany

AlGaN/GaN high electron mobility transistors (HEMTs) are promising candidates for the application as transducers in biosensors. The chemical stability and biocompability of GaN surfaces as well as their high pH-sensitivity serve as the basis for this application. By covalent immobilization of enzymes on the gate area of an AlGaN/GaN HEMT one obtains an enzyme-modified field-effect transistor (EnFET) with the type of enzyme defining the specificity of the biosensor. Essential to this concept is the formation of an acid or a base as a product of the enzymatic reaction. The pH-change is detected by the AlGaN/GaN HEMT in terms of a change in the drain-source current I_{DS}.

Here, we report the preparation of penicillinase-modified as well as acetylcholinesterase-modified FETs (PenFETs, AcFETs) by a wet chemical process. The obtained EnFET response curves can be fitted by applying a kinetic model which is used to extract microscopic parameters representing both the enzymatic activity and the transis-

tor/enzyme/electrolyte system.

Our results show that EnFETs based on AlGaN/GaN HEMT structures provide a suitable base not only for the realization of specific biosensors but also for analysis of the functionality of immobilized enzymes.

HL 17.8 Mon 16:45 H15

Silicon surface properties after irradiation with single femtosecond laser pulses under SF_6 atmosphere — •Kay-Michael Günther[1], Hartmut Witte[2], Jürgen Blaesing[2], Alois Krost[2], Thomas Gimpel[3], Wolfgang Schade[1,3], and Stefan Kontermann[3] — [1]Clausthal University of Technology, EFZN, Am Stollen 19B, 38640 Goslar, Germany — [2]Otto-von-Guericke University Magdeburg, Institute for Experimental Physics, Universitätsplatz 2, 39106 Magdeburg, Germany — [3]Fraunhofer Heinrich Hertz Institute, Am Stollen 19B, 38640 Goslar, Germany

Irradiating a silicon surface with femtosecond laser pulses under a SF_6 atmosphere can lead to the incorporation of sulfur donors into the top layer. After several pulses on the same spot, the surface becomes roughened. Hence, with a single fabrication step, a pn-junction as well as a low reflecting surface can be created. This technique is already used to fabricate solar cells and photodetectors.

In this work, we investigate the properties of p-type silicon samples which are irradiated with a single pulse per spot. With X-ray diffraction (XRD) measurements, atomic force microscopy (AFM) and Nomarski microscopy images we show that the crystal quality of the material remains unchanged and that only the close surface region of the samples is structured by the laser. The sulfur incorporation is investigated by secondary ion mass spectroscopy (SIMS), Hall-effect measurement, photoluminescence spectroscopy as well as capacitance-voltage spectroscopy (CV) which indicates, that the incorporated sulfur atoms are partly electrically active.

HL 18: Lasers and LEDs I

Time: Monday 15:00–16:30 Location: H16

HL 18.1 Mon 15:00 H16

Interplay of different degradation mechanisms in short wavelength InGaAlP light emitting diodes in model and experiment — •Cynthia Karl, Jens Ebbecke, Claudia Kauss, Thomas Lutz, and Roland Zeisel — OSRAM Opto Semiconductors, 93055 Regensburg, Germany

The interplay of different degradation mechanisms in short wavelength $(Al_xGa_{1-x})_{0.5}In_{0.5}P$ LED structures is investigated by overstress experiments. The experimental data are analyzed with regard to the characteristic dependence of each of the concurring degradation mechanisms on the stress and measurement power density. Therefore a multi component defect evolution approach is used describing simultaneous growth and annealing of defects with different characteristic time constants. In combination to this approach the rate equation model for radiative and non-radiative recombination and leakage losses is applied. In such a way access to a further understanding of the origin of the different occurring aging mechanisms is provided, whose superposition can lead to a quite complex overall LED degradation behavior.

HL 18.2 Mon 15:15 H16

Red quantum dot based semiconductor disk laser — •Thomas Schwarzbäck, Roman Bek, Fabian Hargart, Christian A. Kessler, Hermann Kahle, Elisabeth Koroknay, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen and Research Center SCoPE, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

Since the pioneering work of Kuznetsov et al. in 1997, semiconductor disk lasers also known as vertical external cavity surface-emitting lasers (VECSELs) have excited growing interest in science. These kinds of lasers combine some advantages, which none of the remaining semiconductor laser sources can offer. High continuous-wave (cw) output power and near-diffraction-limited beam quality with a TEM00 Gaussian beam profile are somewhat unique. Meanwhile not only quantum wells but rather quantum dots (QDs) are used as gain material, where theory promises stunning properties like higher and broader gain or temperature insensitive low threshold. This make QD-VECSELs predestinated for lots of applications in various fields such as medicine, life sciences, display or projection applications and in research.

The QD-VECSEL is fabricated via metal-organic vapor-phase epitaxy. The fundamental laser emission around 650 nm is provided by InP QDs embedded in a separate confinement heterostructure. We will present laser characteristics as well as output powers exceeding 1.3 W.

HL 18.3 Mon 15:30 H16

Passively mode-locked red AlGaInP-VECSEL emitting $<$ 50 ps pulses — •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

Since the first introduction of a semiconductor saturable absorber mirror (SESAM) into a vertical external cavity surface-emitting laser (VECSEL) in 2000, there has been substantial progress regarding pulse duration, repetition rate and output power. Despite the numerous advantageous properties of these mode-locked VECSELs like the possibility of bandgap engineering and near-diffraction-limited beam quality, most research has been limited to the infrared spectral range from 830 nm to 1.5 μm. We present SESAM mode locking of a VECSEL producing pulses with a FWHM duration below 50 ps and a repetition rate of 810 MHz at around 665 nm. The metal-organic vapor-phase epitaxy fabricated structures include a Bragg mirror consisting of 55 $\lambda/4$ pairs of AlGaAs/AlAs on a GaAs substrate. The following active region of the VECSEL has a resonant periodic gain structure containing 20 GaInP quantum wells. Two of the same quantum wells serve as absorber layers in the SESAM using fast surface recombination. The SESAM structure has a resonant design with an additional SiO_2 coating for low saturation fluence and a flat group delay dispersion. We use a V-shaped cavity with an overall length of 185 mm to strongly focus onto the SESAM where the folding mirror is used for outcoupling.

HL 18.4 Mon 15:45 H16

Implementation of diffractive optical elements into AlGaInP-based vertical-cavity surface-emitting lasers for beam shaping — •Susanne Weidenfeld[1], Hendrik Niederbracht[1], Thomas Schwarzbäck[1], Frederik Schaal[2], Christoph Pruss[2], Wolfgang Osten[2], Michael Jetter[1], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, University of Stuttgart, Stuttgart, Germany — [2]Institut für Technische Optik, University of Stuttgart, Stuttgart, Germany

Vertical-cavity surface-emitting lasers (VCSELs) have all kinds of applications, like in the field of optical data transmission, in optical computer mice, laser printing and sensor applications. The idea is now the development of a compact micro optical device for non-pixelated spatial polarization control of an incoming light field. Here, the red-emitting AlGaInP-based VCSEL will act as a lighting module for a photo-addressable layer. With the monolithic integration of an oxide aperture, the transverse beam profile can be defined. The vertical structure of these lasers and thus the on-wafer processing offers also the opportunity to implement beam shaping optics monolithically in the top surface. The aim of these additional features is the manipulation of the laser beam for special device applications. We present first steps towards integrating a diffractive optical element (DOE) directly into the top mirror of the VCSEL. Different measurements will be presented to determine the optical and electrical characteristics of the VCSEL, especially to analyze the effect of the DOE on the beam profile.

HL 18.5 Mon 16:00 H16

Harmonic emission intensity modulation of a microlaser using picosecond acoustics — •Thomas Czerniuk[1], Christian Brüggemann[1], Andrey V. Akimov[2,3], Christian Schneider[4], Sven Höfling[4], Alfred Forchel[4], Dimitri R. Yakovlev[1,2], and Manfred Bayer[1] — [1]Experimentelle Physik 2, TU Dortmund, 44221 Dortmund, DE — [2]A. F. Ioffe Physical Technical Institute, 194021 St Petersburg, RU — [3]School of Physics and Astronomy, University of Nottingham, NG7 2RD, UK — [4]Technische Physik, Universität Würzburg, 97074 Würzburg, DE

We demonstrate a harmonic ∼10 GHz modulation of the microcavity laser emission intensity using picosecond strain pulses. The gain medium of the microlaser is an 11 meV broad inhomogenious InGaAs quantum dot ensemble. These QD's are placed inside a resonant optical AlAs/GaAs Bragg reflector microcavity with a linewidth of 1.2 meV. This results in a inefficient coupling for a large fraction of the quantum dot ensemble to the laser mode. An optically excited broadband strain pulse propagates through the cavity and, once hitting the QD's, shifts their transition energies by ∼10 meV within picoseconds. This couples more QD's into the laser mode, thereby increasing the emission intensity. Due to the acoustic mismatch of AlAs and GaAs, the Bragg reflectors also work for phonons, increasing the lifetime of 16.6 GHz phonons inside the cavity. The effect is maximal, if the laser is pumped slightly above the lasing threshold, where we observe GHz modulations with a relative amplitude of 1.5 for more than 300 ps, much longer than the duration of the strain pulse.

HL 18.6 Mon 16:15 H16

High Modal Gain 1.55 μm InAs/InP(100) Based Quantum Dot Lasers with High Wavelength Stability — •Vitalii Sichkovskyi, Vitalii Ivanov, and Johann Peter Reithmaier — Institute of Nanostructure Technologies and Analytics, CINSaT, University of Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel, Germany

Self-organized InAs/InP quantum dot systems are promising candidates for telecommunication applications at 1.55 μm. Based on a novel quantum dot (QD) growth technique, high density dot-like QDs can be grown on (001) InAlGaAs surfaces which results in a strongly improved modal gain per QDs layer. Here we report on the influence of the number of QD layers on static properties of the laser. By reducing the number of QD layers to only three or even two layers, i.e., lowering the modal gain, the wavelength shift with temperature can be reduced. The broad area lasers processed from such laser structure revealed small coefficients of their wavelength variation with temperature, whose values decreased with decreasing the cavity length down to a remarkably low value of 0.07 nm/K, which is 5 times less than for QW lasers. As a proof of high modal gain material, ridge waveguide lasers with only one active InAs QDs layer and cavity lengths of 2025 μm could be operated at room temperature. The threshold current was measured to 130 mA and a total cw output power of 9 mW was obtained. The laser structures with specially optimized design for high-speed telecom applications will be presented and discussed.

HL 19: Invited Talk: Stephan Winnerl

Time: Monday 15:00–15:30 Location: H17

Invited Talk HL 19.1 Mon 15:00 H17

Relaxation dynamics in graphene close to the Dirac point — •Stephan Winnerl — Helmholtz-Zentrum Dresden-Rossendorf

The carrier relaxation in graphene is of strong interest for understanding carrier-carrier and carrier-phonon interactions in this fascinating material as well as for optoelectronic applications such as detectors, and saturable absorbers. Here we give an overview on our investigations on the dynamics in the energetic vicinity of the Dirac point, which is explored by pump-probe experiments with mid-infrared and terahertz radiation [1]. We compare our experimental results with microscopic theory and discuss the role of optical phonons, acoustic phonons and carrier-carrier scattering. For excitations slightly above and below the Fermi edge an interesting change in sign of the pump-probe signals is observed, which can be explained by an interplay of intraband and interband excitation. Furthermore we present recent results on the dynamics in Landau quantized graphene, where a strong dependence of the pump-probe signals on the state of circular polarization of both pump and probe radiation is found. The results indicate the importance of Auger-type processes in this regime.

S. Winnerl et al., Phys. Rev. Lett. 107, 237401 (2011).

HL 20: Topological insulators 2 (MA, jointly with HL, O, TT)

Time: Monday 15:00–18:00 Location: H10

Invited Talk HL 20.1 Mon 15:00 H10

The THz response of topological insulator surface states — •N. Peter Armitage — The Institute of Quantum Matter, Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD 21218, USA

Topological insulators (TIs) are newly discovered states of matter characterized by an *inverted* band structure driven by strong spin-orbit coupling. One of their most touted properties is the existence of robust "topologically protected" surface states. I will discuss what topological protection means for transport experiments and how it can be probed using the technique of time-domain THz spectroscopy applied to thin films of Bi_2Se_3. By measuring the low frequency optical response, we can follow their transport lifetimes as we drive these materials through instabilities either by doping through a quantum phase transition into a topologically trivial regime or by reducing the film thickness. I'll also discuss our work on the magnetic field dependence of the Kerr rotation in Bi_2Se_3, where we find an unprecedentedly large value of the angle of rotation of reflected light, which is due to the cyclotron resonance of the 2D Dirac fermions.

15 min. break

HL 20.2 Mon 15:45 H10

Peierls dimerization at the edge of 2D topological insulators? — •Gustav Bihlmayer[1], Hyun-Jung Kim[2], Jun-Hyung Cho[2], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Department of Physics and Research Institute for Natural Sciences, Hanyang University, Seoul, Republic of Korea

Edge states of two-dimensional topological insulators (2D-TIs) attracted considerable interest as they support dissipationless spin-currents. Recently, it was proposed that the zigzag-edge of a Bi(111) bilayer, identified as a 2D-TI [1,2], is unstable with respect to a Peierls dimerization [3], a phenomenon that occurs quite general in one-dimensional structures. This proposal was based on an *ab initio* investigation without taking spin-orbit coupling (SOC) into account. We investigate the effect of SOC on the atomic structure of zigzag Bi(111) and Sb(111) nanoribbons. Although we find that edge-reconstructions can influence the number of conductive channels, we conclude that the topological protection of the states in the Bi ribbon actually prevents the Peierls mechanism to get effective, since the opening of a Peierls gap at the zone boundary is forbidden by time-reversal symmetry. We compare the situation to the Sb structure, but also in the topologically trivial case of the Sb(111) bilayer ribbon we find a suppression of the dimerization due to SOC effects.

[1] S. Murakami, Phys. Rev. Lett. 97, 236805 (2006) [2] M. Wada et al., Phys. Rev. B 83, 121310(R) (2011) [3] L. Zhu et al., J. Phys. Chem. C 114, 19289 (2010)

HL 20.3 Mon 16:00 H10

Engineering quantum anomalous Hall (QAH) phases with orbital and spin degrees of freedom — •Hongbin Zhang, Frank Freimuth, Gustav Bihlmayer, Marjana Ležaić, Stefan Blügel, and Yuriy Mokrovsov — Peter Grünberg Institut and Institute for Advanced Simulation, FZJ and JARA, 52425 Jülich, Germany

Combining tight-binding models and first-principles calculations, we demonstrate that under external exchange fields, non-zero Chern numbers and nontrivial QAH effects can be induced by on-site spin-orbit coupling (SOC) in buckled honeycomb lattices with *sp* orbitals. In the Haldane model [1], the occurrence of the QAH effect is attributed to complex valued next-nearest-neighbor hopping matrix elements. Detailed analysis of a generic tight binding model reveals that there exist different mechanisms giving rise to complex hoppings, utilising both

orbital and spin degrees of freedom of electrons on a lattice. Furthermore, it is shown that in Bi- or Sb(111) bilayers [2], different topological phases exist as function of the magnitude of SOC and external exchange fields. These phases are characterised using Chern and spin Chern numbers [3] in combination with transverse charge and spin conductivities. At last, we show that introducing ferromagnetic dopants provides a practical way to induce nontrivial topological phases, whereas the physics is altered due to partially filled d states around the Fermi energy. – Support by Helmholtz Young Investigators Group Programmes VH-NG-409 and -513 is acknowledged.

[1] F.D.M. Haldane, PRL **61**, 2015 (1988). [2] H. Zhang, *et al.*, PRB **86**, 035104 (2012). [3] E. Prodan, PRB **83**, 195119 (2011).

HL 20.4 Mon 16:15 H10

Prediction of weak topological insulators in layered semiconductors — •Binghai Yan[1,2], Lukas Müchler[1,2], and Claudia Felser[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, D-01187 Dresden — [2]Institute for Inorganic and Analytical Chemistry, Johannes Gutenberg University of Mainz, 55099 Mainz

We report the discovery of weak topological insulators by ab initio calculations in a honeycomb lattice. We propose a structure with an odd number of layers in the primitive unit cell as a prerequisite for forming weak topological insulators. Here, the single-layered KHgSb is the most suitable candidate for its large bulk energy gap of 0.24 eV. Its side surface hosts metallic surface states, forming two anisotropic Dirac cones. Although the stacking of even-layered structures leads to trivial insulators, the structures can host a quantum spin Hall layer with a large bulk gap, if an additional single layer exists as a stacking fault in the crystal. The reported honeycomb compounds can serve as prototypes to aid in the finding of new weak topological insulators in layered small-gap semiconductors.

HL 20.5 Mon 16:30 H10

Dirac States in a Novel Topological Insulator: Epitaxial alpha-Tin Layers on Indium Antimonide — •J. Schäfer[1], A. Barfuss[1], G. Bihlmayer[2], D. Wortmann[2], L. Dudy[1], P. Höpfner[1], A. Bostwick[3], E. Rotenberg[3], and R. Claessen[1] — [1]Phys. Inst., Universität Würzburg, D — [2]Peter Grünberg Inst. and Inst. Adv. Sim., FZ Jülich, D — [3]Lawrence Berkeley Nat. Lab., USA

This study addresses a new material realization of a topological insulator (TI) thus far only proposed theoretically, which is formed by α-Sn in the diamond lattice on InSb substrates. The epitaxial growth opens various pathways to access and manipulate the topological surface state (TSS). This includes the evolution of the Dirac bands as a function of thickness, or surface coating layers which alter the spin-orbit interaction. Interestingly, the TI band properties are closely related to that of strained HgTe, for which the Quantum Spin Hall effect was demonstrated.

Here we report on the electronic structure of α-Sn(001) based on angle-resolved photoemission (ARPES), complemented by density functional theory (DFT). We observe the formation of a clearly pronounced Dirac cone. The Fermi level in ARPES is located close to the Dirac point. Its position can be controlled by dopants, which allows to adjust the Fermi level crossings of the TSS. The Dirac cone is discernible down to bulk band energies, and its constant energy surfaces seemingly reflect the lattice symmetry. The experimental findings are consistent with DFT calculations including spin-orbit interaction, which document the formation of a TSS.

HL 20.6 Mon 16:45 H10

Observation of terahertz photocurrents in the topological insulator Bi_2Se_3 — •Lukas Braun[1], Luca Perfetti[2], Martin Wolf[1], and Tobias Kampfrath[1] — [1]Physikalische Chemie, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Laboratoire des Solides Irradiés, Ecole Polytechnique, Palaiseau cedex, France

Recent experiments have indicated that optical excitation of topological insulators (TIs) with circularly polarized light can induce spin-polarized electron currents along the TI surface. The direction of this photocurrent can be controlled by varying the circular polarization of the driving light from right- to left-handed. So far, only DC photocurrents have been detected [J. W. McIver *et al.* Nature Nanotechnology **7**, 96 (2012)]. Since electrons moving through a solid typically undergo scattering on sub-picosecond time scales, it is highly desirable to generate and detect TI photocurrents with femtosecond time resolution.

Here, we drive ultrashort current bursts in n-doped Bi_2Se_3 by excitation with a laser pulse (10fs, 800nm, 10nJ). The photocurrent gives rise to the emission of a terahertz (THz) electromagnetic pulse whose transient electric field $E(t)$ is detected by means of electro-optic sampling with a time resolution of 10fs. We observe extremely broadband THz emission covering the range from 10 to 30THz, and the THz intensity is found to depend strongly on the helicity of the pump pulses. A method is presented that allows us to extract the transient current $j(t)$ from the measured $E(t)$. We finally discuss the origin of $j(t)$ and implications for the dynamics of photoexcited TI electrons.

HL 20.7 Mon 17:00 H10

Static screening properties of topologically protected surface states — •Daniel Wortmann, Gustav Bihlmayer, Yuriy Mokrousov, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The electrons occupying surface states of topological insulators (TI) provide charges that can screen electric fields applied perpendicular to the surface. Being a very basic phenomenon, its realistic description is rather difficult: model approaches fail to provide quantitative results while DFT calculations of insulating slabs with external electric fields suffer from difficulties arising from the incomplete screening of the field inside the slab.

We demonstrate that the embedded Green function method [1,2] can be utilized to investigate the effects of an applied field on the surface states. Our approach describes the formation of surface states in terms of their scattering properties at the semi-infinite bulk states by means of a generalized logarithmic derivative. Besides discussing the underlying idea of this elegant theoretical tool and its application to prototypical topological insulators, we present a comparison of the expected screening effects seen in a topological insulator with those in a topological material.

[1] see http://www.flapw.de for details of the code

[2] D. Wortmann, H. Ishida, S. Blügel, Phys. Rev. B **65**, 165103 ('02)

HL 20.8 Mon 17:15 H10

Topological phases of spin chains — Kasper Duivenvoorden and •Thomas Quella — Universität zu Köln, Institut für Theoretische Physik, Köln, Deutschland

The Haldane phase of one-dimensional $S = 1$ spin chains with $SU(2)$ symmetry is one of the first topological states of matter. In particular, it features a bulk-boundary correspondence, with $S = 1/2$ degrees of freedom emerging at the boundaries of the system. Moreover, it exhibits a diluted anti-ferromagnetic order which can be measured using a non-local string order parameter. With the prospect of being able to simulate spin chains with $SU(N)$ symmetry in the laboratory using ultracold earth-alkaline atoms it is a natural and interesting question whether similar topological phases also exist beyond $N = 2$.

In a recent paper we have shown that this is indeed the case. More precisely, spin chains with $SU(N)$ symmetry allow for up to N different topological phases, $N - 1$ of which are topologically non-trivial. These phases exhibit topological order that is reflected in a specific entanglement pattern resulting from the matrix product state representation of the corresponding ground state wave function. It may be detected using a non-local string order parameter which characterizes each of the N phases unambiguously. Analytical and numerical results confirm that our order parameter may be used to extract a quantized topological invariant.

HL 20.9 Mon 17:30 H10

Strongly-correlated topological semiconductors — •Stanislav Chadov[1], Claudia Felser[1], Leon Petit[2], Hubert Ebert[3], and Jan Minár[3] — [1]MPI-CPFS Dresden — [2]STFC Daresbury Laboratory, UK — [3]LMU München

Using the fully-relativistic Green's function formalism we analyze the electronic structure topology in series of the heavy rock-salt type semiconductors PuX, SmX (X=Te, Se, S). Due to the partial filling of their f-shells, these materials exhibit strong dynamical correlations which destroy the Bloch-like eigenstates. Thus, the usual analysis based on the symmetry of the eigenstates cannot be applied. Here we recall the adiabatic approach, which allows to analyze the topology based on a purely bulk information disregarding the Bloch or localized character of the electronic states. The dynamical correlations were treated within the DMFT scheme implemented in the framework of the SPR-KKR Green's function method.

HL 20.10 Mon 17:45 H10

Correlation between linear Magnetoresistance and Mobility of Heusler Topological Insulators — •C. Shekhar, A. K. Nayak, S. Ouardi, G. H. Fecher, and C. Felser — Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany

Topological insulators (TIs) are a class of quantum materials and belong to a new state of matter with topologically protected gapless Dirac fermionic states. Among the TIs series Heusler compounds are promising candidates for the nanoelectronic devices. If these compounds contain heavy metals (Au, Pb, Pd, Pt, Sb and Bi) and a lanthanide element then they exhibit extraordinary physical properties including *zero band gap*. Generally, gapless compounds show high mobility, where no threshold energy is required to conduct carriers from occupied states to empty states. Very recently, the exciting discovery of graphene is an example of high-mobility compounds due to its linear dispersion of the bands, where charge carriers behave like massless particles. However, the Heusler TIs having *zero band gap* are also expected to show high mobility. The Heusler TIs also exhibit nonsaturating and positive magnetoresistance, that shows systematic variations with temperature. The best fitting of observed MR is found with the combination of linear and quadratic field dependence and may be written in form of a quadratic equation: MR $= a|B| + (b/2)B^2$, where B is applied field. It is clear that this MR originates from the contribution of both linear and parabolic terms. The parabolic term is well known and comes from the Lorentz force, while the origin of the linear MR is intriguing.

HL 21: Transport: Quantum dots, wires, point contacts 2 (TT, jointly with HL)

Time: Monday 15:00–17:30 Location: H18

HL 21.1 Mon 15:00 H18

Bound States in a Carbon Nanotube Quantum Dot Coupled to Superconducting Leads — •Amit Kumar[1], Martin Gaim[1], Daniel Steininger[1], Andreas K. Hüttel[1], Christoph Strunk[1], Alfredo Levy Yeyati[2], and Alvaro Martín-Rodero[2] — [1]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Department of Theoretical Condensed Matter Physics, Universidad Autónoma de Madrid, 28049 Madrid, Spain

We report on tunnelling spectroscopy measurements on a carbon nanotube quantum dot device strongly coupled with niobium superconducting leads at two ends and weakly coupled to a tunnel probe (aluminium) in the middle. Gate dependent differential conductance measurements at low temperature down to 25mK reveal the formation of bound states (Andreev / Yu-Shiba Rusinov) inside the superconducting gap. By virtue of the larger superconducting gap of the niobium, we observe several such states. Odd Coulomb valleys show negative differential conductance features, which are characteristics for bound states with localized spins. These localized spins (odd number of electrons on the quantum dot) are known to generate localized Yu-Shiba Rusinov bound states inside the superconducting gap and are expected to dominate in asymmetrically coupled quantum dot devices. More detailed experimental investigations and theoretical calculations are in progress to understand these experimental findings.

HL 21.2 Mon 15:15 H18

Kondo Physics in Clean Carbon Nanotubes — •Daniel Schmid, Alois Dirnaichner, Peter Stiller, Andreas K. Hüttel, and Christoph Strunk — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

Clean carbon nanotube quantum dots provide ideal model systems with orbitally degenerate quantum levels to probe novel Kondo physics. Transport measurements on single quantum dots were done down to a base temperature of $T \simeq 20\,\mathrm{mK}$ in the $10 \leq N_{\mathrm{el}} \leq 50$ electron regime, showing the typical signatures of the Kondo effect, as well as co-tunneling features at finite bias.
We focus on a specific charge state with $N_{\mathrm{el}} = 21$ electrons in the intermediate coupling regime $G_{\max} \simeq 0.9(2e^2/h)$. Besides the usual Kondo peak around zero bias voltage ($V_{\mathrm{SD}} = 0$) the differential conductance displays interesting satellites at finite V_{SD}. These satellites depend only weakly on magnetic field and temperature for the range $B < 8\mathrm{T}$ and $T < 1\mathrm{K}$.

HL 21.3 Mon 15:30 H18

Thermal quasiparticle spectroscopy of a carbon nanotube quantum dot coupled to superconducting leads: part I, experiment — •Markus Gaass, Andreas K. Hüttel, Tom Geiger, Sebastian Pfaller, Andrea Donarini, Milena Grifoni, and Christoph Strunk — University of Regensburg, 93040 Regensburg, Germany

We present electronic transport measurements of a single wall carbon nanotube quantum dot contacted with Niobium electrodes. At elevated temperatures, within the superconductor energy gap and the Coulomb blockade region additional transport resonances arise, which we attribute to thermally generated quasiparticles in the Nb leads. A detailed comparison of the temperature dependence with model calculations leads to excellent agreement for zero as well as finite applied bias.

HL 21.4 Mon 15:45 H18

Thermal quasiparticle spectroscopy of a carbon nanotube quantum dot coupled to superconducting leads: part II, theory — •Sebastian Pfaller, Markus Gaass, Andreas K. Hüttel, Tom Geiger, Andrea Donarini, Christoph Strunk, and Milena Grifoni — University of Regensburg, 93040 Regensburg, Germany

We present in this study a transport theory for a carbon nanotube quantum dot coupled to superconducting leads to lowest order in the tunneling. A generalized master equation is used to model the dynamics. For high enough temperatures, quasiparticles in the superconducting lead get thermally excited across the gap, leading to conductance in the Coulomb blockade including the subgap region. Around zero bias conductance peaks are observed. A comparison of the temperature dependence of these thermally induced conductance peaks with experimental data shows excellent agreement.

HL 21.5 Mon 16:00 H18

Mapping out the band structure of carbon nanotubes in a magnetic field: part I, experiment — •Alois Dirnaichner, Daniel Schmid, Magdalena Marganska, Milena Grifoni, Andreas K. Hüttel, and Christoph Strunk — University of Regensburg, 93040 Regensburg, Germany

We report on electronic transport spectroscopy measurements on an ultra-clean carbon nanotube as a quantum dot at low temperature and finite magnetic field. The direction of the magnetic field can be adjusted both parallel and perpendicular to the nanotube axis with flux densities of up to $B = 17\,\mathrm{T}$. Data focusses on the few-electron spectrum, highly regular down to $N_{\mathrm{el}} = 1$, where sharp Coulomb blockade oscillations enable tracing of multiple excited quantum states. We discuss spin-orbit coupling and KK'-mixing in our sample. The data is compared to state-of-the art CNT modeling.

15 min. break

HL 21.6 Mon 16:30 H18

Mapping out the band structure of carbon nanotubes in a magnetic field: part II, theory — •Magdalena Marganska, Alois Dirnaichner, Daniel Schmid, Andreas K. Hüttel, Christoph Strunk, and Milena Grifoni — University of Regensburg, Germany

We report here an analysis of transport measurements of ultraclean carbon nanotubes in parallel magnetic field. Employing the magnetic field dependence of the energies of ground and excited states of a single excess electron in the CNT-quantum dot we can assign a diameter and chirality to the nanotube present in the device. The data obtained in low fields allow us to extract several of the nanotube parameters, and to refine the minimal Hamiltonian commonly used for CNT quantum dots in parallel magnetic fields. With an additional asymmetry term appearing in the Hamiltonian, we can match the experimental data with high accuracy. Using the results from high magnetic fields we can further refine our analysis and identify the term responsible for electron-hole asymmetry in the spin-orbit splitting.

HL 21.7 Mon 16:45 H18

Tunable electron-vibron coupling in suspended carbon nanotube quantum dots — •Christoph Stampfer[1,2], Peter Weber[1,2], Carola Meyer[2], and Stefan Trellenkamp[2] — [1]JARA-FIT and II. Institute of Physics B, RWTH Aachen, 52074 Aachen, Germany — [2]Peter-Grünberg-Institut (PGI-6/8/9), Forschungszentrum Jülich, 52425 Jülich, Germany

Measurements through nano electromechanical systems and single-molecule junctions have shown that electronic transport is strongly influenced by the mechanical motion, leading to transport assisted by emission of vibrons. Furthermore, a strong electron-vibron coupling is expected to lead to a suppression of transport through the vibronic ground state, known as Franck-Condon blockade. Here we report on transport in a quantum dot formed in a partly suspended carbon nanotube devices. The data show Coulomb diamonds with a clear fourfold degeneracy and an experimental confirmation of Franck-Condon blockade mechanism. More interestingly, we show that our four-terminal quantum device allows us to tune the electron-vibron coupling. In particular, we focus on the investigation of spin states and the tunability of electron-phonon coupling in the suspended carbon nanotube quantum dot.

HL 21.8 Mon 17:00 H18

Spin-dependent coupling to vibrations in suspended carbon nanotube quantum dots — •Hernán L. Calvo[1,2], Julian Bohle[1,2,3], Christoph Stampfer[2,3,4], and Maarten R. Wegewijs[1,2,3] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University, Germany — [2]JARA - Fundamentals of Future Information Technology — [3]Peter Grünberg Institut, Forschungszentrum Jülich, Germany — [4]II. Institute of Physics B, RWTH Aachen University, Germany

Recent transport experiments in a semi-suspended carbon nanotube (CNT) quantum dot have shown an electron-vibration coupling that is markedly different for spin singlet and triplet states. In this talk, we show that such an apparent spin-vibration coupling can be understood in terms of a coupling of the electronic valley degree of freedom of the CNT to the observed longitudinal vibration. Strikingly, this Peierls-type coupling in the valley space leads to Franck-Condon sidebands that mostly develop for the triplet excited state. A vibrational modulation of the exchange interaction on the CNT is shown to result in a similar, but weaker effect. The effect can be understood qualitatively from polaronic shifts obtained in the Born-Oppenheimer approximation. In the regimes of interest, however, this approximation breaks down and we present transport calculations accounting for the full pseudo-Jahn-Teller mixing of the vibronic states that show satisfactory agreement with the experiment.

HL 21.9 Mon 17:15 H18

Graphene quantum dots on hexagonal boron nitride — •Alexander Epping[1,2], Stephan Engels[1,2], Christian Volk[1,2], Jan Dauber[1,2], Bernat Terres[1,2], Matthias Goldsche[1,2], Kenji Watanbe[3], Takashi Taniguchi[3], and Christoph Stampfer[1,2] — [1]JARA-FIT and II. Institute of Physics B, RWTH Aachen, 52074 Aachen, Germany — [2]Peter-Grünberg-Institut (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany — [3]Advanced Materials Laboratory, National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan

Graphene exhibits unique electronic and mechanical properties making it a promising material for future quantum-electronic applications. However, state of the art graphene quantum dots fabricated on SiO_2 substrates suffer from their poor quality due to a large disorder potential. Recently, it has been shown that placing graphene on hexagonal boron nitride (hBN) substantially reduces the disorder potential because of its atomically-flat graphene-like hexagonal structure. Here, we present the fabrication and characterization of single-layer graphene quantum dots on hBN substrates. In particular we show low-temperature transport measurements showing Coulomb diamonds with charging energies between 9 meV and 11 meV.

HL 22: Focused Session: Correlations in topological bands (TT, jointly with HL, MA, O)

Topological ideas have been among the most profound recent additions to the field of condensed matter physics, and they have provided some of the most unexpected new developments, most recently through the proposed existence of fractional Chern insulators: these are lattice systems in which fractional quantum Hall physics occurs in partially filled non-dispersive topological "Chern" bands. Our ability to create such environments is central to advancing the understanding of correlated electron physics.

This session focuses on the twin aspects of the new physics that can be found in such settings on one hand, and recent progress towards realizing such settings on the other. It contains theoretical and experimental contributions, from nano-, semiconductor and cold atomic physics.

Organizer: Roderich Moessner (MPI PKS, Dresden)

Time: Monday 15:00–17:45 Location: H20

Invited Talk HL 22.1 Mon 15:00 H20

Designer Dirac Fermions, Topological Phases, and Gauge Fields in Molecular Graphene — •Hari C. Manoharan — Dept. of Physics, Stanford University, Stanford, California 94305, USA

Using low-temperature scanning tunneling microscopy and spectroscopy, we show the emergence of Dirac fermions in a fully tunable condensed-matter system—molecular graphene—assembled via atomic manipulation of a conventional two-dimensional electron system in a surface state. We embed, image, and tune the symmetries underlying the two-dimensional Dirac equation into these electrons by sculpting the surface potential with manipulated molecules. By distorting the effective electron hopping parameters into a Kekulé pattern, we find that these natively massless Dirac particles can be endowed with a tunable mass engendered by the associated scalar gauge field, in analogy to the Higgs field. With altered symmetry and texturing of the assembled lattices, the Dirac fermions can be dressed with gauge electric or magnetic fields such that the carriers believe they are in real fields and condense into the corresponding ground state, as confirmed by tunneling spectroscopy. Using these techniques we ultimately fabricate a quantum Hall state without breaking time-reversal symmetry, in which electrons quantize in a gauge magnetic field ramped to 60 Tesla with zero applied laboratory field. We show that these and other chiral states now possible to realize have direct analogues in topological insulators, and can be used to guide or confine charge in nontrivial ways [1].

[1] Gomes et al., Nature **483**, 306–310 (2012).

Invited Talk HL 22.2 Mon 15:30 H20

Fractional Topological Insulators — •Claudio Chamon[1], Christopher Mudry[2], Titus Neupert[2], and Luiz Santos[3] — [1]Boston University — [2]Paul Scherrer Institute — [3]Perimeter Institute

The prediction and experimental discovery of topological band insulators and topological superconductors are recent examples of how topology can characterize phases of matter. In these examples, electronic interactions do not play a fundamental role. In this talk we shall discuss cases where interactions lead to new phases of matter of topological character. Specifically, we shall discuss fractional topological states in lattice models which occur when interacting electrons propagate on flattened Bloch bands with non-zero Chern number. Topologically ordered many-particle states can emerge when these bands are partially filled, including a possible realization of the fractional quantum Hall effect without external magnetic fields. We also discuss the importance of geometric band attributes to stabilize certain fractional states, highlighting the importance of geometry and not just topology for reaching

fractional states of matter.

Topical Talk HL 22.3 Mon 16:00 H20
Hierarchy of Fractional Chern Insulators and Competing Compressible States — •Andreas Läuchli — Institut für Theoretische Physik, Universität Innsbruck, A-6020 Innsbruck, Österreich

The recent engineering of simple tight binding models harboring flat bands with non-zero Chern number calls for a detailed study of the possible many-body phases occurring in partially filled Chern bands and their analogies and differences compared to the continuum Landau level problem. We first report the numerical phase diagram for a flat Chern band with $C = 1$ on the checkerboard lattice, where we find hierarchy multiplets of incompressible states at various fillings ν These are accounted for by an analogy to Haldane pseudopotentials extracted from an analysis of the two-particle problem. Important distinctions to standard fractional quantum Hall physics are striking: absent particle-hole symmetry in a single band, an interaction-induced single-hole dispersion appears, which perturbs and eventually destabilizes incompressible states as ν increases [1]. In second study we investigate the occurrence of fractional Chern insulating phases in a series of bands with higher Chern numbers $C = N > 1$. We find compelling evidence for a series of stable states at $\nu = 1/(2N + 1)$ for fermions as well as bosonic states at $\nu = 1/(N + 1)$. By examining the topological ground state degeneracies and the excitation structure as well as the entanglement spectrum, we conclude that these states are Abelian [2].

[1] A. M. Läuchli, Z. Liu, E.J . Bergholtz, and R. Moessner, arxiv:1207.6094 (2012)
[2] Z. Liu, E. J. Bergholtz, H. Fan, and A. M. Läuchli, Phys. Rev. Lett. **109**, 186805 (2012)

15 min. break

Topical Talk HL 22.4 Mon 16:45 H20
Designing Topological Bands for Ultracold Atomic Gases — •Nigel Cooper — Cavendish Laboratory, University of Cambridge, UK

One of the most important techniques in the ultracold atom toolbox is the optical lattice: a periodic scalar potential formed from standing waves of light. Optical lattices are central to the use of atomic gases as quantum simulators, and allow the exploration of strong-correlation phenomena related to condensed matter systems. I shall describe how to design new forms of optical lattice - so-called "optical flux lattices" - in which optically dressed atoms experience a periodic effective magnetic flux with high mean density. Optical flux lattices have narrow energy bands with nonzero Chern numbers, analogous to the Landau levels of a charged particle in a uniform magnetic field. These lattices will greatly facilitate the achievement of the quantum Hall regime for ultracold atomic gases.

Topical Talk HL 22.5 Mon 17:15 H20
Probing Topological Bloch Bands Using Ultracold Quantum Gases — •Immanuel Bloch — Max-Planck Institut für Quantenoptik, Garching, Germany — Ludwig-Maximilians Universität, München, Germany

Over the past years, ultracold quantum gases have emerged as highly controllable testbeds for probing fundamental condensed matter phenomena. In my talk, I will show how strong effective magnetic fields can be realized for neutral atoms held in an especially engineered optical lattice potential. The effective field strengths that can be reached, are 10-100 times larger than what can be achieved even with the strongest magnets in real material systems, allowing one to take the artificial quantum matter into a new parameter regime. Furthermore, I will show how by carrying out matter wave interferometry within the Bloch bands, we have been able to measure the Zak phase - the Berry phase in one dimension - and to directly determine topological invariants. As an example, I will present results for the celebrated Su-Schrieffer-Heeger model of polyacetylene that can be modelled by using optical superlattice potentials.

HL 23: Charge transfer effects in molecular materials II (CPP, jointly with BP, DS, HL)

Related to SYCT organized by Frank Schreiber (Tübingen) and Wolfgang Brütting (Augsburg).

Time: Monday 15:00–17:30 Location: H40

Invited Talk HL 23.1 Mon 15:00 H40
a molecular picture of charge-transfer processes at donor-acceptor interfaces in organic solar cells — •Jean-Luc Bredas — School of Chemistry and Biochemistry/Center for Organic Photonics and Electronics, Georgia Institute of Technology, Atlanta, Georgia 30332-0400

Our objective in this presentation is two-fold. First, after a general introduction to organic solar cells, we use a molecular mechanics / molecular dynamics simulations approach to try and provide a molecular picture of the packing configurations (local morphology) at the interface between the donor and acceptor components in organic solar cells [1-3]. Then, we discuss in detail the impact that these local packing configurations at the interfaces have on the exciton-dissociation and charge-separation processes [4]. Systems under consideration include fullerene derivatives or n-type oligoacene derivatives as acceptors and low optical-gap polymers or small molecules (pentacene or squaraine derivatives) as donors.

References (1) N. Cates Miller, E. Cho, et al., Advanced Materials, in press (DOI: 10.1002/adma.201202293). (2) N. Cates Miller, E. Cho, et al., Advanced Energy Materials, in press (DOI: 10.1002/aenm.201200392). (3) Y.T. Fu, C. Risko, and J.L. Bredas, Advanced Materials, in press (DOI: 10.1002/adma.201203412). (4) J.L. Bredas, J. Norton, J. Cornil, and V. Coropceanu, Accounts of Chemical Research 42, 1691 (2009).

HL 23.2 Mon 15:30 H40
Microscopic simulations of charge transport in disordered organic semiconductors — •Denis Andrienko, Bjoern Baumeier, Pascal Kordt, Anton Melnyk, and Carl Poelking — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Charge carrier dynamics in an organic semiconductor can often be described in terms of charge hopping between localized states. The hopping rates depend on electronic coupling elements, reorganization energies, and driving forces, which vary as a function of position and orientation of the molecules. The exact evaluation of these contributions in a molecular assembly is computationally prohibitive. Various, often semi-empirical, approximations are employed instead. Here, we review the current status of methods used to evaluate energetic disorder in organic semiconductors, such as polarizable force-fields and QM/MM approaches, focusing on their predictive power and accuracy. All methods are illustrated on donor-acceptor small-molecule interfaces as well as crystalline mesophases of conjugated polymers.

HL 23.3 Mon 15:45 H40
Metal-Molecule Charge Transfer through Surface-Induced Conjugation — •Georg Heimel[1], Steffen Duhm[2], Ingo Salzmann[1], Alexander Gerlach[3], Antje Vollmer[4], Frank Schreiber[3], and Norbert Koch[1] — [1]Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Institute of Functional Nano & Soft Materials, Soochow University, Suzhou 215123, P. R. China — [3]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany — [4]Helmholtz Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin, Germany

For the majority of large π-conjugated molecules, the Fermi level of supporting coinage-metal substrates is *pinned* to stay well within their electronic energy gap. In some cases, however, the Fermi level *does* cross into either of the frontier molecular orbitals. On the basis of a combined multi-technique experimental and theoretical study on a particularly clear-cut case – pentacenequinone and pentacenetetrone on the (111) surfaces of Au, Ag, and Cu – we present an attempt for a unifying explanation of such intriguing cases: The conjugation length of the organic semiconductor increases through interaction of specific chemical substituents with the metal surfaces. The ensuing reduction of the energy gap is found to be *the* crucial ingredient needed to overcome Fermi-level pinning. Our findings aid in the design of

charged molecular monolayers, which are of interest both from the fundamental- and the applied-physics point of view.

Invited Talk HL 23.4 Mon 16:00 H40

High efficiency OLEDs based on delayed fluorescence — •Chihaya Adachi — OPERA, Kyushu University, Fukuoka, Japan

We achieved a novel pathway to reach the ultimate EL efficiency by inventing simple aromatic compounds displaying efficient thermally-activated delayed fluorescence (TADF) with high photoluminescence efficiency, namely *hyperfluorescence*. While we had previously assumed that the S1 level should be significantly higher than the T1 level, i.e., 0.5˜1.0 eV higher, due to the presence of electron exchange energy, we found that the proper design of organic molecules can lead to a small energy gap (ΔEST) between them. Relatedly, a molecule displaying efficient TADF requires a very small ΔEST between its S1 and T1 excited states, resulting in enhanced T1 * S1 reverse intersystem crossing (ISC). Such excited states are attainable by the intramolecular charge transfer (CT) of a spatially separated donor and acceptor system. The critical point of the molecular design is the compatibility of a small ΔEST ˜ 0 eV and a reasonable radiative decay rate of over 106/s that overcomes competitive non-radiative decay paths, leading to highly luminescent TADF materials. Since the two properties conflict with each other, a delicate balance of the overlap of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) is required. Furthermore, to enhance the PL efficiency of a TADF material, geometrical change between its S0 and S1 states should be restrained to suppress non-radiative decay processes. In this work, we designed a novel series of highly efficient TADF emitters that resulted in very high electroluminescence efficiency.

HL 23.5 Mon 16:30 H40

Triplet Exciton Generation and Electron Back Transfer in Organic Solar Cells — •Andreas Sperlich[1], Hannes Kraus[1], Stefan Väth[1], Alexander Förtig[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

To increase the power conversion efficiency of organic solar cells it would be extremely advantageous to improve the harvesting of singlet and charge transfer (CT) excitons. Dissociation of CT complexes into free charge carriers or, alternatively, their decay by electron back transfer (EBT) reactions depend on the energy levels of constituting donor and acceptor molecules, on microscopic structure of blends but also on the relative spin orientation of charges carriers within the e-h pair. We report on state-of-the-art organic semiconductors for polymer-fullerene bulk hetero-junction solar cells, such as blends based on the benzodithiophene donor PTB7 or the endohedral fullerene-derivative $Lu_3N@C_{80}$-PCBEH. We applied optical, current-voltage, morphology, and spin-sensitive techniques and found correlations between electrical performance of solar cells and formation of CT and triplet states. Combining results of these complementary experiments, we offer a physical picture on how pushing up the LUMO level of acceptors or tailoring the blends' morphology may end up in unwanted loss mechanisms in bulk-heterojunction solar cells.

HL 23.6 Mon 16:45 H40

Reduced recombination and field independent charge carrier generation in polymer-polymer solar cells — •Steffen Roland[1], Marcel Schubert[1], Zhihua Chen[2], Antonio Facchetti[2], and Dieter Neher[1] — [1]University of Potsdam, Institute of Physics and Astronomy — [2]Polyera Corporation

Charge transport and recombination are investigated for solar cells made of poly(3-hexylthiphene) (P3HT) and the non-fullerene, high mobility acceptor copolymer P(NDI2OD-T2). Optimized devices show high fill factors of up to 70%, indicating that the excellent electron transport properties of pure P(NDI2OD-T2) is prevailed in the blend. By applying of the time delayed collection field technique (TDCF) we measured the field dependence of the charge carrier generation, and of the non geminate recombination as well as the electron and hole mobilities. The results reveal a field-independent photocurrent generation and a strongly reduced recombination coefficient for free charge carriers. The results imply that major charge carrier losses originate from an ultrafast (geminate) recombination on time scales below 10 ns.

Invited Talk HL 23.7 Mon 17:00 H40

The role of intermolecular hybridization in molecular electrical doping — •Ingo Salzmann[1], Georg Heimel[1], Henry Méndez[1], Andreas Opitz[1], Patrick Barkowski[1], Martin Oehzelt[2,1], Katrein Sauer[1], and Norbert Koch[1,2] — [1]Humboldt Universität zu Berlin — [2]Helmholtz Zentrum Berlin, Germany

Molecular electrical doping of functional organic semiconductor (OSC) films is typically done by the admixture of strong molecular donors/acceptors as dopants. In a recent combined experimental and theoretical study on prototypical OSC/dopant pairs we showed that positive polarons, evidencing the common perception of direct electron transfer between the highest occupied molecular orbital (HOMO) of the OSC and the lowest unoccupied molecular orbital (LUMO) of the p-dopant, are not observed in ultraviolet photoelectron spectroscopy even at considerable dopant ratios [1]. Instead of mutual ionization leading to singly occupied states, frontier molecular orbital hybridization between the OSC-HOMO and the dopant-LUMO occurs forming a *doubly occupied* bonding and an *empty* anti-bonding supramolecular hybrid orbital with a reduced fundamental gap, which is tunable by the acceptor strength. As all available states are occupied following Fermi-Dirac statistics, only a fraction of the hybrids is ionized at room temperature rationalizing the high dopant concentrations in practical applications. From this model, controlling the degree of hybridization emerges as strategy for the design of future improved molecular dopants in organic electronic devices.

[1] I. Salzmann, G. Heimel et al., *Phys. Rev. Lett.* 108, 035502, 2012.

HL 24: Graphene: Electronic properties and transport (O, jointly with HL, TT)

Time: Monday 16:00–19:00 Location: H17

HL 24.1 Mon 16:00 H17

Epitaxial silicene - tunable hybridization with the substrate and weak interactions with epitaxial organic overlayers — •Rainer Friedlein[1], Antoine Fleurence[1], Fabio Bussolotti[1,2], and Yukiko Yamada-Takamura[1] — [1]School of Materials Science, Japan Advanced Institute of Science and Technology (JAIST), Nomi, Ishikawa 923-1292, Japan — [2]present address: Graduate School of Advanced Integration Science, Chiba University, Chiba, Japan

The electronic and structural properties of epitaxial silicene formed on ZrB_2(0001) thin films grown on Si(111) wafers upon adsorption of either potassium atoms and anthracene molecules have been studied using photoelectron spectroscopy and electron diffraction. For pristine silicene, a particular, atomic-scale buckling leads to the opening of a direct band gap at the Γ point, while ZrB_2-related surface states are not affected. This is consistent with only a minor degree of hybridization beween Si- and Zr-derived states. The electronic interactions at the interface can be tuned by electron donation from adsorbed potassium atoms, upon which hybridization is progressively switched on.
At 140 K, anthracene molecules are found to grow as epitaxial multilayers that exhibit a point-on-line commensurate relationship with silicene. The results indicate that the charge-density modulation associated with the buckling of silicene render the interactions with organic adsorbates as compared to graphene, which allows for specific epitaxial conditions. On the other hand, the results also confirm that silicene is strikingly different from other Si surfaces for which the presence of dangling bonds leads to chemisorption of organic adsorbates.

HL 24.2 Mon 16:15 H17

***Ab initio* study of graphene nano domes on Ir(111) surface** — •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

Recently, in a combined experimental and theoretical work we have unveiled the bonding mechanism of graphene on Ir(111) surface as physisorption with a local chemical modulation [1]. In this contribution we extend our previous density functional theory (DFT) study to analyse the bonding of graphene nano domes on a clean and an oxygen pre-covered Ir(111) substrate.

As previously shown [1], the inclusion of the long-range van der

Waals interactions is mandatory and in our *ab initio* study these dispersion interactions were considered at a semi-empirical [2] or first-principle [3] level, the latter as implemented in our real-space JuNoLo code [4]. In particular, the non-local correlation vdW-DF functional [3] provides an unique visual insight on the origin of a different graphene bonding on Ir(111) due to a non-local and a semi-local description of the correlation effects in DFT.

[1] C. Busse *et al.*, Phys. Rev. Lett. **107**, 036101 (2011).
[2] S. Grimme, J. Comput. Chem. **27**, 1787 (2006).
[3] M. Dion *et al.*, Phys. Rev. Lett. **92**, 246401 (2004).
[4] P. Lazić *et al.*, Comp. Phys. Commun. **181**, 371 (2010).

HL 24.3 Mon 16:30 H17

Effects of strain on the excitonic Fano resonance in the optical spectrum of graphene — •Daniela Ullrich[1,2], Patrick Herlinger[1], Harald Giessen[2], Jurgen Smet[1], and Markus Lippitz[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart — [2]4th Physics Institute, University of Stuttgart

Using transmission and reflection spectroscopy we examine the optical response of graphene from the visible to the UV regime. The absorbance spectrum of free-standing graphene is dominated by an asymmetric peak in the UV at about 4.7 eV. We show that this resonance can be described by a simple Fano model which includes an excitonic state beneath the saddle point of graphene's band structure [1]. When strain is applied to a graphene sheet, the symmetry of the lattice and thus also of the band structure is broken. As predicted recently [2], this should result in a splitting of the absorbance peak in the optical spectrum as well as a strong dependence on polarization and lattice orientation. Here, we present our findings on the effects of strain on the Raman and reflectivity spectra of graphene on flexible substrates.

[1] Chae et al., Nano Lett. 11, 1379 (2011)
[2] Liang et al., J. Mater. Res. 27, 403 (2012)

HL 24.4 Mon 16:45 H17

Probing Hot Electron Distributions in Graphene on Ni(111) with High Harmonic Radiation — •Carsten Winter[1], Thorben Haarlammert[1], Luca Bignardi[2], Petra Rudolf[2], and Helmut Zacharias[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität, Münster — [2]Zernike Institute for Advanced Materials, University of Groningen

Theoretical calculations and experimental observations of hot electron distributions in graphene show an initial ultrafast carrier relaxation accompanied by a population of optical phonons, which decay on a picosecond time scale. In this talk we present an experimental set-up suited to measure the lifetime of excited electrons and their relaxation dynamics via time-resolved 2PPE. Through frequency conversion by High Harmonic Generation coherent radiation at 39 eV photon energy is generated and subsequently used as the probe pulse in two-photon photoemssion.

A graphene sheet was produced by decomposition of ethylene on a Ni(111) substrate. Hot electron distributions were generated in graphene on Ni(111) by applying 800nm pulses. The energy dependent lifetimes of these distributions have been measured. The lifetimes have been determined to 20-50 fs in the lower energy parts of the distribution (E-E_F < 1eV) and show a strong Ni-like behavior. In the upper energy parts lifetimes of 10-20 fs have been measured and a graphite-like behavior dominates.

HL 24.5 Mon 17:00 H17

Reversible Photooxidation of Graphene — •Stefan Böttcher, Hendrik Vita, and Karsten Horn — Fritz-Haber Institute of the Max-Planck Society, Berlin, Germany

Graphene oxide is often discussed in the context of a technical usage of graphene in future electronic devices. The necessity to obtain a tunable band gap in possible electronic applications makes graphene oxide a promising covalent modification of graphene. However, the homogeneous preparation of graphene oxide has so far been a challenging task, using mainly an aggressive chemical or complex physical treatment of graphene. Here we present a method to selectively produce graphene oxide from epitaxially grown graphene on transition metal surfaces such as Ir(111). Using NO_2 as an adsorbate we transform graphene into graphene oxide by irradiation with UV light at low temperatures, leading to specific signatures in the core and valence level photoemission and -absorption spectra. The graphene oxide thus prepared is stable up to room temperature, but its formation is thermally completely reversible to graphene at higher temperatures.

HL 24.6 Mon 17:15 H17

Edge charge disorder in graphene — •Cornelie Koop, Manuel Schmidt, and Carsten Honerkamp — Institut für Theoretische Festkörperphysik, RWTH Aachen University, Deutschland

We study the interplay of edge roughness and electron-electron interaction in graphene nanoribbons. Our focus is the charge response of a rough edge to (possibly random) potentials induced by adatoms. While the bulk density response in graphene is rather small due to the vanishing density of states at the charge neutrality point, it turns out that edges show a strongly increased response - a fact that may be traced back to the presence of localized states at rough edges. The existence of these localized states depends on the structural properties of the edge. They are the disordered analogs to the well known edge states in clean zigzag ribbons and lead to a random sequence of peaks in the local density of states along the rough edge. As a consequence there may be strongly localized charges randomly distributed along the edge. We discuss the conditions for this effect, which we call edge charge disorder, its strength, and its consequences on the bulk electrons in a graphene nanoribbon.

HL 24.7 Mon 17:30 H17

Electronic and magnetic properties of zigzag graphene nanoribbons on the (111) surface of Cu, Ag and Au — •Yan Li[1], Wei Zhang[1], Markus Morgenstern[2], and Riccardo Mazzarello[1] — [1]Institute for Theoretical Solid State Physics and JARA, RWTH Aachen University, D-52074 Aachen, Germany — [2]II. Physikalisches Institut B and JARA-FIT, RWTH Aachen University, D-52074 Aachen, Germany

We have carried out an *ab initio* study of the structural, electronic and magnetic properties of zigzag graphene nanoribbons (GNRs) on Cu(111), Ag(111) and Au(111). Both H-free and H-terminated GNRs are considered revealing that the nanoribbons invariably possess edge states when deposited on these surfaces. In spite of this, they do not exhibit magnetism at the edge, with the exception of H-terminated GNRs on Au(111), whose zero-temperature magnetic properties are comparable to those of free-standing GNRs. The absence of edge magnetism is due to the hybridization between the 2*pz* orbitals of the carbon atoms and the *d* states of the metal and, for some models, to the charge transfer between the GNR and the surface, which shifts the edge state away from the Fermi level. Only in the case of H-terminated GNRs on Au(111) is the interaction between the substrate and the GNR sufficiently weak so as not to affect the magnetic properties of the edge state significantly.

HL 24.8 Mon 17:45 H17

The atomic and electronic structure of well-defined graphene nanoribbons studied by scanning probe microscopy — •Joost van der Lit[1], Mark Boneschanscher[1], Mari Iljas[2], Ari Harju[2], Andreas Uppstu[2], Daniel Vanmaekelbergh[1], Peter Liljeroth[2], and Ingmar Swart[1] — [1]Debye Institute for Nanomaterials Science, Utrecht University, The Netherlands — [2]Department of Applied Physics, Aalto University, Finland

Recently, graphene nanostructures have gained a lot of interest since they introduce a bandgap in graphene, which is important for (opto-) electronics applications. Graphene nanoribbons can have a bandgap as large as 3 eV[1,2], which can be tuned by varying its width. By using a chemical bottom-up approach, we have synthesized graphene nanoribbons (GNR) on an Au(111) substrate[3]. By combining scanning tunneling microscopy (STM) and atomic force microscopy (AFM) with reactive and non-reactive tips, we can relate the electronic properties of the GNRs with their atomic structure. Furthermore, we can use the STM tip to (i) deliberately create well-defined atomic scale defects and (ii) control the interaction with the substrate. Hence, we are able to directly study the robustness of the properties of the graphene nanostructures. [1] P. Ruffieux, et al. , ACS Nano 6 (2012) 6930. [2]M. Koch, F. Ample, C. Joachim, L. Grill, Nat. Nanotechnol. 7 (2012)713. [3] J. Cai et al., Nature, 446 (2010) 470-473.

HL 24.9 Mon 18:00 H17

Intact Dirac cones at broken sublattice symmetry: photoemission study of graphene on Ni and Co — •Dmitry Marchenko[1], Andrei Varykhalov[1], Jaime Sánchez-Barriga[1], Markus R. Scholz[1], Bart Verberck[2], Björn Trauzettel[3], Tim O. Wehling[4,5], Carlo Carbone[6], and Oliver Rader[1] — [1]Helmholtz-Zentrum Berlin — [2]Universiteit Antwerpen — [3]Universität Würzburg — [4]Universität Bremen — [5]Bremen Center for Computational Materials Science — [6]Consiglio Nazionale delle

Ricerche Trieste

A band gap at the Dirac point of graphene can be created by breaking of the sublattice symmetry through epitaxial growth on a substrate crystal. One of the strongest sublattice-symmetry-breaking interactions with predicted and measured band gaps ranging from 400 meV to more than 3 eV has been attributed to the interfaces of graphene with Ni and Co, which are also promising spin filter interfaces. We apply angle-resolved photoemission to epitaxial graphene on Ni(111) and Co(0001) to show the presence of intact Dirac cones in a strongly n-doped system. Our results challenge the common belief that breaking of sublattice symmetry by a substrate and opening of the band gap at the Dirac energy are in a straightforward relation. A simple effective model of a biased bilayer structure composed of graphene and a sublattice symmetry broken layer, corroborated by density functional theory calculations, demonstrates the general validity of our conclusions.

HL 24.10 Mon 18:15 H17

sp^2 carbon hybrid junctions — Pablo Robert[1,2], Renjun Du[1], Fan Wu[1], Kristina Hönes[1], Jens Mohrmann[1], Frank Hennrich[1], Manfred Kappes[1,3,4], Hilbert von Löhneysen[1,2,4,5], and •Romain Danneau[1,2] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, — [2]Institute of Physics, Karlsruhe Institute of Technology, Germany — [3]Institute of Physical Chemistry, Karlsruhe Institute of Technology, Germany — [4]DFG Center for Functional Nanostructures, Karlsruhe Institute of Technology, Germany — [5]Institute for Solid-State Physics, Karlsruhe Institute of Technology, Germany

Lowering the contact resistance is a key issue to improve graphene field effect device performance. The connection between a metal and graphene depends on many parameters such as the work function mismatch between the two connected material, the adsorption of the metal on graphene, the quality of the deposited material as well as the strain induced on the graphene sheet. We have studied electronic transport through carbon nanotube (CNT)-graphene and graphene-graphene junctions produced by nano-manipulation and transfer. For the CNT-graphene junctions, we first demonstrate that the influence of the CNT on the charge distribution of the graphene sheet is limited to few nanometers. Our experiments show that the junction transparency is strongly gate dependent due to the variation of the CNT-graphene distance, and the charge carrier injection occurs via a single point. For the graphene-graphene junctions, our measurements show low resistance and prove that graphene makes a good connection to graphene.

HL 24.11 Mon 18:30 H17

Graphene on boron nitride microwave transistors driven by graphene nanoribbon back-gates — Christian Benz[1,2], •Maximilian Thürmer[1], Fan Wu[1], Zeineb Ben Aziza[1], Jens Mohrmann[1], Hilbert von Löhneysen[1,2,3,4], Kenji Watanabe[5], Takashi Taniguchi[5], and Romain Danneau[1,2] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany — [2]Institute of Physics, Karlsruhe Institute of Technology, Germany — [3]DFG Center for Functional Nanostructures, Karlsruhe Institute of Technology, Germany — [4]Institute for Solid-State Physics, Karlsruhe Institute of Technology, Germany — [5]Advanced Materials Laboratory, National Institute for Materials Science, Tsukuba, Japan

We have designed ultra-thin graphene microwave transistors by using pre-patterned metal or graphene nanoribbon back-gates and hexagonal boron nitride (h-BN) as a dielectric substrate. Despite the inhomogeneities induced by the graphene transfer process, we show that it is possible to operate these types of devices across a broad range of microwave frequencies. For the graphene nanoribbon gates, we observe a deviation of the current gain from the usual 1/f trend that can be attributed to the large gate resistance of these systems as we demonstrate with our small-signal model. The scattering parameter analysis shows a very limited back-action from the channel onto the graphene nanoribbon gates. Our work thus proves that graphene microwave transistors could be driven by graphene nanoribbon gates.

HL 24.12 Mon 18:45 H17

Strong gate hysteresis in graphene on mica field effect devices — •Jens Mohrmann[1], Kenji Watanabe[2], Takashi Taniguchi[2], and Romain Danneau[1,3] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany — [2]Advanced Materials Laboratory, National Institute for Materials Science, Tsukuba, Japan — [3]Institute of Physics, Karlsruhe Institute of Technology, Germany

One of the outstanding properties of graphene is the unbeatable ratio of surface to volume. As a membrane of only one atomic layer of carbon, graphene is extremely sensitive to external influences. The large area contact with the substrate thus causes a large influence of the used substrate on the electronic properties of graphene. Therefore, a lot of effort is being made in order to understand the interaction between graphene and its substrate, and to find new and possibly better materials. One material under investigation is muscovite mica. The layered structure allows perfect basal (001) cleavage with atomically flat terraces, and using mechanical exfoliation, very thin crystals can be created and used as a substrate and gate dielectric. Transport measurements of graphene on mica show a very high hysteresis with respect to the gate voltage. Here, we investigate this effect using dual gated devices, with both mica and hexagonal boron-nitride dielectrics.

HL 25: Focus Session: Frontiers of electronic structure theory II (O, jointly with HL, TT)

Time: Monday 16:00–19:15 Location: H36

HL 25.1 Mon 16:00 H36

Excited States of the divacancy in SiC — •Michel Bockstedte[1], Thomas Garratt[1], and Adam Gali[2] — [1]Theoretische Festkörperphysik, FAU Erlangen-Nürnberg, Staudstr. 7B2, D-91058 Erlangen — [2]Wigner Research Centre for Physics, Hungarian Academy of Sciences, PO Box 49, Budapest 1525, Hungary

The negatively charged nitrogen-vacancy center in diamond has emerged as a candidate for the implementation of a qbit in quantum computing. Silicon Carbide also fullfils necessary conditions[1] which makes it a suitable material for this purpose. With the neutral divacancy it possess a defect center with a high spin ground state, which can be manipulated by spin-resonance techniques.[2] Optical excitation of the triplet ground state and subsequent spin-selective recombination via yet unknown intermediate spin-singlet states enables spin-initialization with M_z=0, which is requisit for a qbit. Here we investigate the excitation spectrum of the divacancy based *ab initio* methods. DFT and TD-DFT calculations[3] reveal a Jahn-Teller effect for the first excited triplet state that is absent for the NV-complex. TD-DFT and an *ab initio* many body hamiltonian nicely reproduce the prominent photoluminescence transitions. The latter method also describes the spin-singlet states. We discuss the defect excitation spectrum in the light of the Jahn-Teller distortion.

[1] J. R. Weber *et al.*, PNAS **107**, 8513 (2010).
[2] F. Koehl *et al.*, Nature **479**, 84 (2011).
[3] A. Gali, phys. status solidi (b) **248**, 1337 (2011).

HL 25.2 Mon 16:15 H36

Extending the random phase approximation for electronic correlation energies: The renormalized adiabatic local density approximation — •Thomas Olsen — Technical University of Denmark

The adiabatic connection fluctuation-dissipation theorem with the random phase approximation (RPA) has recently been applied with success to obtain correlation energies of a variety of chemical and solid state systems. The main merit of this approach is the improved description of dispersive forces while chemical bond strengths and absolute correlation energies are systematically underestimated. In this work we extend the RPA by including a parameter-free renormalized version of the adiabatic local density (ALDA) exchange-correlation kernel. The renormalization consists of a (local) truncation of the ALDA kernel for wave vectors $q > 2k_F$, which is found to yield excellent results for the homogeneous electron gas. In addition, the kernel significantly improves both the absolute correlation energies and atomization energies of small molecules over RPA and ALDA. The renormalization can be straightforwardly applied to other adiabatic local kernels.

HL 25.3 Mon 16:30 H36

First-principles IXS spectra for TiO_2 and HfO_2 — •Linda

Hung and Francesco Sottile — Ecole Polytechnique, Palaiseau, France

Using time-dependent DFT and many-body perturbation theory, we determine the inelastic x-ray scattering (IXS) spectra for bulk TiO_2 and HfO_2. Excitations from valence and semi-core states are modeled, corresponding to transition energies up to 60 eV. By varying momentum transfer, plasmon dispersion can be observed. We characterize differences in the spectra for the rutile, anatase, and brookite polymorphs of TiO_2, as well as the cubic, tetragonal, and orthogonal polymorphs of HfO_2. These spectra are also Fourier transformed, allowing us to image the real-time and real-space electron density response to external perturbations.

HL 25.4 Mon 16:45 H36

Linear-scaling time dependent density-functional theory in the linear response formalism — •Tim J. Zuehlsdorff, Nicholas D. M. Hine, James S. Spencer, Nicholas M. Harrison, and Peter D. Haynes — Imperial College London, UK

In recent years, linear-scaling approaches to density-functional theory have enabled the computation of ground-state properties of large nanostructures and biomolecules. While these methods are now well established, the linear-scaling computation of excited state properties via time-dependent density-functional theory (TDDFT) in the linear response regime is less developed.

In this talk we will present an implementation of TDDFT in the linear response formalism, enabling the computation of low-energy optical absorbtion spectra for large molecules and nanostructures. The method avoids any explicit reference to canonical representations of either occupied and unoccupied Kohn-Sham states and thus achieves linear-scaling computational effort with system size. In contrast to conventional localised orbital formulations where a single basis set is used to represent the occupied and unoccupied Kohn-Sham states, we make use of two sets of in-situ optimised localised orbitals, one for the occupied and one for the unoccupied Kohn-Sham space. The double basis set approach avoids known problems of representing the unoccupied space with localised orbitals optimised for the occupied space, while the in-situ optimisation procedure allows for efficient calculations with a minimal set of basis functions. The method is applied to a number of large-scale test systems in order to demonstrate its validity.

HL 25.5 Mon 17:00 H36

Dynamical spin and charge excitations with spin–orbit coupling in 3d adatoms on Cu(111) and Pt(111) — •Manuel dos Santos Dias, Benedikt Schweflinghaus, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

The presence of spin–orbit coupling has a fundamental impact on the magnetic excitation spectrum: there is a finite gap at zero frequency and spin and charge excitations become coupled. The excitation spectrum is derived from the dynamical magnetic susceptibility of the electronic system, for which we developed a formalism based on Time–Dependent Density Functional Theory, as implemented in the Korringa–Kohn–Rostoker Green function method [1,2]. As an application, we present first–principles calculations of the charge, longitudinal and transverse magnetic excitations of 3d adatoms deposited on the Cu(111) and Pt(111) surfaces. Focus is on the expected spin–charge coupling induced by the the spin–orbit interaction, and on the dynamical anisotropic effects that generalize the familiar magnetic anisotropy.

Work supported by the HGF-YIG Programme FunSiLab – Functional Nanoscale Structure Probe and Simulation Laboratory (VH-NG-717).

[1] S. Lounis, A. T. Costa, R. B. Muniz and D. L. Mills, Phys. Rev. Lett. **105**, 187205 (2010)
[2] S. Lounis, A. T. Costa, R. B. Muniz and D. L. Mills, Phys. Rev. B **83**, 035109 (2011)

HL 25.6 Mon 17:15 H36

Beyond the *GW* approximation: a second-order screened exchange correction — •Patrick Rinke[1], Xinguo Ren[1], Noa Marom[2], Fabio Caruso[1], and Matthias Scheffler[1] — [1]Fritz Haber Institute, Berlin, Germany — [2]University of Texas, Austin, USA

Despite the success of the *GW* method in describing the photoemission spectra of solids, molecules and clusters, challenges remain. For aromatic molecules for example absolute as well as relative positions of ionisation energies and affinities are not well reproduced in perturbative G_0W_0 schemes with different starting points as well as in self-consistent *GW* [1], sometimes even giving the wrong orbital order. Motivated by renormalized second-order perturbation theory [2] for the ground-state energy, we propose a second-order screened exchange correction (SOSEX) to the *GW* self-energy. This correction follows the spirit of the SOSEX correction to the random-phase approximation for the electron correlation energy and reduces the self-correlation error. The performance of the *GW*+SOSEX scheme has been benchmarked for a set of molecular systems, including the G2 set, commonly used acceptor molecules, benzene and the azabenzene molecules. We find that the SOSEX correction improves the description of the spectral properties including the orbital order with respect to the different *GW* schemes, highlighting the importance of reducing the self-correlation error. [1] N. Marom *et al.*, arXiv:1211.0416 [2] X. Ren *et al.*, J. Mater. Sci. **47**, 7447 (2012)

HL 25.7 Mon 17:30 H36

A strategy for finding a reliable starting point for G_0W_0 demonstrated for molecules — •Thomas Körzdörfer[1] and Noa Marom[2] — [1]Institut für Chemie, Universität Potsdam, D-14476 Potsdam — [2]Center for Computational Materials, Institute of Computational Engineering and Sciences, The University of Texas at Austin, Austin, TX 78712, USA

Many-body perturbation theory in the G_0W_0 approximation is an increasingly popular tool for calculating electron removal energies and fundamental gaps for molecules and solids. However, the predictive power of G_0W_0 for molecules is limited by its sensitivity to the density functional theory (DFT) starting point. In this contribution, the starting point dependence of G_0W_0 is demonstrated for several organic molecules. Analysis of the starting point dependence leads to the development of a non-empirical scheme that allows to find a consistent and reliable DFT starting point for G_0W_0 calculations by adapting the amount of Hartree-Fock-exchange in a hybrid DFT functional. The G_0W_0 spectra resulting from this *consistent starting point (CSP) scheme* [1] reliably predict experimental photoelectron spectra over the full energy range. This is demonstrated for a test set of various typical organic semiconductor molecules.

[1] T. Körzdörfer and Noa Marom, Phys. Rev. B Rapid Communications **86**, 041110 (2012).

HL 25.8 Mon 17:45 H36

Electronic properties of isolated and supported organic dyes modeled through the GW method — •Paolo Umari[1], Filippo De Angelis[2], Luigi Giacomazzi[3], Mariachiara Pastore[2], and Stefano Baroni[3] — [1]Dipartimento di Fisica e Astronomia, Università di Padova, Italy — [2]Istituto CNR di Scienze e Tecnologie Molecolari, Perugia, Italy — [3]Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy

The first-principles GW method is used for investigating the electronic levels of isolated and supported dyes for electrochemical solar cells. We consider a set of all-organic dyes, (L0,L2,L3,L4) exhibiting the same donor and anchor groups. First, we calculate the energy levels in the limit of isolated molecules obtaining nice agreement with available experimental photoelectron spectra. Then, we consider the L0 and the L2 dyes while adsorbed on the anatase TiO_2 (101) surface. Also in this case we find good agreement when comparing with available experimental photoelectron spectra. We find that the HOMO -LUMO gap of the dye is reduced with respect to the isolated molecule and that the HOMO level is slightly shifted towards higher energies due to image charge effects. This permits us to derive a simple model for obtaining approximate GW energy levels for the HOMO and the LUMO of the adsorbed molecule and for the valence band maximum and the conduction band minimum of the substrate performing just one complete GW calculation of the isolated molecule and one of the bulk TiO_2 combined with a calculation at the DFT level of the adsorbed molecule complex. In this way, we can investigate larger, more realistic, model structures.

HL 25.9 Mon 18:00 H36

Ab-initio description of satellites in semiconductors — •Matteo Guzzo[1,2], Josh J. Kas[3], Lorenzo Sponza[1,2], Christine Giorgetti[1,2], Francesco Sottile[1,2], Debora Pierucci[4], Mathieu G. Silly[4], Fausto Sirotti[4], John J. Rehr[3], and Lucia Reining[1,2] — [1]LSI, Ecole Polytechnique, Palaiseau, France — [2]European Theoretical Spectroscopy Facility (ETSF) — [3]UW, Seat-

tle, USA — [4]Synchrotron Soleil, Gif-sur-Yvette, France

The GW method from Many-Body Perturbation Theory has been very successful in describing photoemission spectra in a variety of systems. In particular, GW is known to give good quasiparticle properties like band gaps, but it has shown some limitations in the description of complex correlation effects like satellites. Satellite peaks in photoemission come from higher-order excitations and are still poorly studied in the valence bands. In perturbative GW the spectral function can describe additional features beside the quasiparticle peaks, but these satellites are known to be too weak and too low in energy, as it appears from calculations on the Homogeneous Electron Gas and some real materials. Including additional diagrams in the Green's function we obtain an excellent description of satellites series in the test case of bulk silicon, where GW is unable to cope [1]. This approach can be extended to more complex system, i.e. graphite. Using our newly measured XPS valence data, we investigate the effects of anisotropies on satellites and give a prediction on the spectral changes following the transition towards true freestanding graphene. [1] M. Guzzo et al., Phys. Rev. Lett. 107, 166401 (2011)

HL 25.10 Mon 18:15 H36

Optical spectra of alkali-metal fluorides — •Christoph Sommer, Peter Krüger, and Johannes Pollmann — Institut für Festkörpertheorie, Universität Münster, D-48149 Münster, Germany

We have studied the virtue of different approximations for quasiparticle energies in the calculation of optical spectra including excitonic effects by solving the Bethe-Salpeter equation (BSE). To this end, we have computed exemplarily optical spectra of the three alkali-metal fluorides LiF, NaF, and KF using quasiparticle energies resulting from two different approximations of the self-energy operator in Hedin's *GW* approach as well as electronic energies and wave functions obtained by employing self-interaction corrected pseudopotentials. The energetic positions of characteristic peaks in the calculated and measured spectra are in very good agreement when quasiparticle energies are used that result after an update of the screened interaction W on the basis of a preceding G_0W_0 calculation. Additionally, two simple further approximations for one-particle energies that use input either from experiment or from quasiparticle calculations for a small set of wave vectors are included into this investigation.

HL 25.11 Mon 18:30 H36

Bethe-Salpeter Equation from many-body perturbation theory — •Tobias Sander, Ronald Starke, and Georg Kresse — Computational Materials Physics, University of Vienna, Sensengasse 8/12, 1090 Vienna, Austria

The Green function formalism is a powerful tool to calculate not only electronic structure within the quasi-particle (QP) picture, but it also gives access to optical absorption spectra. Starting from QP energies within the GW method, the polarizability, as central quantity, is calculated from the solution of a Bethe-Salpeter-like equation (BSE). It is usually solved within the Tamm-Dancoff Approximation (TDA) which neglects the coupling of resonant (positive frequency branch) and anti-resonant (negative frequency branch) excitations. In this work we solve the full BSE [1] (beyond TDA) based on self-consistently calculated QP orbitals and energies [2] for typical systems. The dielectric function is averaged over many low dimensional shifted **k**-meshes to obtain **k**-point converged results. We compare the results to recently introduced approximation to the BSE kernel [3]. Additionally, the time-evolution ansatz [4] is employed to calculate the polarizability, which avoids the direct solution of the BSE.

[1] S. Albrecht, L. Reining, R. Del Sole, G. Onida, PRL 80, 4510 (1998)
[2] M. Shishkin, M. Marsman, G. Kresse, PRL 99, 246403 (2007)
[3] L. Reining, PRL 88, 66404 (2002)
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HL 25.12 Mon 18:45 H36

Acceleration of the response function convergence using the effective energy techniques within the ultrasoft pseudopotential and PAW methods — •Jiří Klimeš and Georg Kresse — Faculty of Physics, University of Vienna, A-1090 Vienna, Austria

Calculations of quasiparticle spectra based on the GW approximation or evaluation of total energies using the RPA method are of a wide interest in the computational materials community. However, their applicability is to a large extent limited by the cost of evaluating the response function or the selfenergy where a large number of unoccupied bands needs to be included. A promising way to speed-up the convergence is to use the resolution of identity and replace the sum over an infinite number of unoccupied states by an effective correction [1,2]. However, the available schemes have been only formulated for norm-conserving pseudopotentials and when applied directly within the ultrasoft pseudopotentials (USPPs) or the PAW method they introduce an error since the correction term doesn't vanish when the number of included bands is increased. Here we present an implementation of the schemes within the formalism of USPPs or the PAW method which gives the proper behaviour of the correction term. We also show how the convergence of the scheme given in [2] can be further improved and discuss the efficiency of the methods for RPA total energy calculations.

[1] F. Bruneval and X. Gonze, PRB **78**, 085125 (2008)
[2] J. A. Berger, L. Reining, and F. Sottile, PRB **82**, 041103(R) (2010); PRB **85**, 085126 (2012)

HL 25.13 Mon 19:00 H36

SnO: GW band gap of a van der Waals bonded system — •Kirsten Govaerts[1], Rolando Saniz[2], Bart Partoens[2], and Dirk Lamoen[1] — [1]EMAT, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerpen, Belgium — [2]CMT group, Department of Physics, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerpen, Belgium

In this work we have investigated the structural and electronic properties of SnO, which is built up by layers kept together by van der Waals (vdW) forces. The combination of a vdW functional (within DFT) and GW calculations leads to accurate values for the c/a ratio and the fundamental band gap. A comparison is made between three starting points for the GW calculation: a regular PBE calculation, one with the vdW effect included, and a hybrid functional calculation. The difference between different levels of self-consistency is also investigated.

HL 26: Lasers and LEDs II

Time: Monday 16:45–18:30 Location: H16

HL 26.1 Mon 16:45 H16

Beam steering in mid-IR external cavity quantum cascade lasers — •Verena Blattmann, Frank Fuchs, Stefan Hugger, Jan Jarvis, Michel Kinzer, Quankui Yang, Ralf Ostendorf, Wolfgang Bronner, Rachid Driad, Rolf Aidam, and Joachim Wagner — Fraunhofer-Institut für Angewandte Festkörperphysik IAF, Tullastr. 72, D-79108 Freiburg, Germany

Quantum cascade (QC) lasers have been established as Watt-level coherent light sources in the mid-infrared of the electromagnetic spectrum. Applying band structure engineering, the gain spectrum of a QC laser can be designed according to the specific needs of the given application. Control over the emission wavelength over the entire gain spectrum can be obtained by an external cavity (EC) setup, making QC lasers interesting for broad-band spectroscopy. Such sensing applications require a stable far-field intensity distribution in order to realize a high signal-to-noise ratio during the measurement. However, it has been shown that QC lasers are likely to show lateral multi-mode emission. In particular when operated at higher output power, they show far-field beam instabilities and beam steering effects due to coherent coupling of different lateral modes. In order to understand these effects, we investigate the dependence of far-field characteristics of EC-QC lasers on parameters such as laser current, temperature, emission wavelength as well as the precise alignment of the components of the external cavity. In addition, the influence of lateral optical confinement is evaluated by using laser chips differing in ridge width and processing technology (double trench, buried heterostructure).

HL 26.2 Mon 17:00 H16

Power scaling of 2-μm GaSb-based semiconductor disk laser

emitting in TEM_{00} mode — •Steffen Adler, Sebastian Kaspar, Marcel Rattunde, Tino Töpper, Christian Manz, Klaus Köhler, 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. VECSEL in the 2-3-μm wavelength range are of interest for a broad range of applications in materials processing, medicine, trace gas sensing and optical pumping. In this presentation we will report on power scaling of TEM_{00}-emitting GaSb-based VECSELs, which are excellently suited for applications requiring Watt-level output powers emitted from a single-mode fiber.

Investigating different cavity designs in order to scale the output power in TEM_{00} mode we prove the existence of a thermal lens in GaSb-based VECSEL. This finding was unlikely to be expected since the up-to-date scientific consensus has been that the influence of thermal lensing in GaSb-based VECSEL is negligible.

The thermal lens in the VECSEL chip is due to pump-power induced heating inducing a valid refractive index variation. Since thermal lensing hampers TEM_{00} emission at high output power we have investigated different cavity designs minimizing this unwanted effect. Using an optimized setup, we realized a 2.1-μm emitting VECSEL with an output power above 1.5 W at $M^2 < 1.2$ at 20°C heat-sink temperature.

HL 26.3 Mon 17:15 H16

Design, simulation and characterization of RCLEDs — •Paul Börner[1], Michael Kunzer[1], Thorsten Passow[1], Klaus Köhler[1], Wilfried Pletschen[1], Tarik Moudakir[2], Abdallah Ougazzaden[2], Frédéric Genty[3], and Joachim Wagner[1] — [1]Fraunhofer-Institut für Angewandte Festkörperphysik, Tullastrasse 72, D-79108 Freiburg, Germany — [2]UMI 2958, Georgia Tech CNRS, Georgia Inst Technol, 2-3 Rue Marconi, F-57070 Metz, France — [3]Supelec, 2 Rue Edouard Belin, F-57070 Metz, France

Resonant-cavity light emitting diodes (RCLEDs) can be regarded as a hybrid between vertical-cavity surface-emitting lasers (VCSELs) and conventional LEDs. In contrast to VCSELs, the operating principle is based on spontaneous emission. Putting a light source into a cavity enhances the probability of spontaneous emission (Purcell effect). Therefore, emission perpendicular to the surface is increased. On the one hand, RCLEDs are still incoherent light sources with larger line widths and no speckling compared to lasers since the mirror reflectivity and optical gain is too low for stimulated emission. On the other hand the resonant cavity improves emission directionality compared to conventional LEDs. In combination with circular facets fitting to the fibre core diameter, RCLEDs are suited for efficient fibre coupling.

We report on the realization of RCLEDs emitting in the 400 nm range. The vertical cavity consists of a top dielectric SiO_2/ZrO_2 mirror and a bottom AlInN/GaN or AlGaN/GaN distributed Bragg reflector (DBR) enclosing an InGaN/GaN multiple quantum well active layer.

HL 26.4 Mon 17:30 H16

Low Threshold Interband Cascade Lasers — •Robert Weih, Sven Höfling, and Martin Kamp — Technische Physik and Wilhelm-Conrad-Röntgen-Research Center for Complex Material Systems, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Several applications like medical diagnostics, free space communication and high sensitivity tunable laser absorption spectroscopy (TLAS) demand compact and robust laser sources in the mid infrared region. Particularly the window from 3 to 6 μm is of great interest for TLAS, since many organic molecules have strong rotational-vibrational absorption lines in this so called fingerprint region. A very promising source for this spectral region is the interband cascade laser (ICL). This device relies on the special band alignment in the InAs/GaSb/AlSb material system that allows the combination of (spatially indirect) interband transitions with tunnel junctions for carrier conversion, enabling cascaded active regions. Within the last years, the performance of ICLs has improved significantly, and continuous wave operation over a wide wavelength range has been demonstrated even at elevated temperatures. We'll present several design optimizations of the layer sequence and the doping scheme that were made to reduce the photon losses and increase the external efficiency. As a result, the threshold current densities for broad area lasers could be reduced below $200 A/cm^2$. Narrow ridge waveguide laser operate up to 60°C in continuous wave mode and emit more than 20 mW of optical power at 20°C.

HL 26.5 Mon 17:45 H16

Interband Cascade Lasers for Tunable Laser Spectroscopy — •Michael von Edlinger[1], Julian Scheuermann[1], Lars Nähle[1], Robert Weih[2], Adam Bauer[2], Marc Fischer[1], Sven Höfling[2], Johannes Koeth[1], and Martin Kamp[2] — [1]nanoplus GmbH, Oberer Kirschberg 4, 97218 Gerbrunn, Germany — [2]Technische Physik University of Würzburg, Wilhelm-Conrad-Röntgen-Research Center for Complex Material Systems, Am Hubland, 97074 Würzburg, Germany

Tunable laser sources have proven themselves as a very successful tool for high performance gas sensing and are used in a variety of challenging applications. Especially the mid infrared (MIR) region between 3 and 4 microns is technologically and industrially relevant, since many gas species have their strongest absorption features in this range, including e. g. important hydrocarbons like methane or acetylene as well as formaldehyde.

In this contribution, a promising approach to MIR distributed feedback (DFB) laser devices based on interband cascade laser material is presented. Continuous wave laser operation above room temperature has already been demonstrated in the wavelength range from 3 to 6 microns based on this concept. A crucial requirement for tunable laser spectroscopy (TLS) is the availability of spectrally monomode emitters such as DFB lasers. In this work distributed feedback is achieved by etched sidewall gratings defined by electron-beam lithography. With this method devices with SMSR around 30 dB have been fabricated in the 3.5 micron wavelength range, well suited for formaldehyde detection.

HL 26.6 Mon 18:00 H16

InAs-based Interband-Cascade-Lasers for emission around 6 um — •Matthias Dallner, Martin Kamp, and Sven Höfling — Technische Physik and Wilhelm-Conrad-Röntgen-Research Center for Complex Material Systems, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Interband-cascade-lasers (ICLs) based on the GaSb material system are currently able to provide room-temperature continuous wave operation at wavelengths up to 5.6μm. One limitation of the performance at longer wavelengths is the requirement of thick cladding layers, which have a large thermal resistance if realized as superlattices. An alternative solution is the combination of established active region designs with plasmon enhanced waveguides on InAs substrates. The cladding layers of these devices are made out of highly doped InAs whose refractive index is significantly reduced due to the proximity of the emission wavelength to the plasmon resonance. This allows a combination of strong optical confinement and high thermal conductivity.

We'll present data from InAs-based ICLs emitting around 6 um at room temperature that have been grown using molecular beam epitaxy. Various optimization concepts known from GaSb-based ICLs, like shortend injectors, split hole extractors or carrier rebalancing have been applied to our structures, yielding a considerable improvement in device performance. The latest devices show threshold current densities as low as $1.4 kA/cm^2$ at 20°C under pulsed operation and a maximum operation temperature of 40°C.

HL 26.7 Mon 18:15 H16

Evanescently coupled semiconductor laser arrays fabricated in the InGaAs/GaAs material system — •Alexander Reinhold[1], Christian Zimmermann[1], Julian Scheuermann[1], Michael von Edlinger[1], Andreas Heger[1], Wolfgang Zeller[1], Johannes Koeth[1], and Martin Kamp[2] — [1]nanoplus GmbH, Oberer Krischberg 4, D-97218, Gerbrunn, Germany — [2]Technische Physik, Universität Würzburg, Am Hubland,D-97074, Würzburg, Germany

Semiconductor laser diodes are nowadays well established as highly efficient, compact and low cost coherent light sources in various fields of applications. However, the combination of high output power with a good beam quality and narrow spectral linewidth is still challenging. A possible device geometry that can meet these demands is an array of ridge waveguides with lateral gratings in between the ridges. The ridge array leads to a large mode size for the still strongly index guided mode, whereas the grating provides wavelength selection. We have fabricated such devices based on an AlGaAs/GaAs laser structures with a double InGaAs quantum well as active material, emitting in the wavelength range around 890 nm. We achieved spectrally narrow operation around a wavelength of 887 nm with side mode suppression ratios (SMSR) of 33 dB and optical output powers up to 100 mW. The devices operate on a higher order lateral supermode with a multi-lobed farfield. We have also investigated phase matching segments and ver-

tically etched sidewall gratings in order to achieve discrimination of high order lateral supermodes and diffraction limited emission.

HL 27: Joint Poster Session: Functionalized semiconductor nanowires (DS, jointly with HL); Resistive switching (DS, jointly with DF, KR, HL)

Time: Monday 17:00–20:00 Location: Poster B1

HL 27.1 Mon 17:00 Poster B1

Optical properties of Sn-doped CdS nanowires — •Marcel Wille[1], Sebastian Geburt[1], Robert Röder[1], Mengyao Zhang[2], Jia Grace Lu[2], and Carsten Ronning[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena — [2]Department of Physics and Electrical Engineering, University of Southern California, Los Angeles, USA

Nanowires (NWs) are promising candidates for future optoelectronic applications due to their possibility of light generation, waveguide properties and light amplification in a Fabry-Perot resonator. The controlled modification of their electrical and optical properties, for example by doping, will continue the consequent progress in NW research. The in-situ doping during the VLS synthesis is a difficult task due to the restricted solubility of dopants in gold (Au), which is typically used as catalyst. Therefore, we investigate an alternative catalyst (Sn) in order to succeed in successful doping during growth. SEM an TEM were performed to analyse the morphology of CdS NWs synthesized under usage of Sn as catalyst. The stoichiometry and successful doping with Sn was proven by EDX point measurements and mappings. In micro-PL, macro-PL and CL measurements at low and room temperatures the NBE, DLE and DAP (donor-acceptor pair) transitions were investigated to state about the optical properties. The occurring DAP transition, which was proven by power- and temperature dependent PL measurements, indicates the successful incorporation of Sn into the CdS NWs.

HL 27.2 Mon 17:00 Poster B1

Tailoring CdS nanowire lasing resonators — •Robert Röder[1], Sebastian Geburt[1], Andreas Johannes[1], Markus Glaser[2], Alois Lugstein[2], and Carsten Ronning[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, D-07743 Jena — [2]Institut für Festkörperelektronik, TU Wien, Floragasse 7, A-1040 Wien

The nanophotonics research for the development of on-chip optical components has to be intensified due to the forthcoming limits of conventional electronic integrated circuits. Semiconductor nanowires mark the physical size limit of a multimode photonic laser system. Thus, they are promising for circumventing these limits via optical data transmission and processing. The green spectral range around 2.4 eV is made accessible by high quality VLS synthesized cadmium sulfide nanowires (CdS NW) 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)]. The resulting task for the processing of CdS nanolasers with reproducible properties remains in defining the resonator: The mode spacing can be adjusted by reducing the cavity length. The reflectivity of the guided modes can be enhanced as well by polishing the facet ends. Thus, preparation techniques for tailoring the resonator are demonstrated using focused ion beams (FIB) and a focused laser beam.

HL 27.3 Mon 17:00 Poster B1

Luminescence decay dynamics of colloidal CdSe quantum dots in different environments — •Michael Diez[1], Stephanie Bley[1], Dongchao Hou[1], Sebastian Resch[2], Siegfried Waldvogel[2], Jürgen Gutowski[1], and Tobias Voss[1] — [1]Institute of Solid State Physics, Semiconductor Optics, University of Bremen, 28359 Bremen, Germany — [2]Institute of Organic Chemistry, Johannes Gutenberg University Mainz, 55128 Mainz, Germany

The functionalization of semiconductor surfaces with colloidal quantum dots has gained substantial interest because of its wide application in optical sensing and energy harvesting. The quantum dots can be selectively attached to semiconductor surfaces with the help of linker molecules. We have studied the luminescence decay dynamics of colloidal CdSe quantum dots functionalized with ω-mercapto alkanoic acid in different environments. As optical excitation source we use a frequency-doubled Ti:sapphire laser ($\lambda = 350\,nm$, $\Delta t = 60\,fs$, $f = 82\,MHz$ and $E_{pulse} = 12\,nJ$). We detect the luminescence signal with a streak camera and an attached spectrometer ($\Delta t < 2\,ps$, $\Delta\lambda < 0.2\,nm$). For colloidal CdSe quantum dots in aqueous solution, we find that the luminsescence decay time can be well fitted with a bi-exponential decay (shorter decay time $t_1 \approx 200\,ps$, longer decay time $t_2 \approx 3\,ns$). Furthermore, we discuss the importance of surface and bulk states for the observed biexponential decay and study the change of t_1 and t_2 for quantum dots attached to different oxide surfaces. The observed results will allow for the optimization of quantum dot properties for specific optoelectronic applications.

HL 27.4 Mon 17:00 Poster B1

Einfluss der Prozessparameter auf das Wachstum von ZnO-Nanodrähten — •Matthias Ogrisek, Andreas Johannes und Carsten Ronning — Friedrich-Schiller-Universität, Jena, Deutschland

ZnO Nanostrukturen können sehr einfach über Gasphasentransport und -Abscheidung in einem horizontalen Rohrofen synthetisiert werden. In den vergangenen Jahren stand hier insbesondere die Herstellung von ZnO Nanodrähten über den Vapor-Liquid-Solid (VLS) Mechanismus im Fokus. Dabei ist das Verständnis über die wechselseitigen Einflüsse der einzelnen Prozessparameter auf die resultierenden Nanostrukturen nicht vollständig geklärt. ZnO Nanodrähte und andere Strukturen wurden durch thermisches Verdampfen von ZnO:C Pulver (carbothermal method) auf verschiedenen Substraten (SiO2, AZO) gewachsen. Die sich gegenseitig beeinflussenden Prozessparameter erlauben dabei das Wachstum von Nanodrähten bei sehr unterschiedlichen Bedingungen. Untersucht wurden die erzeugten ZnO Nanostrukturen mittels Rasterelektronenmikroskopie (REM) und Photolumineszenz-Spektroskopie (PL). Über den Vergleich der Bandkantennahen- und Defektbandemission lassen sich Rückschlüsse auf die relative Defektkonzentration ziehen.

HL 27.5 Mon 17:00 Poster B1

Growth of GaAs nanowires using the ANKA portable MBE system — •Jean-Wolfgang Hornung[1], Emmanouil Dimakis[2], Philipp Schroth[1], Lutz Geelhaar[2], and Tilo Baumbach[1] — [1]Karlsruhe Institute of Technology, Institute for Photon Science and Synchrotron Radiation, Karlsruhe, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

We present results on first growth experiments with the portable Molecular Beam Epitaxy (PMBE) System at ANKA performed at the PDI in Berlin. This system enables the growth of nanostructures in the (In,Ga)As-material system and in-situ monitoring of growth processes using synchrotron radiation at various synchrotron radiation facilities such as ANKA, ESRF, PETRA III. The properties of such NWs are of great importance for the fabrication of high performance electronic devices such as vertical transistors and solar cells.

For future time-resolved XRD-measurements on single NWs, the control of the axial growth rate and number density is very important. We show that by changing the growth parameters (growth temperature, V/III-ratio) we were able to influence these properties. In particular we grew self-catalyzed GaAs-Nanowires (NWs) on Si(111) substrates covered with thin oxide layers of different thicknesses. In-situ the growth process was monitored using RHEED measurements. Ex-situ the samples were characterized by SEM measurements.

We gratefully acknowledge the help of C. Hermann, A.-K. Bluhm and H. - P. Schönherr at PDI, as well as the support by Dr. B. Krause and H.-H. Gräfe at ANKA.

HL 27.6 Mon 17:00 Poster B1

Structural and resistive switching properties of $SrTiO_3$ deposited by RF sputtering — •Benjamin Roessler, Jura Rensberg, Frank Schmidl, and Carsten Ronning — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Strontium titanate ($SrTiO_3$) exhibits bipolar resistive switching between a high- and a low-resistance state when applying an appropriate

electric field. The possibility to deposit $SrTiO_3$ at room temperature by magnetron sputtering on silicon substrates without buffer layers makes it one of the promising candidates for future nonvolatile data memory application. Therefore, we deposited polycrystalline $SrTiO_3$ on p-Si(100) as well as p-Si(110) at room temperature with a fixed oxygen-to argon content ratio of 1:2. The microstructure as well as the crystalline quality of the films was analyzed using cross-sectional electron microscopy and X-ray diffraction analysis. For both substrates a broad grain size distribution was found for the as-deposited films. To improve the crystalline quality post-deposition annealing was performed up to temperatures of 1000°C. In this contribution we discuss the structural changes and electrical properties of $SrTiO_3$, i.e. the resistive switching properties as a function of the annealing temperature.

HL 27.7 Mon 17:00 Poster B1

Memory Effects in Resistive Ion-beam Modified Oxides — •S. Gemming[1,2], D. Blaschke[1,2], K. Potzger[1], P. Zahn[1], A. Bogusz[2], H. Schmidt[2], T. Mikolajick[3], S. Slesazeck[3], H. Wylezich[3], B. Abendroth[4], D. C. Meyer[4], S. Rentrop[4], R. Dittmann[5], K. Skaja[5], R. Waser[5], J. Rensberg[6], C. Ronning[6], N. A. Spaldin[7], and D. Basov[8] — [1]HZ Dresden-Rossendorf, D-01314 Dresden — [2]TU Chemnitz, D-09107 Chemnitz — [3]TU Dresden, D-01062 Dresden — [4]TU Bergakademie Freiberg, D-09596 Freiberg — [5]FZ Jülich, D-52425 Jülich — [6]Friedrich Schiller University Jena, D-07743 Jena — [7]ETH Zürich, CH-8092 Zürich, Switzerland — [8]U.C. San Diego, La Jolla CA 92093-0354, U.S.A.

The Virtual Institute 'Memriox' establishes a joint research initiative in the field of ion-tailored oxide-based memristive elements, to be pursued within a novel and unique combination of core competences from the Helmholtz centers Dresden-Rossendorf and Jülich and their university partners in Dresden, Freiberg, Jena, San Diego, and Zürich. A nanoscale memristive element may prove the concept of the ultimate future non-volatile memory cell with a resistance set directly by electric currents. The Virtual Institute aims at stepping beyond the established layer-by-layer control of intrinsic defects during the synthesis of memristive homojunctions. The project is financed by the Initiative and Networking Funds of the Helmholtz Association (VH-VI-442).

HL 27.8 Mon 17:00 Poster B1

Transmission X-ray microscopy of resistively switched epitaxial Fe-doped SrTiO3 MIM structures — •Holger Wasmund[1], Annemarie Köhl[1], Peter Guttmann[2], Katja Henzler[2], Stephan Werner[2], Sebastian Schmelzer[1], Regina Dittmann[1], and Rainer Waser[1] — [1]FZ Jülich, PGI-7, Germany — [2]HZB, Institute for soft Matter and functional Materials, Germany

There exists strong experimental evidence that the resistance change in transition metal oxides is caused by a valency change on a nanoscale. Transmission X-ray microscopy exhibit the potential of observing bulk spectral information of the sample with a spatial resolution of 25nm unlike other methods which exclusively probe the surface e.g. XPS. One central issue in TXM probe preparation is the sample thickness which should not exceed 100nm. As a first approach we studied polycrystalline STO devices on SiN membranes which were switched in two different resistive states. To analyse epitaxial grown STO devices we prepared SRO|STO|Pt MIM structures on top of NGO substrates with an intermediate sacrifical layer by pulsed laser deposition and sputtered Pt electrodes. A chromium adhesion layer and a carbon film were deposited on top of the stack in order to serve as a carrier foil, followed by a selective etching step of the sarifical layer to release the specimen from the substrate. XAS spectra measurements at the Ti L edge and the Fe L edge for electrode pads in different resistive states were realized at the U41 beamline at Bessy II. We observed significant changes in the Ti spectra which are indications for a valency change in a filament like region.

HL 27.9 Mon 17:00 Poster B1

Adaptive Robot learning via (simulated) memresistive Elements — •Marius Schirmer and Andy Thomas — Bielefeld University, Bielefeld, Germany

Memristors are new circuit elements that fill the gap in relations between the circuit variables flux ϕ and charge q. Like their name consisting of *Mem*ory and Res*istor* presumes, they are resistors with memory. The resistance depends on the current *i(t)* that was applied to an element earlier. This behavior is similar to the synapse of a living nerve cell and therefore networks of memristors can be used as neuronal networks in hardware circuits.

To visualize the learning process of such a memresistive neuronal network we used a *Lego Mindstorms NXT* robot and designed an interface for using memristors that can be connected to the *NXT brick*. We also designed a circuit board that is simulating memresistive behavior. The Software written in Java allows several different learning tasks.

HL 27.10 Mon 17:00 Poster B1

Thermal conductivity measurements using the Raman shift method — •Simon Filser, Benedikt Stoib, Martin Stutzmann, and Martin S. Brandt — Walter Schottky Institut, Technische Universität München, Am Coulombwall 4, 85748 Garching

With the aim to determine the in-plane thermal conductivity of laser-sintered thin films of SiGe nanoparticles [1], we study the applicability of a contactless optical method employing the temperature-dependent frequency shift of the LO phonon mode, as observed by Raman spectroscopy, as a measure for the local temperature. We present our results on a variety of model systems such as, e.g., bulk Si, free-standing Si films and rectangular cantilevers validating the method. The pressure-dependent influence of parasitic thermal conduction through the ambient atmosphere is studied, indicating a small effect for single crystalline material, but a significant contribution for the macro-porous laser-sintered system studied here. Free-standing samples of laser-sintered Si nanoparticle thin films were fabricated either by scanning electron microscope-based micro-manipulation or via a liquid-transfer technique. The results of Raman mapping of such membranes are consistent with the sample morphology and provide insight into the thermal transport.

[1] B. Stoib et al., Appl. Phys. Lett., **100**, 231907 (2012)

HL 27.11 Mon 17:00 Poster B1

A real space method for third-order IFCs and phonon relaxation times for Si from first principles — •Marcel Giar, Michael Bachmann, and Christian Heiliger —)I. Physikalisches Institut, Justus-Liebig-Universität, D-35392 Giessen, Germany

We present a real space method to obtain third-order phonon anharmonicities from first principles calculations. The anharmonic interatomic force constants (IFCs) of third order are determined from a real space method involving small displacements of atoms inside a supercell. We calculate the anharmonic IFCs from force fields due to the displaced atoms using the Vienna *Ab Initio* Simulation Package (VASP). We determine the third-order anharmonicities of the potential for the case of silicon (Si). From these the phonon relaxation times for Si are obtained for different phonon branches.

HL 27.12 Mon 17:00 Poster B1

Phonon Transport in Si-Isotope-Multilayer — •Michael Bachmann, Michael Czerner, Robert Henrich, and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

In thermoelectrics the maximum achievable efficiency is linked to the material parameters by the so called figure of merit. There are in principle four different material parameters, which can be divided into three electronic parameters and one phononic parameter. The three electronic parameters are the electric conductivity, the Seebeck coefficient, and the thermal conductivity of the electrons. The phononic parameter is the thermal conductivity of the lattice. In silicon the electronic parameters are suitable for thermoelectric applications, but the high lattice thermal conductivity prevents the application of pure silicon in thermoelectric devices. Si-isotope-multilayers are a promising structure, where the lattice thermal conductivity can be decreased and the electronic parameters remain unaffected. We present phonon transport calculations based on an atomistic Greens function method for $^{28}Si/^{29}Si$ and $^{28}Si/^{30}Si$ isotope-multilayers. These results show that a periodic arrangement of the layer-system cannot decrease the phonon thermal conductivity substantially, whereas a random arrangement of the layer-system can lead to a strong decrease in the phonon conductivity.

HL 27.13 Mon 17:00 Poster B1

Glancing Angle Deposited Silicon/Germanium Nanostructures for Electronic Applications — •Christoph Grüner and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung, Permoserstraße 15, D-04318 Leipzig, Germany

Obtaining control over the physical properties of semiconductors is a big challenge for future electronics. The use of nanostructures can provide this control, since quantum mechanical and surface effects be-

come important. Nanostructured thin films can show higher optical absorption or reduced reflectivity, higher thermal resistivity and altered electrical properties compared to bulk material. Most preparation techniques for such structures, like etching or VLS growth, are limited by a small window of usable materials or process conditions. With Glancing Angle Deposition (GLAD) it is possible to produce nanostructures from a wide range of materials and with highly customizable shapes, such as slanted and vertical wires, spirals or zig-zag structures. In this technique a highly oblique incidence of deposited material causes small obstacles to cast shadows during the high vacuum deposition, so that areas behind them do not receive material. This leads to the growth of a highly porous thin film. The shape of the individual structures can be influenced by a controlled substrate rotation. We present silicon/germanium GLAD heterostructures with different shapes, a varying germanium distribution and adjustable doping. We also show some approaches to prepare electrical contacts to nanostructure arrays for device integration.

HL 27.14 Mon 17:00 Poster B1

Thermoelectric characterization of $Sn_1(V)_2(VI)_4$ substitutional systems — •Stefan Jakobs[1], Felix Rolf Lutz Lange[1], Karl Simon Siegert[1], Peter Jost[1], and Matthias Wuttig[1,2] — [1]I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]JARA - Fundamentals of Future Information Technology, RWTH Aachen University, Germany

The environmental impact of global warming and the steady rise of the world-wide energy demand requires an increased efficiency of energy consumptive applications.

Thermoelectric generators may contribute to increased efficiency since they are able to convert waste heat into electrical energy. The conversion efficiency of thermoelectric materials is characterized by the dimensionless figure of merit $zT = \frac{\alpha^2\sigma}{\kappa}T$. Hence, to gain large zT values, it is mandatory to have a high electrical conductivty σ, a large Seebeck coefficient α and a low thermal conductivity κ. Since charge carriers also contribute to thermal transport, low lattice thermal conductivities are crucial for a high thermoelectric performance.

Thin film $(IV)_1(V)_2(VI)_4$ chalcogenides allow access to a metastable rocksalt phase. While one sublattice consists of Te, the cation site is randomly occupied by Sn, Sb and 25% of vacancies. This unconventionally high degree of disorder in combination with the large amount of vacancies is favourable for low lattice thermal conductivities [1].

Here, we present the thermoelectric properties of $Sn_1Sb_2Te_4$ and $Sn_1Bi_2Te_4$ thin films prepared under different annealing conditions.

[1] E. R. Sittner *et al.*, *Phys Status Solidi* **A**, DOI 10.1002/pssa.201228397

HL 27.15 Mon 17:00 Poster B1

Transport through nano sized pillars — •Thorben Bartsch, Alina Wetzel, David Sonnenberg, Christian Heyn, and Wolfgang Hansen — Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Jungiusstraße 11, 20355 Hamburg, Germany

We fabricate GaAs nanopillars with typical lengths between 4-8 nm and diameters of about 100 nm using molecular beam epitaxy [1]. The pillars are linked to a GaAs substrate on one end and to a GaAs layer of variable thickness at the other end. The epitaxial growth of the structure ensures that there are no crystal interfaces at these contacts. The pillars are embedded in a matrix of AlAs that can be selectively removed with hydrofluoric acid.

When the AlAs matrix is removed, the pillars open a gap between the GaAs layer and the substrate [1]. Appling a thermal gradient across the gap, thermal transport through the pillars can be studied. Using the 3-omega method we verified that the thermal transport through the pillars is ballistic in a temperature range at least up to 150 K [2]. Here influences from variations of the heterostructure geometry, especially from variable top layer thicknesses are discussed.

Moreover, in case of doped structures, charge transport through the pillars between two charge reservoirs held at different electric potential can be studied. We present first results of electronic transport experiments. At low temperature, the conductance is found to strongly depend on the strength and orientation of a magnetic field.

[1] Ch. Heyn et al., Appl. Phys. Lett. 98, 033105 (2011)
[2] Th. Bartsch et al., Phys. Rev. Lett. 108, 075901 (2012)

HL 27.16 Mon 17:00 Poster B1

Thermoelectric Transport Properties of GeTe Rich GeTe-Sb_2Te_3 Thin Films — •Felix R. L. Lange[1], Ernst-Roland Sittner[1], Karl Simon Siegert[1], Peter Jost[1], and Matthias Wuttig[1,2] — [1]I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]JARA - Fundamentals of Future Information Technology, RWTH Aachen University, Germany

Phase change materials (PCM) are a class of alloys that can be reversibly and rapidly switched between the amorphous and the crystalline state. Since these two states differ significantly in their physical properties such as reflectivity and resistivity they are well suited for future nonvolatile data storage applications. Some PCM along the pseudo-binary line between GeTe and Sb_2Te_3 exhibit a rather unusual combination of physical properties which render these alloys a potential p-type thermoelectric. These alloys allow access to a meta-stable cubic phase where one lattice site is randomly occupied by Ge, Sb and a certain amount of structural vacancies. Only recently Siegrist *et al.* identified disorder in these alloys as the cause of a metal to insulator transition. The degree of disorder can be affected by two independent parameters: stoichiometry and annealing conditions. Since disorder affects both, electrical and vibrational degrees of freedom, this opens up a pathway to tailor electrical and thermal transport properties independently. Using this concept we report enhanced thermoelectric efficiencies for GeTe rich GeTe-Sb_2Te_3 thin films prepared under different annealing conditions [1].

[1] E. R. Sittner *et al.*, *Phys Status Solidi* **A**, DOI 10.1002/pssa.201228397 (2012)

HL 27.17 Mon 17:00 Poster B1

Thermoelectric power factor and full ZT characterization of Bi2Te3-nanowires — •Rüdiger Mitdank[1], Danny Kojda[1], Zhi Wang[3], William Toellner[2], Kornelius Nielsch[2], Peter Woias[3], and Saskia F. Fischer[1] — [1]Novel Materials, Institute of Physics, Humboldt Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany — [2]Institute of Applied Physics, Universität Hamburg, Jungiusstr. 11, 20355 Hamburg, Germany — [3]) IMTEK, University of Freiburg, D-79110 Freiburg

Thermoelectric (TE) properties of single Bi2Te3 nanowires (NW) were investigated using a TNCP (Thermoelectric characterization platform) which allows the determination of the Seebeck coefficient S, the conductivity σ and the thermal conductivity. The NW is deposited between 2 thin and freestanding Si-cantilevers. On each cantilever, 2 Pt-electrodes are arranged serving as microheater and thermometer. The calibration of the TNCP is discussed. In the temperature range 4,2K $<$ T $<$ 300K, the conductivity and the thermopower were measured. The function σ(T) corresponds to a rather metallic behaviour. The thermopower exhibits a maximum near 200 K. For a conductivity of nearly 1000S/cm the thermopower S(300K) varied between -35 μV/K and -50 μV/K. Experiments to determine the thermal conductivity are discussed.

HL 27.18 Mon 17:00 Poster B1

Thickness-dependent thermoelectric properties of BiSb thin films — •Heiko Reith[1,2], Friedemann Voelklein[2], and Michael Huth[1] — [1]Physikalisches Institut, Goethe-University, Frankfurt am Main, Germany — [2]IMtech, Hochschule Rhein Main, Ruesselsheim, Germany

We investigated the thermoelectric properties of BiSb thin films in the thickness range between 50 nm and 500 nm. For the determination of the thermoelectric properties we measured the Seebeck-coefficient and the thermal and electrical conductivity to obtain the figure of merit of the films. The thermal conductivity was measured using a specially designed microchip. For the electrical conductivity and Seebeck-measurement a four point structure deposited on a Si/Si_3N_4-wafer was used. The BiSb films were deposited onto these substrates using a thermal evaporation process. During the deposition of the films the substrates and microchips were placed next to each other and the thickness was detected by a quartz microbalance. Afterwards the thickness was measured with a surface profilometer. We present the used measurement techniques and results. From the measurement results we determine the figure of merit of the films and discuss the results using finite size effect models.

HL 27.19 Mon 17:00 Poster B1

Unexpected temperature dependence of thermal boundary conductance for epitaxial Bi(111) films on Si(001) — •Verena Tinnemann, Tim Frigge, Boris Krenzer, Anja Hanisch-Blicharski, Friedrich Klasing, Annika Kalus, and Michael Horn-von Hoegen — Faculty of Physics and Center for Nanointegration CENIDE, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

Ultrafast time-resolved reflection high energy electron diffraction was used to study the heat transfer from epitaxial Bi(111) films into the Si(001) substrate. Films with thicknesses in the range from 25 nm to 120 nm were prepared in-situ under UHV conditions. In a pump-probe setup the Bi films were excited by 50 fs-laser pulses with a wavelength of 800 nm. Short electron pulses were created by photoemission, accelerated to 7 keV, and focused by an electrostatic lens. For variable time delays between laser pump and electron probe diffraction patterns were recorded. The transient drop of spot intensity is explained in terms of the Debye-Waller effect and reflects the instant heating and subsequent cooling of the Bi films. The thermal boundary conductance of the interface is then determined from the exponential cooling of the film. We show that the thermal boundary conductance increases by more than 35% if the substrate temperature is increased from 80 K to 300 K. This is not explained by numerical simulations of the heat transport using temperature dependent parameters. For the 120 nm thick Bi-film a bi-exponential intensity is observed and explained by diffusion in the film and across the interface.

HL 27.20 Mon 17:00 Poster B1

Structural and electrical properties of thermoelectric $Fe_xCo_{1-x}Sb_3$ thin films — Ayham Dalla, •Marcus Daniel, Andreas Liebig, Fabian Ganss, Gunter Beddies, and Manfred Albrecht — Chemnitz University of Technology, Institute of Physics

Increasing interest in efficiency enhancement of existing energy sources led to an extended research in the field of thermoelectricity. A suitable thermoelectric material like $CoSb_3$ is characterised by a high power factor and a low thermal conductivity. To control and improve the power factor a targeted electrical doping is necessary to achieve charge carrier densities up to 10^{20} cm^{-3}. In case of $CoSb_3$ controlled doping can be obtained by a partially substitution of Co by Fe atoms. In this study, 30 nm thick $Fe_xCo_{1-x}Sb_y$ films have been deposited via MBE onto thermally oxidized Si(100) substrates at room temperature. The samples were post-annealed in ultra-high vacuum for one hour at 450°C. Two sample series with varying Fe content ($0<x<0.5$) were fabricated, a Sb rich ($y = 3.3$) and a Sb deficient series ($y = 2.5$). The composition was verified by RBS and the XRD analysis confirmed $CoSb_3$ as major phase. A systematic decrease of the extracted lattice parameter with increasing Fe content indicated the substitution of Co by Fe atoms. The electrical characterization was performed in a temperature range between 4 K and 300 K. Both series show an increase in charge carrier concentration with increasing Fe content, and thus a decrease in resistivity. The temperature dependence of the resistivity revealed for both sample series a change from semiconducting to metallic behaviour at a critical charge carrier concentration.

HL 27.21 Mon 17:00 Poster B1

Measurement setup fpr simultaneous determination of electrical conductivity, Hall coefficient and Seebeck coefficient. — •H. Kolb, J. de Boor, A. Sesselmann, T. Dasgupta, G. Karpinski, and E. Müller — DLR, Institute of Materials Research, Cologne

Thermoelectric materials can convert heat directly into usable electrical energy. An important aim in thermoelectric research is to find and optimize suitable materials and improve their performance to get higher efficiency. For a complete characterization it is in general required to do several different measurements in different apparatuses which can be challenging and time consuming. Therefore we developed a measurement system that can measure three of the thermoelectric key quantities (electrical conductivity, Seebeck- and Hall coefficient) simultaneously from room temperature up to 1000K, which is a typical temperature region for many potential applications of these materials. All three quantities are coupled via the charge carrier concentration and therefore a simultaneous measurement is important for a deep insight in the charge carrier transport in the sample. This is particularly important for thermally instable materials, where consecutive measurements can easily lead to misinterpretations. Four sheathed thermocouples arranged in a van der Pauw geometry are pressed by small springs on a round sample for electrical contact. This special arrangement allows for the electrical measurements, while the thermocouples allow for a determination of the Seebeck coefficient if an additional temperature gradient is applied. We will discuss technical details, features and limitations of the setup.

HL 27.22 Mon 17:00 Poster B1

Anomalous enhancement of the thermoelectric figure of merit by V co-doping in $SrTiO_3$ — •Udo Schwingenschlögl and Mousumi Upadhyay-Kahaly — KAUST, PSE Division, Thuwal, Saudi Arabia

The effect of V co-doping in Nb-$SrTiO_3$ and Pr-$SrTiO_3$ is studied by full-potential density functional theory. While in Nb-$SrTiO_3$ a high carrier density counteracts a high thermoelectric figure of merit, the trend is inverted by V co-doping. A similar but even more pronounced effect is found in Pr-$SrTiO_3$. The mechanism leading to this behavior is explained in terms of a local spin-polarization introduced by the V ions. Our results indicate that magnetic co-doping can be a prominent tool for improving the thermoelectric figure of merit.

Reference: Applied Physics Letters **100**, 193110 (2012)

HL 27.23 Mon 17:00 Poster B1

The effect of interfaces on the thermoelectric properties of laterally microstructured ZnO-based thin-films — •David Hartung, Florian Gather, Achim Kronenberger, Martin Eickhoff, Bruno K. Meyer, and Peter J. Klar — I. Physikalisches Institut, Justus-Liebig-University, Heinrich-Buff-Ring 16, 35392 Giessen

A series of samples was laterally microstructured with a self-aligned pattern transfer method consisting of alternating stripes of ZnO grown by molecular-beam epitaxy and radio-frequency sputtered Ga-doped ZnO stripes. The MBE-grown ZnO thin film samples were laterally microstructured by photolithography followed by ion-beam etching in order to obtain different lateral arrangements of stripes of defined interface geometry. In a second step the free regions between the stripes of MBE-grown ZnO were sputtered with Ga-doped ZnO. A lift-off step completes the micro-fabrication of a planar alternating ZnO/ZnO:Ga bar structure on each sample.
Throughout the series the bar width and hence the number of interfaces was kept constant, but the interface profile was varied yielding different interface lengths and geometries.
We measured in-plane as a function of temperature the Seebeck coefficient S and the electrical conductivity σ of the samples with the transport direction perpendicular to the stripe direction.
The measured data were compared to simulated data using an empirical network model.

HL 27.24 Mon 17:00 Poster B1

Thermoelectric properties of $ZnO_{1-x}S_x$ thin films — •Florian Gather, Achim Kronenberger, Peter J. Klar, and Bruno K. Meyer — I. Physikalisches Institut, Justus-Liebig-University, Heinrich-Buff-Ring 16, 35392 Giessen

We investigated the thermoelectric properties of rf-sputtered $ZnO_{1-x}S_x$ thin films on sapphire substrates. Due to its good availability and its non-toxicity, $ZnO_{1-x}S_x$ is a promising candidate for thermoelectric applications. The electric conductivity σ, the Seebeck coefficient S and carrier concentrations of a series of hydrogen doped samples and aluminum doped samples respectively were determined in in-plane direction over a wide temperature range. For the investigation of the influence of the sulphur concentration x on the thermal conductivity κ we employed the 3-omega method on a series of undoped thin-films. The measurements reveal a reduced κ in cross-plane direction of the samples containing sulphur compared to zinc-oxide samples. Using Raman spectroscopy we found indications for local phonon modes of oxygen in zinc-sulfide and of sulphur in zinc-oxide, respectively. These local phonon modes cause the reduction of κ observed in the experiments. Both sample series are compared in terms of crystal quality and grain size using XRD-analysis and atomic force microscopy.

HL 28: Poster Session: Graphen; Transport properties; Transport in high magnetic fields / Quantum Hall effect; Metal-semiconductor hybrid systems

Presenters are kindly asked to be near their posters at least 17:00–18:00 or to leave a note at the poster indicating a time period of availability for discussions. — Beverages will be served starting at 18:00.

Time: Monday 16:00–20:00 Location: Poster A

HL 28.1 Mon 16:00 Poster A

Fabrication and characterization of free-standing graphene — •Dominique Schüpfer, Katharina Huhn, Torsten Henning, and Peter J. Klar — I. Physikalisches Institut, JLU, Heinrich-Buff-Ring 16, 35392 Gießen

Up to now no simple method for characterizing graphene without the influence of its supporting material has been established. We demonstrate a simple alternative for fabricating free-standing graphene using SU-8 resist as a supporting structure. The SU-8 resist is microstructured via photolithography to prepare hollow cylinders inside the SU-8 layer. In a next step graphene can be deposited on top of this structure by mechanical exfoliation of graphite, which creates free-standing graphene on top of the hollow cylinders. Raman measurements of these graphene monolayers will be discussed aswell as the fabrication of this very suitable supporting structure.

HL 28.2 Mon 16:00 Poster A

Preparation of folded graphene layers via atomic force microscope — •Johannes C. Rode, Dmitri Smirnov, Christopher Belke, Hennrik Schmidt, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, D-30167 Hannover, Germany

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 properties of thusly created bilayers. The crystal lattices of these are often twisted against each other and form decoupled systems which hold interesting electronic properties like a screening effect and reduced Fermi velocities. Our samples are obtained by micromechanical cleavage of natural graphite and placed on a silicon substrate with a top layer of silicon dioxide. Graphene is located and identified using the optical microscope. Detailed height profiles can then be obtained by AFM, which also serves as a tool to mechanically manipulate the graphene by programmed tip movements. We show AFM-induced folding of graphene on a μm-scale and investigate ways to a controlled preparation of folded samples. These can be electrically contacted and characterized. To interpret the results thoroughly, the geometries must be examined with respect to twist angle and crystallographic orientation.

HL 28.3 Mon 16:00 Poster A

Nano patterning graphene by gas-assisted focused-electron-beam-induced etching — •Jens Sonntag, Benedikt Sommer, Arkadius Ganczarczyk, Martin Geller, and Axel Lorke — Faculty of Physics and CENIDE, Universität Duisburg-Essen

The transport properties of graphene devices vary dramatically with their geometric structure. E.g. confining the charge carries in lateral dimension gives rise to a band gap, which is advantageous for the current ratio between on and off state of a graphene field-effect transistor. We present a method to pattern graphene by focused-electron-beam-induced-etching (FEBIE) with water vapor as a reactive gas. While the resolution for graphene on SiO_2 is comparable to the widely used electron beam lithography (EBL) followed by reactive ion etching, no organic resist is needed for the FEBIE technique. A resolution of about 15 nm is achieved. More importantly, we are able to cut suspended graphene with an even better resolution of approximately 8 nm. In both cases, the roughness of the edges is at least better than the obtained resolution.

Transport measurements on a 1D conductive channel patterned by FEBIE indicate the expected band gap, showing that the process does not destroy the characteristic electronic properties of graphene. Therefore it is possible to fabricate devices like suspended graphene nanoribbons in a controlled top-down process.

HL 28.4 Mon 16:00 Poster A

Graphene nanostructures produced from suspended and 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. 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 [1]. To reduce these effects, there are different possibilities, from which two were tested on flakes with different numbers of layers.

a) Etching of the SiO_2 under the flake with hydrofluoric acid is used to make the samples suspended [2]. Afterwards, the flake is cleaned by current annealing, in which a high current flows through the flake, so that contaminations are removed by the generated heat.

b) Transfer of the flakes [3]. For this, graphene is exfoliated on a thin PMMA layer, which can be detached from the silicon wafer. This layer is then placed on another flake or substrate of choice.

Using these two methods, different nanostructures were produced and characterized.

[1] P. Barthold et al. NJP **13**, 043020 (2011).
[2] K. I. Bolotin et al. Science-Direct, **146**, 351 (2008).
[3] C. R. Dean et al. Nature nanotechnology, **5**, 722 (2010).

HL 28.5 Mon 16:00 Poster A

Synthesis and characterization of graphene quantum dots based ink for printable applications — •Tessy Theres Baby[1], Suresh Garlapati[1], Falk von Seggern[1,2], Robert Kruk[1], Subho Dasgupta[1], and Horst Hahn[1,2] — [1]Institute for Nanotechnology, Karlsruhe Institute of Technology (KIT), D-76344 Eggenstein-Leopoldshafen, Germany — [2]KIT-TUD Joint Research Laboratory Nanomaterials, Institute of Materials Science, TU Darmstadt, Petersenstr. 32, 64287 Darmstadt, Germany

Graphene, the one atom thick layer of carbon, is ideally suited for numerous electronic applications on account of its high conductivity, carrier concentration (~ 1013 cm-2) and extraordinary mobility (~ 15,000 cm2/Vs). However, the absence of an electronic band gap has been an impediment in realizing graphene based devices. Therefore, the aim of this work is to synthesize graphene quantum dots with tunable electronic properties. A high temperature gasothermal (exfoliation of graphite oxide at 1050 °C in Ar atmosphere for 30 s) method is found suitable for large scale synthesis of such few nanometer diameter graphene nanodiscs. Acid functionalization has been carried out to obtain stable dispersions with tailored morphology. Finally, in the course of fabricating field-effect devices, a printable (ink-jet) grade of nanoink consisting of graphene nanodiscs has been prepared. In order to preserve the electronic properties, no surfactants or additives have been added. Electrochemically-gated field-effect transistors using composite solid polymer electrolytes have been characterized systematically.

HL 28.6 Mon 16:00 Poster A

Silicon nitride as top gate dielectric for epitaxial graphene — •Peter Wehrfritz[1], Felix Fromm[1], Stefan Malzer[2], and Thomas Seyller[1,3] — [1]FAU Erlangen-Nürnberg, Technische Physik, Erlangen, Deutschland — [2]FAU Erlangen-Nürnberg, Angewandte Physik, Erlangen, Deutschland — [3]TU Chemnitz, Institut für Physik, Chemnitz, Deutschland

Epitaxial graphene grown under atmospheric pressure offers an opportunity for large scale electronic device fabrication [1]. A suitable top gate dielectric, however, is still to be found. Al_2O_3 and HfO_2 grown by atomic layer deposition provides high quality dielectrics. Unfortunately it is not possible to grow closed layer on graphene without additional surface activation [2, 3].

We have investigated silicon nitride (SiN) grown by plasma enhanced chemical vapor deposition (PECVD) as top gate material on epitaxial graphene on 6H-SiC(0001). The NH_3 and SiH_4 flow rate ratio was optimized on the basis of x-ray photoelectron spectroscopy (XPS) measurements. The formed SiN layer is closed. Raman spectroscopy and transport measurements which were performed before and after the

SiN deposition revealed that the plasma process leads only to a minor degradation of the graphene. The SiN layer induces strong n-type doping proven by Hall measurements, transfer characteristic and XPS measurements.

[1] K. Emtsev et al., Nat. Mat. **8**, 203 - 207 (2009).
[2] S. Kim et al., Appl. Phys. Lett. **94**, 062107 (2009).
[3] B. Lee et al., Appl. Phys. Lett. **92**, 203102 (2008).

HL 28.7 Mon 16:00 Poster A

Electronic and optical properties of bilayer-array-embedded graphene — •Hengyi Xu and Thomas Heinzel — Heinrich-Heine-Universität Düsseldorf, Germany

The coexistence of monolayer and bilayer graphene is widely found in graphene samples, like large-scale monolayer/bilayer interfaces obtained from mechanical exfoliation or small-scale interfaces due to some graphite atoms sitting on graphene layers in epitaxial growth. These structures show a rich phenomenology and may provide some new possibilities for device applications.

In this work, we focus on structures with additional carbon atoms located on top of a monolayer graphene, thereby forming a regular hexagonal array of monolayer/bilayer quantum dots. The implementation of such structures seems to be rather plausible via the method of epitaxial growth. The electronic and optical transport properties of the periodic monolayer/bilayer interface are systemically studied with the Kubo formalism. The density of states as well as the electronic and optical conductivity are calculated by solving the time-dependent Schrödinger equation. It is found that the monolayer/bilayer interface array induces midgap states and suppresses the transmission in vicinity of Dirac points. Interface scattering has also a far-reaching impact on the Landau levels and Hall conductivity. In addition, the optical conductivity of such systems exhibits some extra peaks at the low frequencies due to the renormalization of density of states.

HL 28.8 Mon 16:00 Poster A

Ultrafast photocurrents of monolayer graphene on sapphire — •Martin Schwarz, Andreas Brenneis, Max Seifert, Jose Garrido, and Alexander Holleitner — Walter Schottky Institut and Physik-Department, TU München, 85748 Garching, Germany

We present picosecond-time resolved optoelectronic measurements of monolayer graphene, grown by chemical vapor deposition (CVD), on sapphire substrates. Our optoelectronic on-chip scheme samples the photocurrents within the graphene with a picosecond time resolution [1]. We verify an ultrafast displacement current at the metal-graphene interfaces and the dynamics of hot charge carriers within the graphene. In particular, we compare our results to the ones of freely suspended bilayer graphene with special emphasis on the thermal coupling of the graphene to its environment. Financial support by the ERC-grant NanoREAL is acknowledged.

[1] L. Prechtel, L. Song, D. Schuh, P. Ajayan, W. Wegscheider, A.W. Holleitner, Nature Comm. 3, 646 (2012).

HL 28.9 Mon 16:00 Poster A

Photocurrent in epitaxial graphene — •Stefan Link[1], Peter Wehrfritz[1], Felix Fromm[1], Stefan Malzer[2], and Thomas Seyller[1,3] — [1]FAU Erlangen-Nürnberg, Lehrstuhl für Technische Physik — [2]FAU Erlangen-Nürnberg, Lehrstuhl für Angewandte Physik — [3]TU Chemnitz, Institut für Physik

Graphene, the two-dimensional sheet of carbon promises a lot for electronic applications. For example, Mueller et al. [1] have demonstrated the potential of graphene for high-speed optical communications. In particular, they investigated the behavior of graphene-based photodetectors. Epitaxial graphene on SiC, which can be grown on a wafer scale [2], is the ideal platform for the development of such devices. We have investigated the photocurrent generation in graphene-metal junctions using different types of epitaxial graphene grown on SiC(0001). The photoresponse was shown to be due to a photovoltaic effect and improved by optimization of device design and by the use of quasi-freestanding graphene [3].

[1] T. Mueller et al., Nat. Photon. **4** (2010) 297. [2] K. V. Emtsev et al., Nat. Mater. **8** (2009) 203. [3] C. Riedl et al., Phys. Rev. Lett. **103** (2010) 246804.

HL 28.10 Mon 16:00 Poster A

Phototransmission and Photoconductivity in the THz Spectral Range of Graphene Samples — •Markus Göthlich[1], Fathi Gouider[1], Miriam Grothe[2], 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

Graphene has first been isolated in 2004. Since then this material has become a major field of interest in research, not least due to it's remarkable Landau quantization $E_n = \mathrm{sgn}(n)\sqrt{2\hbar e v_F^2 |n| B}$ with n being the Landau level (LL) index. Thus, an intraband transition between LLs with an enery of 10meV (corresponding to electromagnetic radiation with a frecquency of about 2.4THz) can theoretically be achieved with a magnetic field as low as 0.2T. In the case of cyclotron resonance the phototransmission drops and the conductivity of the sample changes due to a change of the carrier density at the Fermi energy. In this contribution, we present the magnetoconductivity and the terahertz (THz) photo-conductivity of devices with graphene. For the photoconductivity measurements, a THz laser system (p-Ge-Laser) is applied. This laser uses transitions between Landau levels of light holes and emits laser impulses in the wavelength range $120\mu\mathrm{m} \leq \lambda \leq 180\mu\mathrm{m}$. The THz laser radiation is used in order to excite charge carriers over the Landau gap. To characterize the examined graphene samples, the Shubnikov-de Haas-effect measurements at a temperature of $T = 4\mathrm{K}$ and in the region of the magnetic fields of $0 \leq B \leq 10\mathrm{T}$ were performed.

HL 28.11 Mon 16:00 Poster A

Terahertz-sensitive devices based on epitaxial graphene — •Christian Sorger, Alexander Glas, Stefan Hertel, Sascha Preu, and Heiko B. Weber — Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Epitaxially grown graphene is a hybrid system comprising graphene as a metal and silicon carbide as a semiconductor. Through patterning the graphene layer by means of local intercalation (i.e. without metallic gates), electronic functionality can be achieved [1].

First, we focus on the transmission of Terahertz radiation through a grid-like, p-n-patterned graphene layer. The physics is predominantly governed by the excitation of plasmons and we currently explore the potential influence of Klein-Tunneling. Secondly, we form Schottky-Diodes following the strategy of reference [1]. When equipped with a metallic antenna, we examine their suitability as Terahertz detectors.

[1] S. Hertel *et al.*, Nature Communications **3**, 957 (2012)

HL 28.12 Mon 16:00 Poster A

Hot Carrier Photoluminescence in Graphene — •Andreas Neff, Reiner Bormann, Sascha Schäfer, and Claus Ropers — Materials Physics Institute and Courant Research Centre, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The photoluminescence of hot carriers in graphene yields insight into the ultrafast carrier and phonon dynamics after optical excitation [1,2], providing complementary information to transient spectroscopy [3]. In this contribution, we study the blue-shifted spectral component of hot-carrier photoluminescence of graphene on sapphire substrates, excited by sub-10-fs near-infrared laser pulses. We characterise the nonlinear spectral dependence of the emission as a function of laser fluence and pulse duration. The experimental findings are analysed using a microscopic model of carrier dynamics based on Boltzmann rate equations, including carrier-carrier and carrier-phonon scattering processes. Specifically, the role of Auger recombination and impact ionization on the photoluminescence properties is discussed.

[1] C.H. Lui, *et al.*, Phys. Rev. Lett. **105**, 127404 (2010)
[2] W. Liu, *et al.*, Phys. Rev. B. **82**, 081408 (2010)
[3] M. Breusing, *et al.*, Phys. Rev. B. **83**, 153410 (2011)

HL 28.13 Mon 16:00 Poster A

Acoustic charge transport in epitaxial graphene on SiC — •Paulo V. Santos, Timo Schumann, Myriano H. Oliveira Jr., Joao Marcelo J. Lopes, and Henning Riechert — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

Graphene is emerging as an important material for electronic applications due to its high carrier mobility. Here, we investigate carrier control in epitaxial graphene on SiC (epiG) using dynamic strain field produced by a surface acoustic wave (SAW). The strain field periodically modulates the epiG band structure[1]. Electron beam collimators based on this effect have been proposed [2]. We report on the piezoelectric excitation and on acoustic charge transport by SAWs in epiG. SAWs with GHz frequencies were generated by interdigital transducers

(IDTs) fabricated on a piezoelectric ZnO island on semi-insulating SiC. These SAW frequencies are substantially higher than those reported for acoustic transport in graphene flakes[3]. Acoustic transport studies in a Hall bar geometry show that SAWs transport carriers in epiG, with the transport direction being determined by the direction of the acoustic beam. The mechanisms for the carrier transport, including the effects of the strain field and the weak piezoelectric field in SiC will be discussed.

[1] C.-H. Park *et al.*, *Phys. Rev. Lett.*, **101**, 126804 (2008).
[2] C.-H. Park*et al.*, *Nano Lett.*, **8** 2920 (2008).
[3] V. Miseikis *et al.*, *Appl. Phys. Lett.*, **100**, 133105 (2012).

HL 28.14 Mon 16:00 Poster A

Proximity induced superconductivity in bilayer graphene — •Julien Bordaz[1], Michael Wolf[1,2], Fan Wu[1], Hilbert von Löhneysen[1,2,3,4], Detlef Beckmann[1,2], Kenji Watanabe[5], Takashi Taniguchi[5], and Romain Danneau[1,3] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany — [2]DFG Center for Functional Nanostructures, Karlsruhe Institute of Technology, Germany — [3]Institute of Physics, Karlsruhe Institute of Technology, Germany — [4]Institute for Solid-State Physics, Karlsruhe Institute of Technology, Germany — [5]Advanced Materials Laboratory, National Institute for Materials Science, Tsukuba, Japan

Proximity induced superconductivity effect occurs when graphene is connected with close enough superconducting electrodes. Observations of Andreev reflection and induced supercurrents flowing through graphene sheets have already been reported in graphene. However, these effects have not been explored in bilayer graphene so far. By applying a perpendicular electric field, it is possible to open a gap in a bilayer graphene. This can be achieved in practice by designing a top gate in addition to the usual back gate. Our devices are produced on top of sapphire wafers by using transfer techniques and standard electron-beam lithography. The bilayers are sandwiched between two atomically flat hexagonal boron nitride multilayers which are both used as gate dielectric. By inducing a band gap into a bilayer graphene connected by two superconducting leads, the supercurrent could be switched off inducing a superconductor-insulator transition.

HL 28.15 Mon 16:00 Poster A

Generalized Boltzmann equation approach to rectification at a potential step — •Stephan Rojek, Alfred Hucht, and Jürgen König — Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany

In a recent experiment[1, 2] a density modulated two-dimensional electron gas has been shown to work as a tunable rectifier. Tow top-gates define two regions of different carrier density separated by a potential step. A bias voltage parallel to the potential step leads to a transverse voltage proportional to the square of the applied bias voltage. The experiment could be well explained within a diffusion thermopower model in terms of a Boltzmann equation approach.[2] The latter is based on a local equilibrium distribution function with a spatially dependent effective chemical potential and temperature.

In our current theoretical investigation, we go beyond this diffusion thermopower model and derive a general theory, which, in principal, allows for a systematic calculation of all contributions to a non-equilibrium distribution function.

[1] A. Ganczarczyk, C. Notthoff, M. Geller, A. Lorke, D. Reuter, and A. D. Wieck, AIP Conf. Proc. **1199**, 143 (2009).
[2] 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).

HL 28.16 Mon 16:00 Poster A

Quasi-ballistic electron transport through bipolar localized magnetic fields — Tudor Chirila, Bernd Schüler, •Mihai Cerchez, and Thomas Heinzel — Heinrich Heine University Düsseldorf, Condensed Matter Laboratory, Universitätsstr. 1, 40225 Düsseldorf

We investigated the electron transport in hybrid ferromagnet/semiconductor devices produced by a series of two magnetic barriers of opposite polarity, placed on top of a Hall bar etched into a GaAs/AlGaAs heterostructure. The size of the Hall bar is comparable to the size of the magnetic structure and smaller than the mean free path of the electrons which places the structure in the quasi-ballistic regime [1]. The strength of the magnetic field profile is tuned by an external applied magnetic field, and the electron density is tuned by a metallic top gate. The magnetoresistance of the device shows non-ohmic behavior with characteristic transmission and reflection resonances. The measurements are in agreement with semi-classical simulations using the Landauer-Büttiker formalism with scattering [2, 3], and reveal the origin of the resonances residing in the quasi-ballistic transport of electrons confined by the edges of the Hall bar and the magnetic field profile.

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HL 28.17 Mon 16:00 Poster A

Mobility Studies on High Electron Mobility Structures — •Christian Schulte-Braucks, Arne Ludwig, and Andreas D. Wieck — Angewandte Festkörperphysik, Ruhr-Universität Bochum

Two Dimensional Electron Gases in modulation doped High-Electron-Mobility-Transistor-Structures (HEMT) have huge potential in current and prospect research and application. Therefore, a good understanding of properties and scattering processes depending on the sample structure is essential to design samples with desired characteristics such as high electron mobility. A systematic study of Hall-mobility (μ) depending on 2D charge carrier concentration (n) of Molecular-Epitaxy-grown δ-doped $GaAs-AlGaAs$-HEMTs is in progress. There are two aspects which are focussed on intensively. First varying structural aspects such as spacer thickness, material composition and doping. Second, changing measurement parameters such as sample current and illumination intensity. n has been tuned by succsessive illumination, exploiting persistent photo effect in DX-centres and measurements are planned to be compared by tuning n by Gate bias. Moreover, Shubnikov-de-Haas-Oscillations are projected to get access to the occupation of subbands, the existence of parallel conductance and scattering mechanisms. A power function law $\mu \propto n^{\alpha}$ where α depends on the spacer thickness has been observed, which can be assigned to remote impurity scattering. In congruence with [1] α is approximately 0.6 but contradictory to [2] increases with increasing spacer thickness.

[1] Shayegan, M et al., Appl.Phys.Lett., **52**(13), (1988)
[2] Schmult, et al., J.Cryst.Growth., **331**(7), (2009)

HL 28.18 Mon 16:00 Poster A

Determination of trap and band states in printable thin film transistors by scanning Kelvin probe microscopy — •Sebastian Hietzschold[1,2,3], Florian Mathies[1,2,4], Rebecca Saive[1,2,3], Norman Mechau[2,4], and Wolfgang Kowalsky[1,2,3] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Germany — [2]InnovationLab, Heidelberg, Germany — [3]Institut für Hochfrequenztechnik, Technische Universität Braunschweig, Germany — [4]Lichttechnisches Institut, Karlsruhe Institut für Technologie, Germany

The development of printed thin film transistors (TFTs) is of utmost importance enabling large-area electronics by low cost fabrication. Former work, e.g. M. Koehler *et al.*, has shown that a fundamental understanding of charge carrier transport in the active material and at interfaces is essential improving device performance [1]. Therefore we investigate TFTs with scanning Kelvin probe microscopy (SKPM) in an ultra-high vacuum environment. We apply different gate bias leading to a filling and emptying of electronic states and measure in-situ the shift in the surface potential respectively. Hereby we indirectly gain the density of trap as well as band states (DOS). The DOS energy distribution provides information on many electronic properties in semiconductor films and is therefore crucial for a performance improving of printed thin film transistors.

[1] M. Koehler and I. Baggio, Phys. Rev. B 68, 075205 (2003)

HL 28.19 Mon 16:00 Poster A

Weak antilocalization and disorder-enhanced electron interactions in crystalline $Ge_1Sb_2Te_4$ — Nicholas Breznay[1], •Hanno Volker[2], Alexander Palevski[3], Riccardo Mazzarello[4], Aharon Kapitulnik[1], and Matthias Wuttig[2,5] — [1]Department of Applied Physics, Stanford University, Stanford, CA 94305, USA — [2]I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany — [3]School of Physics and Astronomy, Raymond and Beverly Sackler Faculty of Exact Science, Tel-Aviv University, 69978 Tel-Aviv, Israel — [4]Institut für theoretische Festkörperphysik, RWTH Aachen University, 52056 Aachen, Germany — [5]JARA FIT, RWTH Aachen

Phase-change materials (PCMs) are characterized by their high optical and electrical contrast between an amorphous and a crystalline phase, the long-term stability of both phases at room temperature and their fast crystallization kinetics[1]. Recently, it has been demonstrated that many PCMs undergo a disorder-induced metal-insulator transition[2].

In the present study[3], we focus on the metallic state, in which disorder-enhanced electron-electron interaction and weak antilocalization caused by strong spin-orbit scattering are observed at low temperatures. Employing well-established theories[4], we are able to consistently fit experimental data and extract the relevant scattering rates.

[1] M. Wuttig and N. Yamada, Nat. Mater. 6, 824 (2007)
[2] T. Siegrist et al., Nat. Mater. 10, 202 (2011)
[3] N.P. Breznay et al., Phys. Rev. B 86, 205302 (2012)
[4] P.A. Lee and V. Ramakrishnan, Rev. Mod. Phys. 57, 287 (1985)

HL 28.20 Mon 16:00 Poster A

Charge Transport and Passivation of ZnO-TFTs Deposited by Spray Pyrolysis — •Yulia Trostyanskaya, Marlis Ortel, Nataliya Kalinovish, Gerd Roeschenthaler, and Veit Wagner — Research Center for Functional Materials and Nanomolecular Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

ZnO serves as a suitable semiconductor for thin film transistors (TFTs) due to its high mobility, wide band gap and simple and cheap way of deposition e. g. via spray pyrolysis. However the electronic properties of the material have a disadvantage of being highly sensitive to the surrounding environment due to the formation of surface states. In this work flour terminated diketones e.g. 4,4,4-trifluoro-1-(3-fluorophenyl)1-3-butanedione were bound on the zinc oxide surface to reduce the impact of the environment. The effect on the charge transport processes in the semiconductor was analyzed by bias stress measurements and temperature dependent electrical measurements which were correlated to optical and morphological investigations. The passivation of the TFTs induced an increase of the linear mobility from 4cm2/Vs to 7.3cm2/Vs and improved the bias stress stability remarkably which is in good agreement with a shift of the optical band gap. Furthermore, significant difference in the conduction processes with and without passivation was found. While similar activation energies are found above 100K clear difference is observed below, reflecting the passivated states.

HL 28.21 Mon 16:00 Poster A

Effects of p-doping on charge carrier concentration and charge carrier transport in organic-inorganic composite thin layers — •Carsten Leinweber[1,2], Diana Nanova[1,2], Daniela Donhauser[1,4], Eric Mankel[2,3], Wolfgang Kowalsky[1,2,4], Uli Lemmer[5], and Norman Mechau[2,5] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Germany — [2]InnovationLab, Heidelberg, Germany — [3]Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany — [4]Institut für Hochfrequenztechnik, Technische Universität Braunschweig, Germany — [5]Lichttechnisches Institut, Karlsruhe Institute of Technology, Germany

Understanding the influence of doping on conductivity, mobility and charge carrier concentration is one of the main challenges towards high-efficiency organic devices. It has been shown that p-type doping of 4,4*-Bis(N-carbazolyl)-1,1*-biphenyl (CBP) with transition metal oxides like MoO3 increases the bulk conductivity of the organic layer. However, a very low doping efficiency for various mixing ratios has been observed. Therefore, we investigated the electronic properties of thermally co-evaporated layers with different doping concentrations using charge extraction by linearly increasing voltage (CELIV). In the CELIV technique charge carriers are extracted by a linearly increasing voltage pulse in reverse bias over a non-injecting contact. From the resulting current transient charge mobilities and charge carrier densities were determined. Furthermore, we correlated our investigations to morphology studies on the dopant distribution to understand the fundamentals of the underlying doping mechanism and its low efficiency.

HL 28.22 Mon 16:00 Poster A

Optical conductivity of the Anderson model calculation using Kernel Polynomial Method — •Paul Wenk[1], John Schliemann[1], and Georges Bouzerar[2] — [1]Institut I - Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany — [2]Institut Néel, 25 avenue des Martyrs, B.P. 166, 38042 Grenoble Cedex 09, France

We investigate the optical conductivity of a three-dimensional system with non-interacting electrons in a random potential (Anderson model) in linear response.[1] The application of the Chebyshev expansion method[2,3] allows for the analysis of large systems at finite temperatures. However, an improper choice of expansion cutoff and Fermi-Energy can lead to unphysical results - not only concerning negative Drude weights. By applying the f-sum rule[4] and a precise analysis of the spectrum degeneracies we resolve the conductivity-artifacts and calculate the suppression of the Drude weight as a function of impurity strength, the Drude weight being the order-parameter for the Metal-Insulator transition.

[1] P. Wenk *et al.* in prep. (2013)
[2] A. Weiße *et al.* Rev. Mod. Phys. **78**, 275 (2006)
[3] A. Weiße Eur. Phys. J. B **40**, 125 (2004)
[4] G. Bouzerar *et al.* Phys. Rev. B **49**, 12 (1994)

HL 28.23 Mon 16:00 Poster A

Metal complexes and organic radicals as electronic components — •Karin Goss, Simon Seyfferle, Martin Dressel, and Lapo Bogani — 1. Physikalisches Institut, Universität Stuttgart

Using molecules as building blocks for electronic devices offers ample possibilities for new device functionalities due to a chemical tunability much higher than that of standard inorganic materials, and, at the same time, offers a decrease in the size of the electronic component down to the single-molecule level. Metal clusters with an organic shell are a very versatile playground since both the metallic ions as well as the organic ligands can be chemically tuned to fulfill a particular functionality. For example, metallic ions can induce magnetism in the system on a single-molecular basis and ligands can be tailored to increase the affinity for binding to metallic electrodes or other organic material. But also purely organic molecules containing no metallic centers can serve as an electronic component. We present our results on electronic devices based on magnetic materials of different kind and functionality. We show the conducting behaviour of several sample layouts, all of which contain a molecular material as the functional element, and we provide a correlation between the electronic behaviour and the pre-designed chemical functionality. In particular, organic radical molecules can be reversibly switched between two oxidation states by applying a bias voltage across a thin layer of molecular material. Some members of this family of molecules also offer spintronic applications, which can be probed by injecting and detecting spin-polarized electrons with ferromagnetic leads.

HL 28.24 Mon 16:00 Poster A

Wigner solid phases near fractional and integer Landau level filling — •Guenther Meissner and Uwe Schmitt — Department of Physics, Saarland University, P.B.O. 151150, D-66041 Saarbruecken, Germany

Electrons in a high magnetic field are quasi two-dimensional (2D) due to the perpendicular cyclotron motion. If the cyclotron radius becomes less than half of the mean distance of the electrons, Wigner solid formation may minimize their Coulomb repulsion. Since the Cartesian components of the guiding center positions of the cyclotron motion turn out to be non-commuting (because of the magnetic vector potential), their density fluctuations are non-commuting, too. Correlation functions of these two quantities have thus been used for studying quantitatively the nature of Coulomb-interacting 2D electrons at high magnetic fields [1]. Here, it will be shown how recent observations of Wigner solid pinning modes [2] near the fractional filling factor 1/3 and the integer filling factor 1 of the Landau levels exhibiting the fractional respectively integer quantum Hall effect could be explained in our many-body approach via Chern-Simons magnetic fields. [1] G. Meissner, Physica B 184,66 (1993).[2] H. Zhu, Y.P. Jiang, L.W. Engel, D.C. Tsui, L.N. Pfeiffer, and K.W. West, Phys Rev. 105, 12608 (2010) and references therein.

HL 28.25 Mon 16:00 Poster A

Application of $CuInS_2$ nanocrystals in hybrid and Schottky-type solar cells — •Katja Frevert, Florian Witt, Nikolay Radychev, Dorothea Scheunemann, Marta Kruszynska, Rany Miranti, Joanna Kolny-Olesiak, Holger Borchert, and Jürgen Parisi — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory (EHF), 26111 Oldenburg, Germany

So called hybrid solar cells built from blends of conductive polymers and inorganic nanoparticles are a possible candidate to improve the performance of solution processed thin film photovoltaics. In most studies on this topic toxic nanoparticle compounds like CdSe or PbS are used. Here we demonstrate results with less toxic $CuInS_2$(CIS)

nanocrystals. CIS offers advantages such as high absorption coefficients in the visible range, size-dependent spectral bandwidth, and suitable charge transport properties. We will show the influence of stabilizing ligands on the morphology of the active layer and the electrical characteristics of hybrid solar cells based on elongated and pyramidal CIS nanocrystals blended with poly(3-hexylthiophene) (P3HT). Another approach for solution processed photovoltaic devices involves all inorganic nanoparticle Schottky-type solar cells. Here thin films of CIS nanoparticles are deposited layer-by-layer and finished by a suitable top electrode like aluminum. We will show first results from an early stage of this development.

HL 28.26 Mon 16:00 Poster A

Influence of Förster interaction on the light emission statistics of hybrid systems — •T. Sverre Theuerholz, Alexander Carmele, Marten Richter, and Andreas Knorr — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany

Hybrid systems consisting of semiconductor quantum dots (SQD) and metallic nanoparticles (MNP) are in the focus of current experimental and theoretical [1] research, since they may combine the advantages of both constituents.

In our contribution, we theoretically investigate a hybrid system of two SQDs and a MNP driven by coherent light. Within our theoretical framework, we focus on the second-order correlation plasmon-plasmon function $g^{(2)}$ and its dependency on the external field and on the internal interactions between the constituents. We find, that even relatively weak internal interactions, like the Förster coupling [2] between the SQDs, can have a significant impact on the second-order correlation function. Since the strength of this coupling depends on the size, shape and distance between the SQDs, it can be engineered to tune the $g^{(2)}$-function. We also investigate how MNPs in the vicinity of SQDs influence the Förster interaction between the dots.

[1] A. Ridolfo, O. Di Stefano, N. Fina, R. Saija and S. Savaste, Phys. Rev. Lett. 105 (26), (2010)

[2] J. Danckwerts, K. J. Ahn, J. Förstner and A. Knorr, Phys. Rev. B 73 (16), (2006)

HL 28.27 Mon 16:00 Poster A

Purcell effect in rolled-up active hyperbolic metamaterials — •Marvin Schulz, Hoan Vu, Stephan Schwaiger, David Sonnenberg, Christian Heyn, and Stefan Mendach — Institute of Applied Physics, University of Hamburg, Jungiusstraße 11, 20355 Hamburg, Germany

Using the relaxation process of strained semiconductor layers [1] we fabricate microtubes whose walls represent three-dimensional hyperbolic metamaterials consisting of alternating semiconductor ((Al)(In)GaAs) and metal (Ag) layers [2]. Here, we investigate the Purcell effect for a GaAs quantum well embedded in the semiconductor compound of the metamaterials [3]. We varied the Ag/GaAs thickness ratio $\eta = d\_(Ag)/d\_(GaAs)$ to tune the anisotropic effective permittivity tensor of the metamaterial at the quantum well emission energy (1.63 eV). Time-resolved photoluminescence measurements reveal a sharp decrease of the embedded quantum well's lifetime τ from $\tau = 430$ ps for metamaterials with $\eta < 0.53$ to $\tau = 250$ ps for metamaterials with $\eta > 0.53$. This well corresponds to an increase of the photon density of states as expected at the transition to the hyperbolic dispersion regime [4, 5]. The authors acknowledge financial support by the Deutsche Forschungsgemeinschaft via Graduiertenkolleg 1286.

[1] V. Ya. Prinz et al., Physica E 6, 828 (2000).
[2] S. Schwaiger et al., Phys. Rev. Lett. 102, 163903(2009).
[3] S. Schwaiger et al., Phys. Rev. B 84, 155325 (2011).
[4] M. A. Noginov et al., Opt. Lett. 35, 1863 (2010).
[5] T. Tumkur et al., Appl. Phys. Lett. 99, 151115 (2011).

HL 29: Poster Session: Spintronics; Spin-controled transport; Topological insulators; Interfaces / Surfaces; Magnetic semiconductors

Presenters are kindly asked to be near their posters at least 17:00–18:00 or to leave a note at the poster indicating a time period of availability for discussions. — Beverages will be served starting at 18:00.

Time: Monday 16:00–20:00 Location: Poster A

HL 29.1 Mon 16:00 Poster A

Spin noise spectroscopy at ultra low temperatures — •Jan Gerrit Lonnemann, Jens Hübner, and Michael Oestreich — Institute for Solid State Physics, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany

In recent years the all optical method of semiconductor spin noise spectroscopy (SNS) has proven to be a powerful tool to investigate spin dependent processes in semiconductors [1]. Especially at low temperatures most optical methods obscure the real spin dynamics due to carrier heating and excitation. SNS on the other hand utilizes off-resonant Faraday rotation for probing the intrinsic spin fluctuations at thermal equilibrium.

Consequently SNS is ideally suited to analyze systems at ultra low temperatures due to its perturbation free nature. We present measurements performed at temperatures as low as 100 mK. At these very low temperatures we try to gain access to spin physics obscured otherwise like for example quantum phase transitions, magnetic ordering, or highly localized states. The investigated GaAs sample is doped slightly below the metal-to-insulator transition [2] and shows localization of the donor electrons especially below 1 K. We observe a strong negative shift of the electron g-factor with increasing temperature while in the same sample the opposite dependence is observed above 10 K, where the donors are delocalized. The intrinsic spin lifetime of the weakly localized electrons is measured to be well above 300 ns.

[1] G.M. Müller, *et al.*, *Physica E* **43**, 569 (2010).
[2] M. Römer, *et al.*, *Phys. Rev. B* **81**, 075216 (2010).

HL 29.2 Mon 16:00 Poster A

Spin Noise Spectroscopy at Single Photon Intensities — •Julia Wiegand[1], Ramin Dahbashi[1], Xavier Marie[2], Klaus Pierz[3], Hans Werner Schumacher[3], Jens Hübner[1], and Michael Oestreich[1] — [1]Insitute for Solid State Physics, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany — [2]Université de Toulouse, INSA, UPS, CNRS; LPCNO, 135 avenue de Rangueil, F-31077 Toulouse, France — [3]Physikalisch Technische Bundesanstalt, Bundesallee 100, D-38116 Braunschweig, Germany

Spin noise spectroscopy is capable of performing quantum nondemolition measurements of spin dynamics by off-resonant optical probing [1]. However, recent reports on heavy-hole spin dephasing in self-assembled (InGa)As quantum dots (QDs) show a non-negligible influence of the probe beam intensity on the dephasing time. This is due to residual light absorption disturbing the equilibrium [2].
A Hanbury Brown and Twiss type detection setup is implemented for single QD photoluminescence detection. This setup is further modified in order to enable Faraday fluctuation measurements by single photon counting which, in principle, provides access to the truly undisturbed spin dynamics by preventing light absorption.

[1] Müller *et al.*, Semiconductor spin noise spectroscopy: Fundamentals, accomplishments, and challenges, Physica E **43**, 569 (2011).
[2] Dahbashi *et al.*, Measurement of heavy-hole spin dephasing in (InGa)As quantum dots, Appl. Phys. Lett. **100**, 031906 (2012).

HL 29.3 Mon 16:00 Poster A

First Steps towards Spin Noise Spectroscopy in Sillicon — •André Grieger, Jan Gerrit Lonnemann, Jens Hübner, and Michael Oestreich — Insitute for Solid State Physics, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany

Semiconductor spin noise spectroscopy (SNS) has evolved as a powerful experimental technique to explore spin dynamics in close vicinity to thermal equilibrium [1]. Not beeing masked by optical excitations SNS is a very verstile technique that uses off resonant Faraday rotation and consequently avoids carrier heating and optical excitation.

SNS has already been utilized to analyse the spin dynamics of conduction electrons in GaAs [2]. Recent measurements have been per-

formed on highly n-doped ($10^{17} cm^{-3}$) bulk GaAs at a temperature of 20 K in dependence on the applied magnetic field (0-8T) with integration times below 5 minutes [3]. We are extending SNS to silicon which is doped well above the metal isolator transition. The theoretical calculations of the selection rules in silicon are difficult due to the indirect band gap of sillicon where transitions between valence and conduction band are phonon-assisted processes [4]. The expected long integration times require a very stable experimental setup. Thus steps taken towards such a long-term stable system will be presented.

[1] Georg M. Müller et al.; *Physica E*, **43**, 569 (2010).
[2] M. Römer et al., *Rev. Sci. Instrum.*, **78**, 103903 (2007).
[3] F. Berski et al., *arXiv*, 1207.0081 (2012).
[4] J.L. Cheng et al., *Phys. Rev. B*, **83**, 165211 (2011).

HL 29.4 Mon 16:00 Poster A

Spin Noise Spectroscopy - towards solid-state entanglement — •Agnes Beichert[1], Fabian Berski[1], Andreas D. Wieck[2], Jens Hübner[1], and Michael Oestreich[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany — [2]Angewandte Festkörperphysik, Ruhr-Universität Bochum, Universitätsstr. 150, D-44780 Bochum, Germany

In the context of quantum information processing dopants in semiconductor hosts are attractive candidates for providing a sufficient number of indistinguishable pure states on a nanoscale level [1]. Entanglement can be used to build up a non-local interaction between these states.

First, spin noise spectroscopy (SNS) is applied as a quantum nondemolition measurement to determine the temporal limit for coherent manipulation of the system state. Therefore, the spin dynamics of localised donor bound electron spins in GaAs is examined. The experiment shows spin dephasing dominated by hyperfine coupling [2].

Next, we want to expand the experiment to create entanglement between a solid state spin ensemble. Subsequently, we plan to use density matrix tomography to verify the prepared state [3].

[1] K.-M. C. Fu et al., *Millisecond spin-flip times of donor-bound electrons in GaAs*, Phys. Rev. B **74**, 121304(R) (2006).
[2] G. M. Müller et al., *Semiconductor spin noise spectroscopy: Fundamentals, accomplishments, and challenges*, Physica E **43**, 569 (2010).
[3] S. Simmons et al., *Entanglement in a solid-state spin ensemble*, Nature **470**, 69 (2011).

HL 29.5 Mon 16:00 Poster A

Anomalous spin diffusion in high-mobility (110) GaAs-based quantum wells — •Markus Schwemmer[1], Roland Voelkl[1], Tobias Korn[1], Michael Griesbeck[1], Sergey Tarasenko[2], Dieter Schuh[1], Werner Wegscheider[3], and Christian Schueller[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

We have performed spin diffusion measurements in high-mobility two-dimensional electron systems embedded in a symmetrical GaAs/AlGaAs quantum well grown in [110] direction. For mapping the diffusion of spin-polarized electrons in the sample and to determine the corresponding spin lifetimes, we use a two-beam Hanle-MOKE method. The spin diffusion was studied by moving the pump beam with respect to the probe beam using a motorized mirror. With this technique we could observe diffusion lengths as high as 50 μm for low temperatures. The diffusion length was constant over a wide temperature range (4 - 40 K). Due to a reduced influence of the photogenerated holes, a maximum of the net spin polarization is observed at a distance of a few μm away from the pump spot. Additionally, we manipulated the resident electron density by above-barrier-illumination and investigated its effect on the diffusion length. Financial support by the DFG via SFB 689 and SPP 1285 is gratefully acknowledged.

HL 29.6 Mon 16:00 Poster A

Spin dynamics in high-mobility two-dimensional electron systems embedded in GaAs/AlGaAs quantum wells — •M. Griesbeck[1], M. Glazov[2], E. Sherman[3], T. Korn[1], D. Schuh[1], W. Wegscheider[4], and C. Schüller[1] — [1]Department of physics, Regensburg university, Germany — [2]Ioffe Physical-Technical Institute, St. Petersburg, Russia — [3]Department of Physical Chemistry, University of the Basque Country, Bilbao, Spain — [4]ETH Zürich, Switzerland

Advances in the technology of GaAs/AlGaAs based heterostructures allow for the design of high quality and well-defined two-dimensional electron systems (2DES), which are perfectly suited for the study of the underlying physics that govern the dynamics of the electron spin system. In this work, spin dynamics in high-mobility 2DES is studied by means of the all-optical time-resolved Kerr/Faraday rotation technique. In (001)-grown 2DES, an in-plane spin dephasing anisotropy is studied, resulting from the interference of comparable Rashba and Dresselhaus contributions to the spin-orbit field (SOF). The dependence of this anisotropy on the confinement length of the 2DES, the sample temperature and the carrier density is demonstrated. Moreover, coherent spin dynamics of an ensemble of ballistically moving electrons is studied within a weak magnetic field applied perpendicular to the sample plane, which forces the electrons to move on cyclotron orbits. Finally, anisotropic spin dynamics is investigated in symmetric (110)-grown 2DES, using the resonant spin amplification method. In such systems, very long out-of-plane spin dephasing times can be achieved, in consequence of the special symmetry of the Dresselhaus SOF.

HL 29.7 Mon 16:00 Poster A

Magnetometry on spin-orbit effects in InGaAs/InP quantum wells — •Ayman Ibrahim[1], Florian Herzog[1], Benedikt Rupprecht[1], Marc Wilde[1], Thomas Schäpers[2], Hilde Hartdegen[2], Sebastian Heedt[2], Christian Heyn[3], and Dirk Grundler[1] — [1]Physik.-Dep. E10, TU München, D-85748 Garching — [2]Peter Grünberg Institute (PGI-9), FZ Jülich, D-52425 Jülich — [3]Institute of Applied Physics, University of Hamburg, D-20355 Hamburg

Spin-orbit coupling provokes beating patterns in both magnetic field dependent resistance (MR) and magnetization (MAG) measurements performed on a two-dimensional electron system (2DES) at low temperature. Recently, we have found an unexpected frequency shift and phase anomaly in the quantum oscillations when comparing separately conducted MR and MAG experiments. To understand the anomaly in detail, we aim at performing both experiments simultaneously on one-and-the-same 2DES. For this, we prepare a micromechanical torque magnetometer with integrated electrical contacts and mount the 2DES using a conductive bonding technique. We report our latest results. Financial support by the DFG via GR1640/3 in SPP 1285 "Semiconductor Spintronics" and NIM is gratefully acknowledged.

HL 29.8 Mon 16:00 Poster A

Full cancellation of the Spin-Orbit field in (110) GaAs/AlGaAs Quantum Wells via the application of strain — •Arthur Varkentin[1], David English[1], Richard Harley[2], Jens Hübner[1], and Michael Oestreich[1] — [1]Institute for Solid State Physics, Leibniz University Hannover, Appelstr. 2, 30167 Hannover, Germany — [2]School of Physics and Astronomy, University of Southampton, Southampton, SO17 1BJ, UK

We present measurements of the spin relaxation rate Γ^s in (110) GaAs/AlGaAs quantum wells (QW). QW grown parallel to the (110) axis offer the unique opportunity to completely suppress the usually dominant Dyakonov-Perel (DP) spin relaxation mechanism via the application of strain [1]. The DP mechanism occurs because the electrons sense a momentum dependent spin-orbit field that is randomised due to the thermal motion of the electrons [2]. The bulk contribution to the spin orbit field for (110) QW is aligned along the growth axis z. This results in the suppression of DP for electron spin populations initially aligned parallel to z [3]. The exciting property of (110) QW is that the strain contribution to the spin-orbit field is also aligned parallel to z [1]. The application of strain can potentially cancel all spin-orbit fields and thus completely suppress DP spin relaxation for all orientations of electron spins.

[1] S.-W. Chang & S.-L. Chuang, Phys. Rev. B, **72** (2005).
[2] M. I. Dyakonov & V. I. Perel, Sov. Phys. Sol. St., **13**, 3023 (1972).
[3] Y. Ohno *et al.* & H. Ohno, Phys. Rev. Lett., **83**, 4196 (1999).

HL 29.9 Mon 16:00 Poster A

Charge and spin dynamics in quantum wells under surface acoustic waves — •Johannes Wanner, Cosimo Gorini, Peter Schwab, and Ulrich Eckern — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Various recent experiments have shown the flexibility of surface acoustic waves as a mean for transporting charge and spin in quantum wells [1]. In particular, they 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 surface acoustic wave. A number of experimentally observed features can thus be explained.

[1] J. A. H. Stotz et al., Nat. Mat. **4**, 585 (2005); H. Sanada et al., Phys. Rev. Lett. **106**, 216602 (2011)
[2] P. Schwab et al., Phys. Rev. B **74**, 155316 (2006)

HL 29.10 Mon 16:00 Poster A

Magnetic-Field Contol of Photon Echo from the Electron-Trion System in a CdTe Quantum Well: Shuffling Coherence between Optically Accessible and Inaccessible States — •Lukas Langer[1], Sergey V. Poltavtsev[1,2], Irina A. Yugova[1,2], Dmitri R. Yakovlev[1,3], Grzegorz Karczewski[4], Tomasz Wojtowicz[4], Jacek Kossut[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

We report on magnetic field-induced oscillations of the photon echo signal from negatively charged excitons in a CdTe/(Cd,Mg)Te semiconductor quantum well. The oscillatory signal is due to Larmor precession of the electron spin about a transverse magnetic field and depends sensitively on the polarization configuration of the exciting and refocusing pulses. The echo amplitude can be fully tuned from the maximum down to zero depending on the time delay between the two pulses and the strength of the magnetic field. The results are explained in terms of the optical Bloch equations accounting for the spin level structure of electrons and trions.

HL 29.11 Mon 16:00 Poster A

Spin Dynamics of Heavy-Holes in (InGa)As Quantum Dots — •Ramin Dahbashi[1], Julia Wiegand[1], Xavier Marie[2], Klaus Pierz[3], Hans Werner Schumacher[3], Jens Hübner[1], and Michael Oestreich[1] — [1]Insitute for Solid State Physics, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany — [2]Université de Toulouse, INSA, UPS, CNRS; LPCNO, 135 avenue de Rangueil, F-31077 Toulouse, France — [3]Physikalisch Technische Bundesanstalt, Bundesallee 100, D-38116 Braunschweig, Germany

The spin dynamics of heavy-holes confined in (InGa)As quantum dots (QDs) are of particular interest for future applications in solid state quantum information processing. We employ spin noise spectroscopy as a quantum non-demolition experiment to get access to the intrinsic spin dynamics [1]. The spin noise method is transferred from ensembles of QDs [2] to single dot heavy-hole measurements. Numerical simulations show an extremely long spin dephasing time if light absorption is negligible [2]. The investigated QDs are characterized by polarization resolved photoluminescence measurements and via a Hanbury Brown-Twiss setup. The discharging of the QDs via Auger recombination due to residual light absorption is deactivated by co-pumping the dots with low intensity light.

[1] Müller *et al.*, Semiconductor spin noise spectroscopy: Fundamentals, accomplishments, and challenges, Physica E **43**, 569 (2011).
[2] Dahbashi *et al.*, Measurement of heavy-hole spin dephasing in (InGa)As quantum dots, Appl. Phys. Lett. **100**, 031906 (2012).

HL 29.12 Mon 16:00 Poster A

Optical spin polarization of donor electrons through donor bound exciton states in ZnO — Sebastian Kuhlen[1], •Ralph Ledesch[1], Christoph Schwark[1], Vera Klinke[1], Christian Weier[1], Gernot Güntherodt[1], Matthias Althammer[2], Sebastian T. B. Gönnenwein[2], Matthias Opel[2], Rudolf Gross[2], Thomas Wassner[3], Martin S. Brandt[3], and Bernd Beschoten[1] — [1]II. Physikalisches Institut A, RWTH Aachen University, Aachen — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching — [3]Walther Schottky Institut, Technische Universität München, Garching

ZnO exhibits a large variety of natural dopants, which present a promising playground for coherent spintronics as each donor type presents an individual spin state with different spin lifetimes and Landé factors. Furthermore, long spin dephasing times as high as 20 ns have been observed. We demonstrate that the electrons can be polarized by optical pumping and detected using the Faraday effect in a standard pump-probe experiment. We furthermore observe that the polarization mechanism is most effective when the pump photon energy matches one of various donor bound exciton state energies, while the spin dephasing time exceeds the exciton lifetime by several orders of magnitude. Hence we conclude that electron spins are polarized by optical selection rules during the transition to the exciton state, but are eventually transferred to the donor electron of the impurity to which the exciton has been bound.

Work supported by DFG through SPP 1285.

HL 29.13 Mon 16:00 Poster A

Spin manipulation in spin light-emitting diodes: electron spin resonance in the ZnMnSe spin aligner — •Franziska Reiter, Andreas Merz, Robert Schittny, Benjamin Wolter, Daniel Rülke, Heinz Kalt, and Michael Hetterich — KIT, Karlsruhe, Germany

We investigate the possibility to perform electron spin resonance experiments within a spin-injection light-emitting diode. The latter contains a ZnMnSe spin aligner for spin injection into single optically active InGaAs quantum dots with a spin polarization degree of up to 100% [1]. For the manipulation experiments, a specially prepared spin light-emitting diode is placed in a microwave cavity and is exposed to microwave pulses with different powers and frequencies. At 53 GHz we observe the resonance of the manganese ions in the ZnMnSe spin aligner at 2 T via optically detected magnetic resonance in the photo luminescence signal. Furthermore, this influence is optimized towards coherent manipulation of spin states and spin injection into single quantum dots. This method could pave the way towards future spin manipulation experiments in such semiconductor structures.

[1] W. Löffler et al., Appl. Phys. Lett. 90, 232105 (2007).

HL 29.14 Mon 16:00 Poster A

A novel metastable spin triplet in diamond — •Matthias Widmann[1], Sang-Yun Lee[1], Helmut Fedder[1], Torsten Rendler[1], Moritz Eyer[1], Sen Yang[1], Petr Siyushev[1], Marcus Doherty[2], and Jörg Wrachtrup[1] — [1]3. Physikalisches Institut, University Stuttgart, Germany — [2]Laser Physics Center, National University, Canberra, Australia

The poster introduces a newly found, photo stable single spin center in a HTHP diamond nano-pillar. This new defect poses many properties, similar to those of the well-known NV-center in diamond. However, optically detected magnetic resonance showed positive contrast at room temperature in contrast to NV-centers. The photo physics and spin physics of this new defect have been studied to understand the enhancement of photon emission (contrast up to 45 %) at three different electron spin resonance frequencies. It will be shown that the defect contains a singlet ground-, and excited state, and a metastable spin 1 triplet state which act as a shelving state. The strong enhancement of photon emission by ESR can be attributed to the huge difference in the deshelving rates of each triplet states. It will be also shown that the coherent spin manipulation of the metastable triplet state is possible at room temperature. Even though the electron spin coherence time is limited by the life time of the triplet state (up to 2.5 μs), these findings suggest that the electron spin in this spin system can be used to read-out the coupled nuclear spin state because the nuclear spin can be protected during the initialization and storage processes thanks to the spin-less electron ground state.

HL 29.15 Mon 16:00 Poster A

Inverse spin Hall effect in p-GaAs nanostructures — •Markus Ehlert[1], Thomas Hupfauer[1], Cheng Song[1,2], Martin Utz[1], Dominique Bougeard[1], and Dieter Weiss[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, D-93040 Regensburg, Germany — [2]Laboratory of Advanced Materials, Department of Material Science & Engineering, Tsinghua University, Beijing 100084, China

We performed experiments with "H-geometry" structures in lightly doped p-GaAs (4×10^{16} cm^{-3}), which allow for inverse spin Hall effect (ISHE) measurements without using ferromagnetic contacts [1]. A current is driven in the first branch of the "H" to create a spin current via direct spin Hall effect, which then leads to a charge accumulation in the adjacent branch of the "H" due to ISHE. External magnetic field, either *in-plane* or *out-of-plane*, is applied to induce spin precession and modulate the resulting signal. From analysis we mainly identify classical transport mechanisms being responsible for detected large ISHE-like signal, as previously reported [2]. A small underlying contribution is presumably related to thermally induced effects, due to

the small width of our conduction channels (300 nm), and cannot be unambiguously attributed to ISHE. This work was supported by DFG SPP1285.

[1] E. M. Hankiewicz *et al.*, Phys. Rev. B **70**, 241301(R) (2004).
[2] G. Mihajlović *et al.*, Phys. Rev. Lett. **103**, 166601 (2009).

HL 29.16 Mon 16:00 Poster A

Modification of spin dynamics in ion-implanted wurtzite semiconductors — •Jago Döntgen[1], Jan Heye Buss[1], Jörg Rudolph[1], Stepan Shvarkov[2], Andreas D. Wieck[2], and Daniel Hägele[1] — [1]AG Spektroskopie der kondensierten Materie, Ruhr-Universität Bochum, Germany — [2]Angewandte Festkörperphysik, Ruhr-Universität Bochum, Germany

The wide-gap wurtzite semiconductors GaN and ZnO possess high potential for opto-electronics as well as high-frequency and high-power electronics. Their spin-related properties are in the focus of intense research originally motivated by theoretical predictions of ferromagnetism above room-temperature in rare-earth- or transition-metal-doped material [1]. We use time-resolved Kerr-Rotation spectroscopy to investigate electron spin oscillations in a magnetic field after implantation of GaN with Gadolinium and coimplantation with Si. We find strongly increased spin lifetimes for moderate Gd-implantation doses and a transition to isotropic spin relaxation from the anisotropic case known from unimplanted GaN [2]. The increased spin lifetimes in combination with the disappearance of anisotropy is a fingerprint of localized defect-states caused by implantation with Gd. An enhanced alignment of electron spins along the magnetic field by Gd could not be observed.

[1] T. Dietl *et al.*, Science **287**, 1019 (2000)
[2] J. H. Buss *et al.*, Appl. Phys. Lett. **95**, 192107 (2009)

HL 29.17 Mon 16:00 Poster A

The topological insulator HgTe - grown on GaAs substrates — •Philipp Leubner, Christopher Ames, Maximilian Kessel, Hartmut Buhmann, and Laurens Molenkamp — Phys. Inst. (EP III), Univ. Würzburg, D-97074 Würzburg, Germany

In the past few years MBE-grown HgCdTe/HgTe heterostructures have revealed to be suitable systems to study the magnetotransport properties of both two-dimensional topological insulators [1] with spin polarized edge channels [2] and just recently of three-dimensional topological insulators [3].

In this work we present the successful change of substrate material. So far, growth has been carried out on either CdTe or CdZnTe, with both systems being limited with respect to wafer size and pricing. By growing a ZnTe/CdTe heterostructure on GaAs substrates, we were able to prepare a high-quality <001> CdTe surface, as revealed by RHEED, AFM and HRXRD measurements. The subsequently grown HgCdTe/HgTe quantum-well systems showed carrier mobilities comparable to such grown on commercial CdTe substrates.

The new material system allows not only a much higher yield in working wafer size per growth run, but offers also new possibilities with respect to backgating, doping and lattice-matching and avoids the problematic wet-etching needed to prepare CdTe and CdZnTe prior to growth.

[1] König et. al., Science 318 766 (2007)
[2] Brüne et. al., Nature Phys. 8 485 (2012)
[3] Brüne et. al., Phys .Rev. Lett. 106 126803 (2011)

HL 29.18 Mon 16:00 Poster A

MBE - growth of capped, strained HgTe, a 3D topological insulator — •Christopher Ames, Philipp Leubner, Christoph Brüne, Hartmut Buhmann, and Laurens Molenkamp — Universität Würzburg, D-97074 Würzburg, Germany

The discovery of two (2D) [1] and three dimensional (3D) [2] topological insulator (TI) behavior in HgTe - systems opens a large field for studying magneto transport properties of both.

We grow HgTe as a 3D topological insulator by molecular beam epitaxy. Unstrained bulk HgTe is a semimetal but opens a gap of roughly 22 meV when grown fully strained on <001> CdTe substrate due to 0.3 % lattice mismatch and shows magnetotransport properties of a 3D TI. Hall measurements show electron mobilities of around 50.000 cm^2(V s)^-1. To increase electron mobilities, various growth optimizations have been carried out. Firstly we grew an HgCdTe buffer layer between the substrate and bulk HgTe. Different buffer thicknesses were analyzed ex-situ by HRXRD, AFM and standard Hall measurements. Secondly, we added a cap-layer of HgCdTe on top of the bulk HgTe. Doing so, we were able to raise the electron mobility of the bulk HgTe up to one order of magnitude. Time-dependent XPS measurements allowed us to hold the suppressed oxidization of the surface responsible for this effect.

Through the advanced material quality we have now more prospects for better understanding of the transport properties in strained HgTe.

[1] König et. al., Science 318 766 (2007)
[2] C. Brüne et. al., Phys. Rev. Lett. 106 126803 (2011)

HL 29.19 Mon 16:00 Poster A

Growth of High-Mobility Bi_2Te_2Se Nanoplatelets on hBN Sheets by van der Waals Epitaxy — •Pascal Gehring[1], Bo Gao[1], Marko Burghard[1], and Klaus Kern[1,2] — [1]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — [2]Institute de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

The electrical detection of the surface states of topological insulators is strongly impeded by the interference of bulk conduction, which commonly arises due to pronounced doping associated with the formation of lattice defects. As exemplified by the topological insulator Bi_2Te_2Se, we show that via van der Waals epitaxial growth on thin hBN substrates the structural quality of such nanoplatelets can be substantially improved. The surface state carrier mobility of nanoplatelets on hBN is increased by a factor of about 3 compared to platelets on conventional Si/SiO_x substrates, which enables the observation of well-developed Shubnikov-de Haas oscillations. We furthermore demonstrate the possibility to effectively tune the Fermi level position in the films with the aid of a back gate.

HL 29.20 Mon 16:00 Poster A

Synthesis of topological insulators at the nanoscale — •Christian Nowka[1], Silke Hampel[1], Udo Steiner[2], Lars Giebeler[1], Jochen Geck[1], Jorge E. Hamann Borrero[1], Sandeep M. Gorantla[1], Andreas Teichgräber[1], Romain Giraud[1], Joseph Dufouleur[1], and Bernd Büchner[1] — [1]Institute of Solid State Research - IFW Leibniz institute, Helmholtzstr. 20, D-01069 Dresden — [2]Hochschule für Technik und Wirtschaft Dresden, Friedrich-List-Platz 1, D-01069 Dresden

In this work we investigated the growth of Bi_2Se_3 topological insulator by gasphase transports. The obtained crystals have been characterized by SEM, TEM, AFM, EDX and XRD. To understand the growth mechanisms we performed thermodynamic modelling with the program Tragmin. The experimental growth of Bi_2Se_3 has been simply done by decomposition sublimation. By synthesis of Bi_2Se_3-layers thin ($\approx$ 10 nm), singlecrystalline crystals was deposited on the Si/SiO_2–substrate. For instance nanoribbons with a crystal size in a, b–direction between 3–40 μm and up to 70 μm for nanowires. The manganese-doped Bi_2Se_3 crystals were grown by chemical transport reaction. For this purpose powder of Mn/Bi/Se with different Mn content and Iodine as a transport agent was used. Several experiments showed the possibility of a gasphase transport of Mn/Bi/Se-powder with a high Mn content in a gradient $\triangle T < 100\ K$. In this case, crystals of $MnBi_2Se_4$ was deposited on the Si/SiO_2–substrate.

HL 29.21 Mon 16:00 Poster A

Group theoretical and topological analysis of the band structure of silicene — •Florian Geissler[1], Jan Carl Budich[2], and Björn Trauzettel[1] — [1]Institute for Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany — [2]Department of Physics, Stockholm University, Se-106 91 Stockholm, Sweden

Silicene is a monolayer of silicon atoms in a buckled honeycomb structure. It was recently shown, that a perpendicular electric field is able to couple to the sublattice pseudospin, allowing to electrically tune and close the band gap. Increasing electric fields may therefore generate a topological phase transition from a topological insulator to a normal insulator or semimetal. We perform a group theoretical analysis to systematically construct the Hamiltonian at the K-points of silicene by symmetries only. We discuss, that when further lowest-order terms are respected, the parameter space exhibiting a topological insulator phase is reduced. This is analyzed by an explicit calculation of the topological invariant of the underlying bandstructure.

HL 29.22 Mon 16:00 Poster A

Surface modification of ZnO bulk single crystals in vacuum

— •Lennart Fricke[1], Tammo Böntgen[1], Jan Lorbeer[2], Jörg Lenzner[1], Rüdiger Schmidt-Grund[1], and Marius Grundmann[1] — [1]Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig — [2]Leibniz-Institut für Oberflächenmodifizierung e.V., Permoserstr. 15, 04318 Leipzig

We discuss the modification of the surface of ZnO bulk single crystals under different environmental conditions. For that purpose, in-situ and ex-situ spectroscopic ellipsometry (SE) have been applied to get access to thin surface layers and the bulk as well as the surface near dielectric function. Ambient Atomic force microscopy (AFM) and scanning electron microscopy (SEM) have been used ex-situ to characterize the surface morphology and the electrical properties of the surface.

Commercial ZnO single crystals where pre-treated to exhibit atomically flat terraces with unit cell step heights. During exposition to low pressure conditions between 1 mbar and 10^{-2} mbar for 2 hours, a considerable change in the SE data was observed, revealing a irreversible change in the optical thickness of the surface near region of the samples. Applying lower pressure ($< 10^{-3}$ mbar) or nitrogen atmosphere, no change in the optical response was detected. In all cases, no distinct change in the surface morphology or AFM phase contrast have been observed. The change of SE data can be explained by adsorption or a structural rearrangement, that is hindered by the presence of adsorbates or surface water in atmospheric air, both leading to a change in the electronic configuration of the surface.

HL 29.23 Mon 16:00 Poster A

In situ observation of monolayer removal on Si(100) in H_2 ambient — •Sebastian Brückner[1,2], Peter Kleinschmidt[3], Oliver Supplie[2], Henning Döscher[1,2], and Thomas Hannappel[2,3] — [1]Helmholtz-Zentrum Berlin, Institut für Solare Brennstoffe — [2]TU Ilmenau, Institut für Physik, Fachgebiet Photovoltaik — [3]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, Erfurt

Step formation is crucial for subsequent heteroepitaxial growth of III-V semiconductors on Si(100). Single-layer steps on Si(100) are associated with the presence of two domains with different dimer orientations on the reconstructed surface, leading to the initiation of anti-phase domains (APDs) in the epitaxial III-V layer. Therefore, double-layer steps are required to prevent APD formation.

Here, we used reflection anisotropy spectroscopy (RAS) to study the preparation of Si(100) surfaces during chemical vapor deposition (CVD) processing. Interaction between H_2 process gas and Si(100) surface strongly influences the surface structure. Oscillations in the RAS signal during annealing in H_2 ambient indicate alternating formation of preferential A- and B-type domains on Si(100) due to Si removal. Based on scanning tunneling microscopy measurements we conclude that formation and anisotropic expansion of vacancies on the terraces induces a layer-by-layer removal mechanism. In situ RAS enables precise control of Si removal and domain formation on Si(100) surfaces.

HL 29.24 Mon 16:00 Poster A

Electronic Properties of Si/ZnO Interfaces by ab initio Quasiparticle Calculations — •Benjamin Höffling and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik and European Theoretical Spectroscopy Facility (ETSF), Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany

Transparent Conducting Oxides like ZnO are routinely used in Si-based photovoltaics. However, key electronic properties are still controversially discussed in the literature. Modern ab-initio simulations can help to address this problem.

The applicability of these methods rests on the construction of realistic atomic models for such systems. Modeling interfaces between materials with different crystal structures, bonding mechanisms and chemical character within the repeated-slab supercell method is a particularly difficult challenge.

We develop a method for the construction of atomic models of heterostructural interfaces based on coincidence lattices, maximum bond saturation, and total energy minimization, which enables us to construct model geometries for the interface between diamond structure Si and wurtzite-ZnO. In particular we investigate the Si(001)/ZnO(20-23) by means of density functional theory (DFT). We predict electronic properties of the interfaces using both DFT and modern quasiparticle theory based on semilocal exchange-correlation functionals. We examine band discontinuities and interface states. The influence of dangling bond passivation, strain, and charge transfer is studied by their respective influence on the electronic density of states.

HL 29.25 Mon 16:00 Poster A

Milli-Kelvin transport experiments on GaAs/(Ga,Mn)As core-shell nanowires — •Christian Butschkow[1], Elisabeth Reiger[1], Andreas Rudolph[1], Stefan Geissler[1], Dieter Schuh[1], Werner Wegscheider[2], and Dieter Weiss[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, D-93040 Regensburg, Germany — [2]ETH Zürich, 8093 Zürich, Switzerland

We performed transport measurements on ferromagnetic GaAs/-(Ga,Mn)As core-shell nanowires at temperatures T<1K. These nanowires were grown in a bottom-up process using molecular beam epitaxy and the Vapor-Liquid-Solid technique. The nanowires show a length of up to 4.5μm at a diameter of ∼100nm and a shell thickness of ∼30nm. For T<200mK we observe a pronounced localization of charge carriers resulting in an increase of the resistance by two orders of magnitude. This localization can be suppressed by applying a finite bias voltage or an external magnetic field. Additionally we observe conductance oscillations as a function of the magnetic field. The oscillations are observable for T<900mK, with increasing amplitude at lower temperatures. Considering previous investigations on (Ga,Mn)As nanostructures, fabricated lithographically from bulk material, it is likely that our observations can be ascribed to phase coherent transport effects. It was shown on lithographically defined nanowires of similar dimensions as the core-shell nanowires, that weak antilocalization like features as well as universal conductance fluctuations are observable [1].

[1] D. Neumaier et al. New Journal of Physics 10, 055016 (2008).

HL 29.26 Mon 16:00 Poster A

Anisotropic Magnetotransport in Mn doped, p-type InAs quantum wires — •Sabine Weishäupl[1], Ursula Wurstbauer[2], Werner Wegscheider[3], and Dieter Weiss[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D-93040 Regensburg — [2]Department of Physics, Columbia University, New York, USA — [3]Solid State Physics Laboratory, ETH Zurich, Zurich, Switzerland

The ratio of Rashba and Dresselhaus spin-orbit interaction strengths, α and β, can be deduced by measuring the conductance of narrow wires, where the weak antilocalization correction to the conductance is switched off. The in-plane magnetic field direction where the conductance displays a minimum is related directly to the ratio α/β [1].

Motivated by this proposal we have measured the conductance of quantum wires (widths w=150 nm, w=200 nm) in Mn doped, p-type InAs quantum wells as a function of magnetic field, topgate voltage and manganese concentration.

In the out-of-plane configuration, a strong localization in the low field regime is present. At higher fields the localization is lifted and Shubnikov-de-Haas oscillations start to appear. In the in-plane magnetic field, the wires feature an anisotropy which can be tuned by gate voltage, magnetic field strength and temperature.

We compare these samples with similar ones that have lower manganese concentration. With these, weak antilocalization is observed.

[1] M. Scheid et al., Phys. Rev. Lett. 101, 266401 (2008)

HL 29.27 Mon 16:00 Poster A

Anomalous Hall effect under the influcence of a metal-insulator transition in Mn doped InAs quantum wells — •Dieter Vogel, Christina Wensauer, Ursula Wurstbauer, Dieter Schuh, Werner Wegscheider, and Dieter Weiss — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

We report on magnetotransport studies in InAs:Mn quantum wells (QW), containing a two dimensional hole gas, which reveal a considerable anomalous Hall effect (AHE) in coexistence with a magnetic field driven insulator-to-metal transition. Earlier experimental and theoretical studies made clear that there are at least three different regimes for the behavior of AHE as a function of σ_{xx}[1]:(i) high conductivity regime (ii) good-metal regime (iii) bad-metal hoping regime. In our case a transition from $\sigma_{xy}^{(AH)} \propto \sigma_{xx}^{1.6}$ for the insulating regime to a good-metal regime, in which $\sigma_{xy}^{(AH)}$ is roughly independent of σ_{xx}, is observed. The scaling relation in the low-conductivity region is consistent with a recently developed theory of the anomalous Hall effect in the insulation regime [2]. Finally, we discuss the possibility to separate the intrinsic and the extrinsic scattering contribution in the good-metal regime following recent work by [3].

[1] N.Nagaosa et. al., Rev. Mod Phys. 82, 1539 (2010)
[2] X. Liu et. al., Phys. Rev. B 84, 165304 (2011)

[3] A. Shitade and N. Nagaosa, ArXiv ID 1109.5463 (2012)

HL 29.28 Mon 16:00 Poster A

Optical third-harmonic spectroscopy of the magnetic semiconductors EuSe and EuTe — •Marco Lafrentz[1], David Brunne[1], Benjamin Kaminski[1], Victor V. Pavlov[2], Andre B. Henriques[3], Roman V. Pisarev[2], Dmitri R. Yakovlev[1], and Manfred Bayer[1] — [1]Technische Universität Dortmund — [2]A. F. Ioffe Physical-Technical Institute — [3]Instituto de Física, Universidade de São Paulo

EuX (X=O, S, Se, and Te) are magnetic semiconductors possessing the centrosymmetric crystal structure $m3m$ of rock-salt type in which the second-harmonic generation is forbidden in the electric dipole approximation but the third-harmonic generation (THG) is allowed. We studied the THG spectra of EuSe and EuTe near the band gap at $2.1 - 2.6$ eV and at higher energies up to 4 eV. The observed signals are attributed to four-photon THG processes involving specific combinations of electronic transitions between the $4f^7$ ground state at the top of the valence band and the excited $4f^6 5d^1$ states of the Eu^{2+}-ions forming the lowest conduction bands. Strong modifications of the THG intensity were observed in applied magnetic fields up to 10 T revealing the magnetic phases to play the leading role. Temperature, magnetic field, and rotational anisotropy measurements allow us to unambiguously separate the crystallographic and magnetic-field-induced contributions. In addition, we developed a microscopic quantum-mechanical model that is in good agreement with the experimental results.[1,2]

[1] M. Lafrentz, *et al.*, Phys. Rev. B **82**, 235206 (2010).
[2] M. Lafrentz, *et al.*, Phys. Rev. B **85**, 035206 (2012).

HL 30: Organic electronics and photovoltaics I (DS, jointly with CPP, HL, O)

Time: Monday 17:15–18:45 Location: H32

HL 30.1 Mon 17:15 H32

Correlation between interface energetics and open circuit voltage in organic photovoltaic cells — •Andreas Wilke[1], James Endres[2], Ulrich Hörmann[3], Jens Niederhausen[1], Raphael Schlesinger[1], Johannes Frisch[1], Patrick Amsalem[1], Julia Wagner[3], Mark Gruber[3], Andreas Opitz[1], Antje Vollmer[4], Wolfgang Brütting[3], Antoine Kahn[2], and Norbert Koch[1,4] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Brook-Taylor-Str. 15, D-12489 Berlin, Germany — [2]Department of Electrical Engineering, Princeton University, Princeton, NJ 08544, USA — [3]Universität Augsburg, Institut für Physik, Universitätsstr. 1, D-86135 Berlin, Germany — [4]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH BESSY II, Albert-Einstein-Str. 15, D-12489 Berlin, Germany

We have used ultraviolet and inverse photoemission spectroscopy to determine the transport gaps (E_{T}) of C60 and diindenoperylene (DIP), and the photovoltaic gap (E_{PVG}) of five prototypical donor/acceptor interfaces used in organic photovoltaic cells (OPVCs). The transport gap of C60 (2.5 ± 0.1) eV and DIP (2.55 ± 0.1) eV at the interface is the same as in pristine films. We find nearly the same energy loss of ca. 0.5 eV for all material pairs when comparing the open circuit voltage measured for corresponding OPVCs and E_{PVG}.

HL 30.2 Mon 17:30 H32

Direct Observation of Charge Separation in Perylene Monoimide Solid State Dye-Sensitized Solar Cells — •Ian Howard[1], Michael Meister[1], Björn Baumeier[1], Henrike Wonnenberger[1], Neil Pschirer[2], Rüdiger Sens[2], Ingmar Brüder[2], Klaus Müllen[1], Denis Andrienko[1], and Frédéric Laquai[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany — [2]BASF SE

Combining Vis-NIR broadband pump-probe transient absorption spectroscopy with precise measurement of the time-resolved photoinduced Stark effect we demonstrate that it is possible to track not only the rate of charge injection but also the motion of carriers after injection on the critical nanosecond timescale in Solid State Dye Sensitized Solar Cells. In terms of solar cell efficiency our findings have two major impacts. Firstly, we directly observe that the *reductive quenching* pathway previously suggested (wherein a photoexcited dye donates a hole to the hole transport material before then injecting an electron, now from the dye anion state, into the TiO2) is important for obtaining high device efficiencies, especially for NIR absorbing dyes which exhibit a reduced driving force for electron injection directly from the dye exciton. Secondly, we find that many charges return to the interface after following injection, likely due to Coulombic and image charge effects. Screening the charges better, for example by reducing the dielectric contrast or increasing the dye length, should decrease the interfacial charge density and thereby parasitic recombination.

HL 30.3 Mon 17:45 H32

Full electronic structure across a polymer heterojunction solar cell: interface dipoles and influence of light — •Johannes Frisch[1], Patrick Amsalem[1], Jens Niederhausen[1], Marcel Schubert[2], Eduard Preis[3], Antje Vollmer[4], Jürgen P. Rabe[1], Ullrich Scherf[3], Dieter Neher[2], and Norbert Koch[1] — [1]Humboldt-Universität zu Berlin, Germany — [2]Universität Potsdam, Germany — [3]Bergische Universität Wuppertal, Germany — [4]Helmholtz-Zentrum Berlin für Materialien und Energie - Speicherring BESSY II, Berlin, Germany

Controversial discussions concern the dependence of open circuit voltage on the energy offset between the highest occupied molecular orbital level of the donor material and the lowest unoccupied molecular orbital level of the acceptor material in organic photovoltaic cells. Therefore, we investigate the energy level alignment in two bilayer OPVCs comprising the donor poly(3-hexylthiophene) (P3HT) and the acceptors 1-(3-methoxycarbonyl)propyl-1-phenyl[6.6]C61 (PCBM) and poly(9,9'dialklylfluorene-alt- 4,7-bis(2,5-thiendiyl)-2,1,3-benzothiadiazole) (PFTBTT). Ultraviolet photoelectron spectroscopy revealed that notable interface dipoles occur at all interfaces across the OPVC structures for both material combinations. Particularly, the effective electrode work function (after contact formation with the organic material) differs significantly from those of the pristine materials. In addition, we find that negative charges are collected at the metal clusters (that exist in the early stage of cathode formation) due to exciton dissociation at the heterojunction.

HL 30.4 Mon 18:00 H32

Optoelectronic Properties Of Zinc(II)-Phthalocyanine — •Michael Kozlik, Sören Paulke, Marco Gruenewald, Roman Forker, and Torsten Fritz — University of Jena, Institute of Solid State Physics, Helmholtzweg 5, 07743 Jena, Germany

Zinc phthalocyanine (ZnPc) is an organic molecule which is used in organic optoelectronic devices, such as OLEDs and organic solar cells. Bulk material is represented mainly in form of the metastable α-ZnPc, while the stable β-ZnPc is less conductive [1]. We show the critical transformation temperature as well as optical and morphological differences between both phases. Description and simulation of the performance of organic devices make use of material parameters. In our work we present the determination of the optical constants and the exciton diffusion length. Experimental methods are UV-Vis spectroscopy and external quantum efficiency. By transmittance and reflectance spectra we derive the real and imaginary part of the refractive index [2]. In combination with the derived parameters we show the performance of a simplified photovoltaic cell and identify the region of exciton dissociation and exciton diffusion length.

References

[1] K. Wihksne et al., J. Chem. Phys. 34 (1961) 2184.
[2] M. Kozlik et al., Org. Electron. 13 (2012) 3291.

HL 30.5 Mon 18:15 H32

The operational mechanism of ionic transition metal complex-based light-emitting electrochemical cells — •Sebastian B. Meier[1,2], Stephan van Reenen[3], Henk J. Bolink[4], Martijn Kemerink[3], Wiebke Sarfert[2], and Albrecht Winnacker[1] — [1]Department of Materials Science VI: Materials for Electronics and Energy Technology, University of Erlangen-Nuremberg, Germany — [2]Siemens AG, Corporate Technology, CT RTC MAT MPV-DE, Erlangen, Germany — [3]Department of Applied Physics, Eindhoven University of Technology, The Netherlands — [4]Instituto de Ciencia Molecular, Universidad de Valencia, Spain

Light-emitting electrochemical cells (LECs) are promising candidates for cost-efficient next generation solid-state lighting and signage applications. They feature only a single, solution-processible active layer comprising a luminescent material in an ionic environment which allows for charge carrier injection from air-stable electrodes and low operating voltages. The operational mechanism of LECs has been the subject of an intense debate ever since their discovery. Evidence for electrochemical doping has been demonstrated for polymer-based devices, whereas LECs comprising ionic transition metal complexes (iTMCs) have almost exclusively been stated to operate via an electrodynamic mechanism. We used fluorescence as well as scanning Kelvin probe microscopy on planar iTMC-LECs to elucidate their mechanism of work. Our results illustrate profound evidence for electrochemical doping in these kind of LEC devices and highlight that the position of the established p-i-n junction is not fixed but migrates during device operation.

HL 30.6 Mon 18:30 H32

Effective Charge Carrier Lifetimes in Organic Solar Cells Prepared by Coevaporation of $C60$ and $CuPc$ in different mixtures and geometries — •André Dragässer and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Giessen, Germany

Evaporated organic solar cells can lead to efficiencies of technical relevance if the interface of donor and acceptor molecules is optimized for the interplay of exciton dissociation, charge transport and recombination. The effective lifetime of the charge separated state is of central relevance. Intensity- modulated photovoltage spectroscopy with parallel impedance spectroscopy is a suitable method of analysis. Organic solar cells consisting of the well-established semiconductor materials $CuPc$ and $C60$ were prepared by physical vapor deposition on an ITO substrate, modified with $PEDOT:PSS$. The cells were completed by a back contact of BCP as a buffer and aluminum. Cell architectures of planar junctions, bulk heterojunctions or planar-mixed heterojunctions were studied for different film thickness of the components. IV-measurements in the dark and under varied illumination intensities provided basic device characteristics. Detailed measurements of the short-circuit photocurrent and the open-circuit photovoltage under static or intensity-modulated illumination with different wavelength were performed to determine the average charge carrier lifetime in the devices which was related to the respective charge carrier density obtained by impedance spectroscopy. Recombination reactions and, in particular, the influence of trap states will be discussed.

HL 31: Focus Session: Dirac fermions in solid-state systems (HL, jointly with TT)

The observation of massless Dirac fermions in monolayer graphene has initiated a new area of research exploring charge carriers that behave relativistically within solid-state systems. Both massless and massive Dirac fermions are studied in a growing range of materials that include most prominently few-layer graphene and topological insulators. The symposium will highlight some of the recent developments in this quickly advancing field. (Organizers: Roland Winkler, Northern Illinois University, and Ewelina Hankiewicz, Universität Würzburg)

Time: Tuesday 9:30–12:15 Location: H2

Topical Talk HL 31.1 Tue 9:30 H2

Localization at graphene system and topological insulator edges — •Markus Buttiker — University of Geneva, Dept. of Theoretical Phys., 24 Quai E. Ansermet, 1211 Geneva, Switzerland

Graphene systems share a number of features with topological insulators. We investigate localization phenomena at the edges of these two systems [1,2]. In bilayer graphene subject to a strong perpendicular electric field we have found that in the presence of a strongly disordered edge a sequence of localized states appears. Interestingly the localization length depends only on the size of the bulk gap but is otherwise universal, i.e. independent of the type and strength of the disorder [1]. The appearance of these localized states reflects the marginal topological properties of bilayer graphene, a bipartite square lattice with similarly disordered edges does not show edge states localized at the edge.

In two-dimensional topological insulators such as HgTe/CdTe there exists a pair of helical edge states which are protected against nonmagnetic disorder. However, if time-reversal symmetry is removed by the application of a magnetic field the protection is removed and these states localize. We investigate the divergence of the localization length as the magnetic field tends to zero and find that the localization length saturates at higher fields [2].

[1] Jian Li, Ivar Martin, Markus Buttiker, Alberto F. Morpurgo, Nat. Phys. 7, 38-42 (2011); Phys. Scr. Physica Scripta T146, 014021 (2012).

[2] Pierre Delplace, Jian Li, Markus Büttiker , Phys. Rev. Lett. 109. 246803 (2012).

Topical Talk HL 31.2 Tue 10:00 H2

Controlling Quantized Edge Transport in Two-dimensional Topological Insulators — Viktor Krueckl, Sven Essert, and •Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

Robustness of edge channels against disorder scattering is an outstanding feature of two-dimensional topological insulators (TIs). Here we consider quantized transport and mesoscopic interference phenomena in HgTe-based TIs, systems where the quantum spin Hall state has first been experimentally observed [1]. On the one hand, we discuss mechanisms to steer the spin orientation, and thereby the charge flow between different edges in TI constrictions that turn out to provide rather robust spin transistor functionality [2]. On the other hand, we study the combined effect of a time-reversal symmetry breaking magnetic field and disorder on transport to explore the limits of topological protection and the competition between reflectionless modes, metallic behavior and Anderson localization. In particular, transport in hybrids composed of normal conducting and TI regions shows peculiar quantization phenomena.

[1] M. König et al., Science **318**, 766 (2007);

[2] V. Krueckl, K. Richter, Phys Rev. Lett. **107**, 086803 (2011).

Topical Talk HL 31.3 Tue 10:30 H2

First-principles studies of Dirac-cones in graphene and 3D topological insulators — •Gustav Bihlmayer — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Jülich, Germany

The unique properties of graphene, in particular the two Dirac-cones determining the transport phenomena in this material, led the way to the first theoretical proposal of the quantum spin Hall effect at the edges of a graphene ribbon by Kane and Mele in 2005. Since spin-orbit coupling (SOC) effects are extremely weak at the Dirac points, this phenomenon is hard to observe experimentally. I discuss several theoretical proposals and experiments that have been made to enhance intrinsic SOC effects. Here, density functional theory (DFT) provides a quantitative tool to predict the properties of these two-dimensional topological insulator phases.

In three-dimensional topological insulators topologically protected edge states form Dirac-cones with chiral spin texture (in contrast to the spin-degenerate Dirac-cone of graphene). We discuss the spin-polarization and -orientations in this state for Bi and Se chalcogenides and its interaction and modification with magnetic adatoms. Also here DFT results will be compared to experiments where available.

Coffee break

Topical Talk HL 31.4 Tue 11:15 H2

Lifetime broadening of topological surface states with and without magnetic moments — •Oliver Rader[1], Markus Scholz[1], Jaime Sánchez-Barriga[1], Andrei Varykhalov[1], Dmitry Marchenko[1], Emile Rienks[1], Andrey Volykhov[2], and

Lada Yashina[2] — [1]Helmholtz-Zentrum Berlin — [2]Moscow State University

The lifetime broadening of the angle-resolved photoemission signal from the surface states of Bi_2Se_3 and Bi_2Te_3 is studied. It is revealed that hexagonal warping in Bi_2Te_3 introduces an anisotropy for electrons propagating along $\overline{\Gamma}$-$\overline{K}$ and $\overline{\Gamma}$-$\overline{M}$. Moreover, we show that the electron-phonon coupling strength is substantial and in good agreement with theoretical predictions. The small Fermi surface is believed to limit the number of phonon modes for electron scattering. In line with this, the imaginary part of the self-energy from the surface state electrons declines with higher binding energies. In addition, we find that Fe surface impurities have a much stronger influence on the lifetimes as compared to Ag. This is independent of the sign of the doping which is p-type when Fe is deposited at low temperature.

Topical Talk HL 31.5 Tue 11:45 H2
Transport in topological insulators - experiments —

•Christoph Brüne — Experimentelle Physik 3, Physikalisches Institut, Universität Würzburg

The prediction and discovery of topological insulators (TIs) has attracted wide interest in the physics community during the past years. The first topological insulator state was predicted and discovered in 2 dimensional systems. I will present our results concerning the quantum spin Hall effect in HgTe quantum wells. The quantum spin Hall effect is the signature state of a 2-dimensional topological insulator.

In 3 dimensions this new state of mater is characterized by conducting Dirac type surface states while the bulk of the material remains insulating. Such surface states have been observed in e.g. Bi2Te3, Bi2Se3 and Sb2Te3. These materials do, however, exhibit large defect densities paired with low carrier mobilities. So far this prevented transport studies in the quantum Hall regime of 3D TIs. Recently, however, we succeeded in using strained bulk HgTe as 3D TI. This enabled us to measure the quantum Hall effect from the 3D TI surface state in transport experiments.

HL 32: Spintronics and magnetic semiconductors (MA, jointly with HL)

Time: Tuesday 9:30–12:00 Location: H3

HL 32.1 Tue 9:30 H3
Low versus high energy excitations in the Skyrmion lattice system Cu_2OSeO_3 — •Dirk Wulferding[1], Peter Lemmens[1], Vladimir Gnezdilov[2], Yurii Pashkevich[3], Christian Pfleiderer[4], and Helmuth Berger[5] — [1]IPKM, TU-BS, Braunschweig — [2]ILTPE, Kharkov, Ukraine — [3]DonFTI, Donetsk, Ukraine — [4]Physikdepartment, TU München — [5]EPFL, Lausanne, Switzerland

Cu_2OSeO_3, a ferromagnetic insulator with a skyrmion lattice phase previously known from intermetallics, shows low as well as high energy excitations that strongly depend on small applied magnetic fields. In particular, the low energy anomalies are discussed in relation to the Skyrmion lattice. Work supported by DFG, B-IGSM and NTH School for Contacts in Nanosystems.

HL 32.2 Tue 9:45 H3
Electron Dynamics in a Ferrocene-Based Mixed-Valence Compound — •Nicolas Yeche[1], Lucas Mäde[1], Alexander Hildebrandt[2], Ulrike Pfaff[2], Simon Liebing[3], Marco Günther[1], Heinrich Lang[2], Jens Kortus[3], and Hans-Henning Klauss[1] — [1]TU Dresden, Dresden, Germany — [2]TU Chemnitz, Chemnitz, Germany — [3]TU Freiberg, Freiberg, Germany

Mixed-valence compounds are metal-organic molecules in which the metal centres, a priori identical, are in different oxidation states. These compounds usually stabilize through a strong electron delocalization between the various metallic atoms. Thanks to Mössbauer spectroscopy measurements, we followed the charge dynamics in the monocationic form of 2,5-Diferrocenyl,1-Phenyl-1H-Pyrrole. There, two a priori symmetrical ferrocene moieties contain one Fe(III) and one Fe(II).

We present results obtained from the solid state as well as in dispersed molecules in a tetrahydrofurane glass. From the fluctuation of the electric field gradient (EFG) at the iron nuclei sites we follow the charge fluctuation rate from room temperature down to 4.2K. Results on the average EFG are then compared with DFT calculations.

HL 32.3 Tue 10:00 H3
Flux quantization in spintronic devices — •Wei Chen, Peter Horsch, and Dirk Manske — Max Planck Institute for Solid State Research, Stuttgart

We show that electric flux vector, defined as the cross product of electric field and trajectory, manifests quantization in various spintronic devices in the same sense as quantization of magnetic flux in a SQUID. This quantization is related to many fascinating phenomena such as field-adjustable spin Josephson effect, the current-voltage characteristics of spin-FET, and persistent spin current in a metallic ring. In the case where the quantization is purely due to Aharanov-Casher effect, the flux quantum is determined only by fundamental constants.

HL 32.4 Tue 10:15 H3
Three-magnon splitting process and efficiency of spin pumping in YIG/Pt bilayer — •Oleksandr Dzyapko[1], Vladislav Demidov[1], Hidekazu Kurebayashi[2], and Sergej Demokritov[1] — [1]Institute for Applied Physics, University of Münster, Münster, Germany — [2]Cavendish Laboratory, University of Cambridge, Cambridge, UK

Spin pumping is a process of generation of electron spin current from magnetic dynamics (spin-wave spin current). Recently, it has been shown that in YIG/Pt bilayers a process of three magnon splitting, influencing magnetic dynamics in the ferromagnet can enhance the efficiency of spin current generation in to adjacent metallic layer [1]. However, in the similar experiment performed by another group, the authors claim to observe the enhancement of a spin current in a YIG/Pt-system with a thin YIG-layer, for which the tree-magnon splitting is forbidden [2]. In order to clarify the role of the three magnon splitting process we performed a set of experiments in YIG/Pt bilayers with YIG-film of different thicknesses. The existing theory predicts that the frequency range in which the three magnon splitting process is allowed shrinks with decreasing film thickness. In agreement with the theory, the enhanced efficiency of spin current generation was observed at those frequencies, where the three magnon splitting processes is allowed, clearly demonstrating a close correlation between these two effects.

1.H. Kurebayashi, et al., Nature Mater. 10, 660 (2011).
2.V. Castel, et al., Phys. Rev. B 86, 134419 (2012).

HL 32.5 Tue 10:30 H3
Optimization of spin pumping in YIG/Pt structures — •Matthias Benjamin Jungfleisch, Viktor Lauer, Roland Neb, Andrii V. Chumak, and Burkard Hillebrands — Fachbereich Physik and Landesforschungszentrum OPTIMAS, Technische Universität Kaiserslautern, D-67663 Kaiserslautern, Germany

Spin pumping in yttrium iron garnet (YIG)/platinum (Pt) structures is an interface effect and, thus, it is of crucial importance to investigate the influence of surface processing of the ferromagnetic YIG layer before the Pt deposition.

Here, we present for the first time, systematic studies on the YIG/Pt interface, which improve the spin pumping efficiency. The spin currents generated by spin pumping in the Pt layer are detected by the inverse spin Hall effect (ISHE). Three sets of YIG/Pt samples with different YIG thicknesses and constant Pt thickness of 10 nm were investigated. Spin pumping was driven by the ferromagnetic resonance excited by an external microwave signal. We measure the FMR spectra using a conventional microwave technique, as well as the ISHE induced voltage, allowing us to calculate the spin pumping efficiency defined as the ratio of the detected ISHE charge current to the absorbed microwave power. We succeeded in improving the spin pumping efficiency by a factor of more than 150.

Financial support by the Deutsche Forschungsgemeinschaft CH 1037/1-1 is gratefully acknowledged.

HL 32.6 Tue 10:45 H3
Physical, chemical and structural characterization of the antiferromagnetic semiconductor LiMnAs. — •Andreea Beleanu,

Guido Kreiner, Walter Schnelle, Gerhard H. Fecher, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany.

The compound LiMnAs is a promising candidate for spintronic applications due to its antiferromagnetic and semiconducting behavior. Polycrystalline LiMnAs was obtained as single-phase material from stoichiometric amounts of high purity elements. The compound was characterized by powder x-ray diffraction, metallographic examinations, chemical and thermal analysis and by measurements of magnetic and transport properties. LiMnAs crystallizes in the tetragonal space group $P4/nmm$ with an antiferromagnetic order. It undergoes a phase transition to a cubic phase at 600°C. DC resistivity measurements indicate a semiconducting behavior. Using the Arrhenius plot two sections of activated conduction with a small band gap E_g of 0.21 eV indicating doped levels at low temperatures and a larger E_g of 0.57 eV at high temperatures were determined.

HL 32.7 Tue 11:00 H3

Creep/recovery and $1/f^\alpha$ noise signatures of resistively switching manganites — •Jon-Olaf Krisponeit, Christin Kalkert, Bernd Damascke, Vasily Moshnyaga, and Konrad Samwer — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Perovskite manganites show various interesting resistance effects, such as a metal-insulator transition driven by temperature as well as magnetic fields (colossal magnetoresistance). They also belong to a wide class of oxides which exhibit electrically induced resistive switching. Despite extensive efforts, the underlying mechanism of the switching effect, which possesses a high potential for applications, is still far from being understood.

We report the results on the dynamics of resistive switching on $La_{0.8}Ae_{0.2}MnO_3$ (Ae = Ca, Sr thin film samples. By means of conductive atomic force microscopy (C-AFM) we studied the time evolution of nanoscaled metallic domains. Creep/recovery features show up in pulse-train experiments and current map sequences. Moreover, the current $I(t)$ exhibits $1/f^\alpha$ noise signatures during the switching process. Such behavior is characteristic for various avalanche-type physical processes, like, for instance, the Barkhausen effect and martensitic transitions. Therefore, our results indicate the resistive switching effect to belong to this class of phenomena, and the dynamics to be governed by pinning and depinning of structural domain walls.

Financial support by DFG via SFB 602 and the Leibniz Program is acknowledged.

HL 32.8 Tue 11:15 H3

Magnetic control of channel conductance in Metal Semiconductor Field Effect Transistors with magnetic ZnO channel — •Tim Kaspar[1], Danilo Bürger[1,2], Ilona Skorupa[1], Artur Erbe[1], Daniel Grimm[2,3], Oliver G. Schmidt[2,3], Manfred Helm[1], and Heidemarie Schmidt[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, P.O. Box 510119, 01314 Dresden, Germany — [2]TU Chemnitz, Reichenhainer Str. 39, 09111 Chemnitz, Germany — [3]IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany

We focus on the development of ZnO based devices, e.g. Schottky diodes with a magnetic ZnO depletion region [1]. Our work is motivated by the observation of s-d exchange interaction in magnetic ZnO below 50 K. For ZnO:Co we have shown that the magnetoresistance depends on the magnetic ion concentration, the free electron concentration and temperature [2]. Here we focus on the control of conductance in Metal Semiconductor Field Effect Transistors (MESFETs)with diluted magnetic ZnO channels by applied external electrical and magnetic fields. Co-doped magnetic ZnO channel layers with a Co concentration of 5 at% have been deposited by pulsed laser deposition. Ag/Au gate and Ti/Au source and drain contacts have been structured by optical lithography. The characteristics of the MESFETs with magnetic channel in external perpendicular magnetic fields up to 1.8 T are presented.

[1] Qingyu Xu, H. S.et al., Jpn. J. Appl. Phys.49, 043002(2010)
[2] Qingyu Xu, H. S.et al., Phys. Rev. B.76, 134417(2007)

HL 32.9 Tue 11:30 H3

Tuning the ultrafast magnetic dynamics in Gd-Doped EuO — •A. Schroer[1], M. Matsubara[2], A. Schmehl[3], J. Mannhart[4], A. Melville[5], D. G. Schlom[5], M. Trujillo Martinez[1], M. Fiebig[2], and J. Kroha[1] — [1]Universität Bonn — [2]ETH Zürich — [3]Universität Augsburg — [4]MPI-FF Stuttgart — [5]Cornell University

EuO is a dense ferromagnetic semiconductor with a Curie temperature of T_C = 69 K. Upon Gd-doping, $Eu_{1-x}Gd_xO$ undergoes a simultaneous ferromagnetic and insulator-metal transition, with a resistivity drop of several orders of magnitude, making it an interesting material or spintronics applications. The magnetic coupling J_{eff} between the Eu 4f moments is mediated by a virtual magnetic exciton (Eu 4f-5d mixing), enhancing the wave function overlap of the magnetic Eu orbitals. We show by pump-probe experiments that pumping electrons resonantly into the Eu 5d conduction band in pure EuO leads to an ultrafast increase of the ferromagnetic coupling J_{eff}, and that this coupling can be tuned from a further increase to a decrease by Gd doping. For this pump-induced non-equilibrium situation we calculate the RKKY-like, conduction electron induced magnetic coupling. We find that the magnetic interaction is in general oscillatory and decays spatially with a power law, like the equilibrium RKKY interaction, but the power law exponent is changed. The tuning of the pump-induced change of J_{eff} by Gd-doping is explained by a subtle interplay of correlation-induced shift of spectral weight and of a pump-induced redistribution of the conduction electron occupation.

HL 32.10 Tue 11:45 H3

Magnetism in geometrically frustrated $HgCr_2Se_4$ — •Michael Wagner[1], Sarah Dunsiger[1], Vladimir Tsurkan[2], Alois Loidl[2], and Christian Pfleiderer[1] — [1]Physik Department E21, Technische Universität München, 85748 Garching, Germany — [2]Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

Geometrically frustrated spin systems on a pyroclore lattice are prone to competing antiferromagnetic and ferromagnetic interactions. Under hydrostatic pressure the relative strength of the various magnetic interactions may be changed driving phase transitions of the ground state. We studied the chromium spinel $HgCr_2Se_4$, a ferromagnetic semiconductor with $T_c \approx 106$ K. We have measured the magnetization under pressure with a bespoke Cu:Be piston cylinder cell. Our measurements were carried out on a single crystal prepared by chemical transport reaction. As a function of temperature the magnetization vanishes at the curie temperature T_c which decreases as a function of pressure consistent with literature [1]. Furthermore we find some indications of critical behaviour.

[1] V. Srivastava. Journal of Applied Physics, 40:3, 1969

HL 33: Invited Talk: Hubert Krenner

Time: Tuesday 9:30–10:00 Location: H13

Invited Talk HL 33.1 Tue 9:30 H13

Acoustic nanoquakes dynamically control optical nanosystems — •Hubert Krenner — Emmy Noether Group at Experimentalphysik 1, Universität Augsburg, 86159 Augsburg, Germany

Radio frequency control of the quantum mechanical, electronic and optical properties of nanostructures lies at the forefront of contemporary nanoscale research. Towards this challenging goal, surface acoustic waves (SAWs) provide a particularly versatile tool to manipulate and probe a broad variety of nanosystems. These "nanoquakes on a chip" promise massively parallel manipulation via acousto-mechanical and acousto-electric couplings. In this presentation I will show that a mechanical deformation induced by a SAW can be directly applied to deform and break the periodicity in two-dimensional photonic crystal membranes (PCMs). In a first experiment we employed this effect to spectrally tune the optical mode spectrum of nanocavities defined in this planar and scalable architecture at radio frequencies exceeding 1.7 GHz with a spectral bandwidth of more than 8 cavity linewidths. Recently, we monitored the coupling between the optical mode and quantum dot nanoemitters under periodic acoustic tuning in the time domain. We observe clear periodic coupling and decoupling between the two constituents of this prototype solid-state cavity-quantum electrodynamic system. This unique real-time control promises for the implementation of dynamic quantum gate operations. In addition, the

SAW represents a monochromatic and coherent acoustic phonon field. This property could further allow for coherent acousto-mechanical control of coupled photonic and phononic modes in optomechanical crystals.

HL 34: Quantum dots and wires: Theory

Time: Tuesday 9:30–10:45 Location: H15

HL 34.1 Tue 9:30 H15

Bulk and interface defects and impurities in Au-catalyzed GaAs nanowire growth: First principles study — Sung Sakong, Yaojun Du, and •Peter Kratzer — Fakultät für Physik and Center for Nanointegration (CENIDE), Universität Duisburg-Essen, Duisburg, Germany

For the growth of GaAs nanowires, often an Au nanoparticle is used as catalyst, which allows for generating co-existing zincblende and wurtzite polytypes of GaAs, but may also introduce Au impurities in the nanowire. We use density functional theory to calculate the formation energy of various growth-related defects and impurities in both GaAs polytypes and at the Au(111)/GaAs(111)B interface. Defects whose formation energy in bulk is much larger than at the interface, e.g., an As vacancy or a substitutional Au impurity at the As site will travel with the growth zone and hence are less harmful. However, the energetics of the Ga_{As} antisite defect and the substitutional Au impurity at the Ga site are comparable in bulk and at the interface. Especially, the formation of the Au impurity at the Ga site costs relatively low energy. Thus, we predict that the most abundant defect in the GaAs nanowire will be the Au impurity at the Ga site, in good agreement with the recent experimental findings by Bar-Sadan *et al.* [Nano Lett. 12, 2352 (2012)]. In conclusion, we suggest that an As-rich growth regime could reduce the defects and impurities in the nanowire by avoiding the Ga-termination of GaAs at the growth zone which could act as a source of defects at the Ga site.

HL 34.2 Tue 9:45 H15

Modeling the interface between GaAs nanowire and Au capping: First principles study — •Sung Sakong, Yaojun A. Du, and Peter Kratzer — Fakultät für Physik and Center for Nanointegration (CENIDE), Universität Duisburg-Essen, Duisburg, Germany

We present first-principles calculations of the interface between a Au nanoparticle and a GaAs nanowire. The interfaces are modeled with Au ad-layers on a GaAs(111)B substrate. The GaAs surface can be terminated with As or Ga which reflects the two extreme cases in the growth process. The interface energies of As- and Ga-terminated interfaces are expressed as a function of As chemical potential μ_{As}. Under Ga(As) rich growth, the Ga(As)-terminated interface becomes more stable than the other. We note that under a specific μ_{As} the two interface energies become equal, i.e. the two terminations are energetically competing configurations and a layer-by-layer growth of the GaAs nanowire is possible. When one interface is dominantly more stable than the other, then a bilayer growth mode is preferred. The layer-by-layer growth of GaAs nanowire is at $\mu_{As} - \mu_{As}^{bulk} = -0.28$ eV in LDA density functional. Using the estimated interface energy of 47 meV/Å^2, we explore the optimal geometric structures of a Au capped GaAs nanowire with minimizing the surface free energy under near-equilibrium growth. With replacing the pure Au layers with a Au_7Ga_2 alloy, we are able to simulate an interface to a more Ga-rich nanoparticle. The interface energy of the Au-Ga alloy interface is smaller than the pure Au interface, which results in a more flat nanoparticle geometry due to the Gibbs-Thompson effect.

HL 34.3 Tue 10:00 H15

Topological phase transitions in α-Sn Nanocrystals: a first-principle approach — •Küfner Sebastian, Jürgen Furthmüller, Martin Fitzner, Lars Matthes, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, D-07743 Jena

Nanostucturing significantly changes the properties of materials. This especially holds for nanocrystals (NCs). The increased surface to volume ratio influences the electronic structure. There is a strong dependence of the electronic properties on the geometry, the size, and the surface passivation of the nanoscale objects. α-Sn is a zero-gap semiconductor with an inverted band structure at the Γ-point with respect to other group-IV semiconductors. Using density-functional theory within local XC-functionals we show that the level-ordering of s- and p- like states at Γ is inverted in nanocrystals with respect to the bulk. Since the fundamental energy gap decreases for increased nanodot-diameter, we show that there has to be a phase transition for a diameter of about 13 nm where the level odering changes. We determine this critical dot-size by tight-binding calculations. Furthermore, we prove that our results for the fundamental energy gaps of the NCs agree perfectly with methods taking many-body effects and screened Coulomb-interaction into account.

HL 34.4 Tue 10:15 H15

Fast kinetic Monte Carlo simulations of quantum dots — Petar Petrov and •Wolfram Miller — Leibniz-Institut für Kristallzüchtung (IKZ), Max-Born-Str. 2, 12489 Berlin

We present a new three-dimensional heteroepitaxial kinetic Monte Carlo method (KMC) for fast simulation of self-assembled quantom dot arrays. The incorporation of elastic effects due to misfit strained are based on a ball-and-spring model [1]. In contrary to our previous work [2] we simplify the computation of the corrections to the hopping barriers because of the elastic strain in order to accelerate the computation. As an application we studied the system $In_{1-x}Ga_xAs/GaAs$ and analysed wetting layer formation, uniformity of quantum dots in size, distance, and aspect ratio, and others as a function of deposition rate and substrate temperature.

[1] G. Russo and P. Smereka, J. Comput. Phys. 214 (2006), 809
[2] P. Petrov and W. Miller, Comput. Mater. Sci. 60 (2012), 176

HL 34.5 Tue 10:30 H15

Limit Cycles and Chaos in the Current Through a Quantum Dot — •Carlos López-Monís[1,2], Clive Emary[3], Gerold Kiesslich[3], Gloria Platero[2], and Tobias Brandes[3] — [1]Institute für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany — [2]Institute für Theoretische Physik, TU Berlin, DE-10623 Berlin, Germany — [3]Instituto de Ciencia de Materiales de Madrid, CSIC, ES-28049 Madrid, Spain

In this talk I shall discuss, nonlinear magnetotransport through a single-level quantum dot coupled to ferromagnetic leads, where the electron spin is coupled to a large, external (pseudo)spin via an anisotropic exchange interaction. We find regimes where the average current through the dot displays self-sustained oscillations that reflect the limit cycles and chaos and map the dependence of this behavior on magnetic field strength and the tunnel coupling to the external leads.

C. López-Monís, C. Emary, G. Kiesslich, G. Platero and T. Brandes, Phys. Rev. B. **85**, 045301 (2012).

HL 35: Graphene: Transport (TT, jointly with HL, MA, O)

Time: Tuesday 9:30–12:45 Location: H17

HL 35.1 Tue 9:30 H17

Transport properties of high-quality reduced graphene oxide — •Michael Enzelberger[1], Siegfried Eigler[2], Philipp Hofmann[1], Stefan Grimm[2], Andreas Hirsch[2], and Paul Müller[1] — [1]Department of Physics and Interdisciplinary Center for Molecular Materials, Universität Erlangen-Nürnberg — [2]Department of Chemistry and Pharmacy, and Institute of Advanced Materials and Processes (ZMP), Universität Erlangen-Nürnberg

Chemical production of graphene, especially reducing graphene oxide has gained a lot of interest in recent years. Yet the transport properties

of such materials are usually not compatible to those of graphene.

We have found a way to overcome this problem using a modification of the standard Hummer's method. Single flakes of reduced graphene oxide have been investigated. The graphene oxide was deposited onto a SiO_2/Si substrate and subsequently reduced using hydrogen iodine. The resulting reduced graphene oxide samples were patterned by electron beam lithography. We have characterized the quality of the samples by combining Raman spectroscopy and Hall mobility measurements in magnetic fields up to $14\,T$ and temperatures down to $0.3\,K$.

High-quality samples had a Raman D/G ratio of better than 1 and showed Hall mobilities exceeding 1000 cm^2/Vs. This is nearly two orders of magnitude higher than what is known for standard reduced graphene oxide. The best samples even show Shubnikov-de Haas oscillations and Hall plateaus.

HL 35.2 Tue 9:45 H17

Magnetoresistance of Nanocrystalline Graphene — •Daniel Steininger[1], Paul Linsmaier[1], Ina Schneider[1], Christoph Strunk[1], Matthias Büenfeld[2], Nils-Eike Weber[2], Andrey Turchanin[2], Miriam Grothe[3], and Thomas Weimann[3] — [1]Institute for Experimental and Applied Physics, University of Regensburg, Universitätsstr. 31, D-93053 Regensburg, Germany — [2]Faculty of Physics, University of Bielefeld,Universitätsstr.25, D-33615 Bielefeld, Germany — [3]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

We report on the magnetotransport in Hall bar structures of nanocrystalline graphene. The graphene sheets were prepared by electron-beam-induced cross-linking and subsequent pyrolysis of aromatic self-assembled monolayers [1]. The I-V characteristics show considerably non-linear behaviour at low temperatures. One low resistive sample ($\approx$ 200 kOhm/sq at T = 4 K) shows positive magnetoresistance values up to + 20 % in the perpendicular magnetic field for temperatures below 6 K, while above this temperature the magnetoresistance becomes negative. Measurements of the transversal voltage in the linear regime exhibit anomalous behaviour which cannot be explained by the conventional Hall effect. If the magnetic field is aligned parallel to the graphene sheet the magnetorestance exhibits large positive values up to + 300 %. Measurements on a highly resistive sample ($\approx$ 30 MOhm/sq at T = 4 K) reveal a non-monotonic behaviour of the magnetoresistance in a perpendicular magnetic field.

[1] A. Turchanin et al., ACS Nano 5 (2011) 3896-3904.

HL 35.3 Tue 10:00 H17

Quantum Monte Carlo Study of Edge-State Magnetism on Chiral Graphene Nanoribbons — Michael Golor[1], Thomas C. Lang[1,2], and •Stefan Wessel[1] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen — [2]Department of Physics, Boston University

We investigate the edge-state magnetism of chiral graphene nanoribbons using projective Quantum Monte Carlo (QMC) simulations and a self-consistent mean-field approximation of the Hubbard model. Previous QMC simulations support edge-state ferromagnetism in sufficiently wide zigzag terminated ribbons. We extended these calculations to include the class of chiral graphene nanoribbons and investigate the influence of chirality and ribbon width on spin-spin correlations. The static magnetic correlations are found to rapidly increase with the width of the ribbons for all chiralities, such that already for ribbons of moderate widths we observe a strong trend towards mean-field-type ferromagnetic correlations along the edges. We extract dynamical edge state signatures which can be used to detect edge-state magnetism by scanning tunneling microscopy.

HL 35.4 Tue 10:15 H17

Even-odd effects in NSN scattering problems: Application to graphene nanoribbons — •Francois Crepin[1], Hans Hettmansperger[1], Patrik Recher[2], and Bjoern Trauzettel[1] — [1]Institute for Theoretical Physics and Astrophysics, University of Wuerzburg, 97074 Wuerzburg, Germany — [2]Institute for Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany

We study crossed Andreev reflection (CAR) of electrons or holes in normal metal-superconductor-normal metal junctions and highlight some very strong effects of the underlying lattice. In particular, we demonstrate that for sharp interfaces and under certain, albeit generic, symmetry conditions, the CAR probability exactly vanishes for an even number of atoms in the superconducting region. This even-odd effect applies notably to NSN junctions made of graphene nano-ribbons with armchair edges and for zigzag edges with somewhat more restrictive conditions. We analyze its robustness towards smoothing of the boundaries or doping of the sample.

HL 35.5 Tue 10:30 H17

Efficient quantum transport simulation for bulk graphene heterojunctions: Klein backscattering revisited — •Ming-Hao Liu and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany

The quantum transport formalism based on tight-binding models is known to be powerful in dealing with a wide range of open physical systems subject to external driving forces but is, at the same time, limited by the memory requirement's increasing with the number of atomic sites in the scattering region. Here we demonstrate how to achieve an accurate simulation of quantum transport feasible for experimentally sized bulk graphene heterojunctions at a strongly reduced computational cost [1]. Without free tuning parameters, we show excellent agreement with recent experiments on Klein backscattering [2,3].

[1] M.-H. Liu and K. Richter, Phys. Rev. B **86**, 115455 (2012).
[2] A. F. Young and P. Kim, Nat. Phys. **5**, 222 (2009).
[3] S.-G. Nam, D.-K. Ki, J. W. Park, Y. Kim, J. S. Kim, and H.-J. Lee, Nanotechnology **22**, 415203 (2011).

HL 35.6 Tue 10:45 H17

Combined effect of vacancies and strain on the conductance of graphene nanoribbons — •Thomas Lehmann, Dmitry A. Ryndyk, and Gianaurelio Cuniberti — Institute for Materials Science, Dresden University of Technology, 01062 Dresden, Germany

The understanding and engineering of electron properties of carbon-based nanostructures, in particular graphene nanoribbons, is an important challenge for modern theory of nanoscale systems. We investigate the influence of vacancy defects and uniaxial strain on the electronic transport properties of intermediate-scale graphene nanoribbons using the numerical approach based on the semi-empirical or ab initio based tight-binding model, the Landauer-Büttiker formalism and the recursion method for Green functions. We calculate the transmission of graphene nanoribbons in the quantum coherent regime with different types and concentration of defects. Further, we apply uniform planar tension to non-ideal graphene ribbons with randomly distributed and oriented single and double vacancies and Stone-Wales defects. Since transport characteristics of graphene are found to be very sensitive to edge termination and aspect ratio and it has been shown that energy gaps can emerge under critical strain, the interplay of both effects needs to be studied.

15 min. break

HL 35.7 Tue 11:15 H17

Spin conductance of diffusive graphene nanoribbons — •Jan Bundesmann[1], Ming-Hao Liu[1], Inanc Adagideli[2], and Klaus Richter[1] — [1]University of Regensburg, Regensburg, Germany — [2]Sabanci University, Istanbul, Turkey

Graphene, when cut along a zigzag edge, shows a strongly increased density of states at energies close to the charge neutrality point. The electron states that are the source of this increased DOS are pseudospin-polarized, i.e. they occupy mainly one sublattice, while their wavefunction decays exponentially from the zigzag edge.

In such systems one expects magnetic ordering which anifests as an antiferromagnetic alignment of the two sublattices. Due to the pseudospin polarization of the states finite local magnetic moments appear along the edges.

We investigate how the formation of these local magnetic moments influences charge and spin transport in graphene. It will be shown how this can lead to a finite spin conductance of a single graphene nanoribbon and that within the localized transport regime the spin conductance fluctuations exhibit universal behaviour in the sense that they don't depend on the exact modelling of the magnetization and even a large amount of edge roughness does not lead to deviations from this universal behaviour.

HL 35.8 Tue 11:30 H17

Superlattice Effects on Electronic- and Transport Properties of Nanomaterials — •Fedor Tkatschenko, Viktor Krueckl, and Klaus Richter — Universität Regensbug, Germany

As recently discoverded by various groups [1,2] the electronic properties of two dimensional systems such as graphene show interesting charac-

teristics in presence of superlattices including the emergence of extra Dirac points accompanied by an anisotropic velocity renormalization. Other interesting effects are Bloch-oscillations in presence of resonant Zener tunneling [3] giving rise to a negative differential conductance in the current voltage characteristics.

We focus on a scalar superlattice system extended by a constant mass term which opens a gap between the valance and conduction band in the minibandstructure. Analytical calculations within the effective Dirac model show that it is possible to tune the energy gap by variation of the superlattice amplitude. By additional numerical calculations based on the tight-binding model we confirm the analytical results.

[1] L. Brey and H. Fertig, Phys. Rev. Lett. **103**, 046809 (2009)
[2] M. Barbier, P. Vasilopoulos, and F. Peeters, Phys. Rev. B **81**, 075438 (2010)
[3] V. Krueckl and K. Richter, Phys. Rev. B **85**, 115433 (2012)

HL 35.9 Tue 11:45 H17

Hot Spots and Boundary Conditions in the Quantum Hall Effect — •Tobias Kramer — Universitaet Regensburg, Inst. Theor. Physik, Germany

I discuss the influence of metallic boundary conditions due to the device contacts on the observation and current distribution in the quantum Hall effects. The current density differs in the presence of hot-spots completely from the often assumed edge-state transport picture. A model for transport in graphene [1] based on the self-consistent solution of the classical Hall effect [2] is put forward.

[1] T. Kramer, C. Kreisbeck, V. Krueckl, E. Heller, R. Parrott, and C.-T. Liang, Phys. Rev. B **81**, 081410(R) (2010)
[2] T. Kramer, V. Krueckl, E. Heller, and R. Parrott, Phys. Rev. B **81**, 205306 (2010)

HL 35.10 Tue 12:00 H17

Current resonances in graphene with time dependent potential barriers — Sergey E. Savel'ev[1], •Wolfgang Häusler[2], and Peter Hänggi[2] — [1]Department of Physics, Loughborough University, United Kingdom — [2]Universität Augsburg, Germany

A method is derived to solve the massless Dirac-Weyl equation describing electron transport in a mono-layer of graphene with a scalar potential barrier $U(x,t)$, homogeneous in the y-direction, of arbitrary x- and time dependence. Resonant enhancement of both electron backscattering and currents, across and along the barrier, is predicted when the modulation frequencies satisfy certain resonance conditions. These conditions resemble those for Shapiro-steps of driven Josephson junctions. Surprisingly, we find a non-zero y-component of the current for carriers of zero momentum along the y-axis.

[1] Sergey E. Savel'ev, Wolfgang Häusler, Peter Hänggi, Phys. Rev. Lett. **109**, 226602 (2012).

HL 35.11 Tue 12:15 H17

Mie scattering analogon in graphene: particle confinement, scattering resonances, and Fano effect — •Rafael Leslie Heinisch, Christian Schulz, Franz Xaver Bronold, and Holger Fehske — Institut für Physik, Universität Greifswald

We study the scattering of an incident electron by a circular step in a graphene monolayer in analogy to Mie scattering of light by a sphere. Klein tunnelling results in the absence of backscattering and often entails enhanced forward scattering. For low electron energies we identify sharp resonances originating from quasi-bound states at the dot. The energy and dot radius dependent temporary electron trapping significantly increases the electron density in the dot and induces a vortex pattern in the current field. The angle-resolved scattering exhibits Fano resonances which - counter-intuitive for Klein tunnelling - dramatically suppress forward scattering.

This work is supported by the DFG through SPP 1459.

HL 35.12 Tue 12:30 H17

Mechanical strain on graphene nanoribbons in contact with metal electrodes — •Arezoo Dianat, Dmitry A. Ryndyk, and Gianaurelio Cuniberti — Institute for Materials Science, Dresden University of Technology, 01062 Dresden, Germany

Carbon-based materials are recently of great interest for electronic devices. One of the important issues in graphene based nanoelectronics is to control its electronic and transport properties. The manipulation of electronic properties of graphene nanoribbons (GNR) has been suggested via mechanical strain, vacancies and chemical doping. From modeling point of view, few studies have been reported to investigate the electronic properties of mechanically stretched GNR in a contact with metal electrodes. In this work, we aim to elucidate the combined effects of mechanical strain and the role of metal contact area on the electronic and transport properties of GNR.

The structural and electronical properties of stretched GNR on Nickel and Palladium surfaces with different contact area and suspended strained graphene junction between metal electrodes are investigated by means of density functional theory using Vienna Ab initio Simulation Package (VASP). The structure stability as well as stress-strain curve are analyzed for several strain coefficients.

HL 36: Focus Session: Functionalized semiconductor nanowires I (DS, jointly with HL)

Nanowires are filamentary crystals with a diameter ranging from few to hundred nanometers. Thanks to their special morphology and geometry, they are at the base of many applications that can revolutionize this century's technology. For this to become a reality, fundamental studies on the growth and properties are essential. This focus session presents the latest developments and discoveries in the area of nanowires, with a special focus on semiconductor materials. (Organizers: Margit Zacharias, U. Freiburg; Tobias Voss, U. Bremen; Anna Fontcuberta i Morral, EPFL)

Time: Tuesday 9:30–12:45 Location: H8

Invited Talk HL 36.1 Tue 9:30 H8

Nanowire photovoltaics with absorption beyond the ray optics limit. — •Magnus T Borgström — Solid state physics, Lund University, Lund, Sweden

Semiconducting nanowires have been recognized as promising materials for high-performance electronics and optics where optical and electrical properties can be tuned individually. The feasibility of III-V nanowire integration with existing silicon processing technology due to the small footprint between the silicon substrate and the nanowire material has further sparked that interest. For NWs to provide the new architecture for next generation photovoltaics there is a strong need to take complete control over synthesis. By optimizing growth conditions with respect to tapering we created nanowire-InP nanowire based solar cells using Au seed particles for growth. The nanowires were processed as-grown with a transparent top contact to create 1x1 square mm devices, with about 4 million nanowires contacted on each device. The solar cells were investigated under 1 sun (AM 1.5) illumination, and the devices show efficiencies higher than 10% and conversion of the solar irradiation into photocurrent beyond the ray optics limit.

Invited Talk HL 36.2 Tue 10:00 H8

Crystal structure control in nanowires — •Erik Bakkers — Eindhoven University of Technology, Den Dolech 2, 5612 AZ Eindhoven, The Netherlands — Delft University of Technology, Lorentzweg 1, 2600 CL Delft, The Netherlands

Important semiconductors like Si, Ge and GaP have an indirect bandgap when having the (normal) cubic crystal structure. It has been predicted that when these materials crystallize in a hexagonal structure that they can have a direct bandgap. But, these materials have never been controllably made with the pure wurtzite structure. Nanowires can be grown in other crystal structures than known in the bulk, offering new routes to tailor the optical and electronic properties. The nanowire growth mechanism will be discussed and the fabrication of the pure hexagonal form will be investigated. Here, we exploit these

possibilities and discuss control of the crystal structure of nanowires and investigate the optical properties. Finally, we demonstrate the direct nature of the bandgap of wurtzite materials.

Topical Talk HL 36.3 Tue 10:30 H8

Spectral and spatial overlap of oxide quantum wells and whispering gallery modes — •Marius Grundmann — Universität Leipzig, Insitut für Experimentelle Physik II

We present the fabrication of zinc oxide nano- and microwires and the epitaxial growth of oxide heterostructures and quantum wells around the zinc oxide cores in radial direction. (Mg,Zn)O/ZnO and (Cd,Zn)O/ZnO QWs are compared and found to not exhibit quantum confined Stark effect, as expected for the non-polar growth directions. Due to the hexagonal cross-section, the ZnO wires exhibit whispering gallery resonances. The spectral and spatial overlap of the quantum wells with the whispering gallery modes is achieved in various geometries. The coupling of exciton and photon modes will be discussed.
This work was conducted together with C.P. Dietrich, M. Lange, T. Böntgen and M. Stölzel and financially supported by DFG in the framework of FOR1616 and by ESF.

Coffee break (15 min)

Topical Talk HL 36.4 Tue 11:15 H8

Semiconducting Nanowire Heterostructures on Silicon - From Growth to Devices — Heinz Schmid, Kirsten Moselund, Cedric Bessire, Pratyush Das Kanungo, Philipp Mensch, Siegfried Karg, Mattias Borg, Volker Schmidt, and •Heike Riel — IBM Research - Zurich, Rüschlikon, Schweiz

Bottom-up grown nanowires (NWs) are very attractive materials for direct integration of III-V semiconductors on Si thus opening up new possibilities for the fabrication and design of electronic and optoelectronic devices. The NW geometry allows the growth of abrupt heterostructures with large lattice mismatch and offers an ideal geometry for field-effect transistors (FETs) from an electrostatics perspective. These characteristics are especially important for tunnel FETs (TFETs) which today are being considered the most promising steep-slope devices. TFETs can achieve a subthreshold swing of less than 60 mV/dec and are thus attractive for low-voltage operation thereby offering significant power dissipation savings. We present our results on the fabrication and characterization of vertical InAs-Si heterojunction nanowire (NW) Esaki tunnel diodes and TFETs with InAs as low bandgap source. InAs NWs are grown on Si <111> by selective area epitaxy within e-beam patterned SiOx openings by MOCVD where the doping level is controlled in-situ. Furthermore, a new approach based on nanotube templates has been developed to grow axial III/V nanowire homo- and hetero-structures on silicon with high quality. The device fabrication will be discussed and the latest electrical results of tunnel diodes and TFETs will be presented.

Topical Talk HL 36.5 Tue 11:45 H8

III-nitride nanowires: From growth phenomena to light-emitting diodes — •Raffaella Calarco — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany

Epitaxy in the form of freestanding vertical nanowires offers compared to planar layers the advantage that the interface between adsorbate and substrate is very small and that strain caused by lattice mismatch can elastically relax at the free sidewalls. Hence, dissimilar materials can be combined in high structural quality, and arguably the most relevant case is the growth of III-V compound semiconductors on Si substrates. We grow GaN nanowires on Si substrates by molecular beam epitaxy (MBE) and investigate nanowire properties that are essential for optoelectronic applications. Light emitting diodes (LEDs) have been fabricated using ensembles of free-standing (In, Ga)N/GaN NWs grown on Si substrates in the self-induced growth. Several characterization techniques indicate that the electroluminescence of such LEDs is governed by the differences in the individual current densities of the single-NW LEDs operated in parallel, i.e. by the inhomogeneity of the current path in the ensemble LED. In addition, the optoelectronic characterization leads to the conclusion that these NWs exhibit N-polarity and that the (In, Ga)N quantum well states in the NWs are subject to a non-vanishing quantum confined Stark effect. LEDs require NW ensembles with very homogeneous properties. Here, we present our selective area growth strategy for the synthesis of high-quality GaN NWs on prepatterned Si(111) substrates.

Topical Talk HL 36.6 Tue 12:15 H8

3D GaN nanorods: fabrication, properties, applications — •Andreas Waag, Johannes Ledig, Xue Wang, Milena Erenburg, Jana Hartmann, Lorenzo Caccamo, Matin Mohajerani, Manal Ali Deeb, Jiandong Wei, Martin Hoffmann, Hao Shen, and Hergo-Heinrich Wehmann — TU Braunschweig

GaN nanorods and 3D columns recently attracted a lot of attention since they are expected to be an exciting new route towards light engines for solid state lighting. In contrast to a planar thin film technology, a completely 3-dimensional nano- or microrod approach gives more freedom in the device design. E.g., a core-shell design of LEDs based on 3D GaN offer a dramatically enhanced active area per wafer footprint, since the active area is scaling with height of the 3D structures. High quality core-shell devices will have a tremendous impact on LED technology. However, there are also challenges related to a 3D device approach. Conventional planar characterization as well as processing techniques can no longer be used. In addition, the growth windows in epitaxy have to be modified in order to enhance vertical growth rates and reduce planar growth rates. Quite often, this leads to growth modes, which are far away from the ones regularly used for high efficiency planar LEDs. This talk will give an overview on the state of the art of our 3D GaN research, particularly focusing on MOCVD growth and 3D characterization. Potential advantages and challenges of this exciting new strategy towards low cost high efficiency solid state lighting will also be discussed.

HL 37: Transport: Quantum dots, wires, point contacts 3 (TT, jointly with HL)

Time: Tuesday 9:30–12:30 Location: H20

HL 37.1 Tue 9:30 H20

Theory of Spin Relaxation in Two-Electron Laterally Coupled GaAs and Si Quantum Dots — •Martin Raith[1], Peter Stano[2,3], and Jaroslav Fabian[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Department of Physics, University of Basel, 4056 Basel, Switzerland — [3]Institute of Physics, Slovak Academy of Sciences, 845 11 Bratislava, Slovakia

We present quantitative results of the phonon-induced spin relaxation in two-electron lateral double quantum dots. Both spin-orbit coupling and hyperfine coupling are taken into account. Our analysis of GaAs [1] and silicon [2] based dots includes the variation of the electric field (detuning), the exchange coupling, and the magnetic field strength and orientation. We find that even in strong magnetic fields, the hyperfine coupling can dominate the relaxation rate of the unpolarized triplet in a detuned GaAs double dot. This feature is absent in silicon (we assume a ^{29}Si abundance of 4.7%). Where the spin-orbit coupling dominates, the rate is strongly anisotropic and its maxima and minima are generated by an in-plane magnetic field either parallel or perpendicular to the dots' alignment dependent on specifics, such as spectral (anti-) crossings (spin hot spots), or the detuning strength. We emphasize the differences between GaAs and Si based dots. This work marks a crucial step toward the realization of two-electron semiconductor qubits.
This work is supported by the DFG under grant SPP 1285.

[1] M. Raith et. al., PRL 108, 246602 (2012)
[2] M. Raith et. al., arXiv:1206.6906

HL 37.2 Tue 9:45 H20

Nonequilibrium effect in a NISIN turnstile — •Andreas Heimes[1], Ville Maisi[2,3], Jukka Pekola[2], Michael Marthaler[1], Dmitry Golubev[1], and Gerd Schön[1] — [1]Institut für Theoretische Festkörperphysik, Karlsruher Institut für Technologie, Wolfgang-Gaede-Str. 1, D-76128 Karlsruhe, Germany — [2]Low Temperature Laboratory (OVLL), Aalto University School of Science, P.O. Box 13500, 00076 Aalto, Finland — [3]Centre for Metrology and Accredi-

tation (MIKES), P.O. Box 9, 02151 Espoo, Finland

A single electron transistor consisting of a superconducting island coupled to two normal leads is investigated. By periodically changing the gate voltage this setup works as a single electron pump. However during the turnstile operation quasiparticles are injected onto the superconductor, which relax via inelastic electron-phonon scattering and effectively heat up the island. We theoretically model the time evolution of the charge transport and the quasiparticle distribution during the pumping process. By analyzing the dependence on pumping frequency we discuss the experimental ability to measure the relaxation dynamics of quasiparticles in the superconducting island.

HL 37.3 Tue 10:00 H20

Keldysh effective action theory for universal physics in spin-1/2 Kondo dots — •Sergey Smirnov and Milena Grifoni — Institut I - Theoretische Physik, Universität Regensburg, Universitätsstraße 31, D-93040 Regensburg, Deutschland

We present a theory for the Kondo spin-1/2 effect in strongly correlated quantum dots. The theory is applicable at any temperature and voltage. It is based on a quadratic Keldysh effective action parameterized by a universal function. We provide a general analytical form for the tunneling density of states through this universal function for which we propose a simple microscopic model [1]. We apply our theory to the highly asymmetric Anderson model and describe its strong coupling limit, weak coupling limit and crossover region within a single analytical expression.

We further extend our theory to describe the Kondo regime when the quantum dot is placed in an external magnetic field. The modern experimental issues of the critical magnetic field, at which the zero bias maximum of the differential conductance starts to split into two maxima, as well as the distance between these maxima as a function of the magnetic field are also addressed.

[1] S. Smirnov and M. Grifoni, arXiv:1203.4360 (2012)

HL 37.4 Tue 10:15 H20

Superfermions in Liouville space as a powerful tool for investigating quantum transport out of equilibrium: new insights into the Anderson model — •Roman Saptsov[1,2] and Maarten Wegewijs[1,2,3] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA- Fundamentals of Future Information Technology — [3]Institute for Theory of Statistical Physics, RWTH Aachen, 52056 Aachen, Germany

Recently, we introduced a new formalism of superfermions in Liouville space for a renormalization group study of the non-linear transport through an Anderson quantum dot (QD) at zero temperature [1]. This formalism turns out to be a very useful tool to study other aspects of non-equilibrium phenomena, as well. In the wide band limit for a strongly interacting QD it allows one to sum up exactly temperature-independent contributions and obtain a general form of the QD effective Liouvillian as well as some exact relations for its eigenvalues. In the non-interacting case, U=0, our approach describes time evolution of the QD in the most simple way: we show that a "Pauli super-exclusion principle" for the superfermions leads to the exact truncation of the time-dependent perturbation series at the second order in a coupling constant. Using our approach we are able also to explore the time-evolution of the initial dot-reservoir correlations. We discuss the extension of this U=0 result to the case of finite U. Finally, we discuss other useful applications of our formalism, such as: path integrals in Liouville space and "super- mean-field theory".

[1] R.B. Saptsov, M.R. Wegewijs, arXiv:1207.3207

Invited Talk HL 37.5 Tue 10:30 H20

Nano-Conductors as Measurement Devices and Driving Sources — •Sigmund Kohler — Instituto de Ciencia de Materiales de Madrid, CSIC, 28049 Madrid, Spain

The capacitive coupling between electrically isolated nano-circuits bears a wealth of novel transport effects. One prominent realization is the coupling of a quantum dot to a quantum point contact, where the latter acts as charge monitor. Most interesting is the backaction of the point contact to quantum superpositions in the measured system and the decoherence induced in this way. For example, it has been predicted that, despite decoherence, a charge monitor may be used for qubit phase readout with good fidelity [1]. Moreover, a point contact may act upon a double or triple quantum dot not only as detector or decoherence source, but may also impose useful non-equilibrium driving and thereby, e.g., induce a pump current. This effect leaves its fingerprints in the charging diagram of double quantum dots [2] and in the full-counting statistics [3]. If the point contact is replaced by a double quantum dot, coherent tunnel oscillations in the latter may induce phenomena known from ac-driven transport.

[1] C. Kreisbeck and S. Kohler, PRB **81**, 125404 (2010)
[2] M. Stark and S. Kohler, EPL **91**, 20007 (2010)
[3] R. Hussein and S. Kohler, PRB **86**, 115452 (2012)

15 min. break

HL 37.6 Tue 11:15 H20

Electronic structure and the Aharonov-Bohm effect in inhomogeneous Möbius rings — •V. M. Fomin[1], S. Kiravittaya[1,2], and O. G. Schmidt[1,3] — [1]Institute for Integrative Nanosciences, IFW-Dresden, D-01069 Dresden, Germany — [2]Department of Electrical and Computer Engineering, Naresuan University, Phitsanulok 65000, Thailand — [3]Material Systems for Nanoelectronics, Chemnitz University of Technology, D-09107 Chemnitz, Germany

Nanostructure fabrication techniques can be exploited to generate non-trivially shaped objects with man-designed topological space metrics. A symbiosis of the geometric potential and an inhomogeneous twist renders an observation of the topology effect on the electron ground-state energy in microscale Möbius rings into the realm of experimental verification. We predict a 'delocalization-to-localization' transition for the electron ground state as the Möbius ring is made more inhomogeneous [1]. This transition can be quantified through the Aharonov-Bohm quantum-interference effect on the ground-state persistent current as a function of the magnetic flux threading the Möbius ring. Our theoretical considerations may receive practical relevance in view of the emerging experimental realizations of topologically nontrivial manifolds at the nanoscale.

[1] V. M. Fomin, S. Kiravittaya, and O. G. Schmidt, Phys. Rev. B 86, 195421 (2012).

HL 37.7 Tue 11:30 H20

Transport across an Anderson quantum dot in the intermediate coupling regime — •Johannes Kern and Milena Grifoni — Universität Regensburg, Institut für Theoretische Physik, 93040 Regensburg

We describe transport across a quantum dot coupled to leads at different chemical potentials. For this we use the master equation approach. The current is determined via the reduced density matrix by "kernels", the contributions to those are visualized by diagrams. Because of the huge variety and complexity of the diagrams, we take into account only the diagrams within a selection which we call the "dressed second order" (DSO)[1]. We apply this to the case of the single impurity Anderson model and show that the DSO allows the description of various effects: the transition from thermally broadened to tunnel broadened peaks of the linear conductance as well as of the differential conductance as function of the bias; the shift of the conductance peaks with temperature; a zero bias anomaly in the differential conductance; the splitting of this anomaly in case a magnetic field is applied. To conclude, we see the strength of the DSO in its simplicity as well as in its applicability to various problems including the transport across more complicated quantum dots.

[1] J. Kern and M. Grifoni, arXiv:1209.4995.

HL 37.8 Tue 11:45 H20

Helical nuclear spin order and conduction reduction in two subband quantum wires — •Tobias Meng and Daniel Loss — Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

In quantum wires, the hyperfine coupling between conduction electrons and nuclear spins can lead to an ordering of the latter at low temperatures. This order acts back onto the electrons and gaps out part of their spectrum. In the presence of two subbands with distinct Fermi momenta k_{F1} and k_{F2}, we discuss how the nuclear spins order in a superposition of two helices with pitches π/k_{F1} and π/k_{F2}, thus exhibiting a beating patter. This ordering results in a reduction of the electronic conductance in two steps of e^2/h upon lowering the temperature.

HL 37.9 Tue 12:00 H20

Electron Waiting Times in Non-Markovian Quantum Transport — •Konrad Thomas and Christian Flindt — Département

de Physique Théorique, Université de Genève, 1211 Genève, Switzerland

We formulate a quantum theory of electron waiting time distributions for charge transport in nano-structures described by non-Markovian generalized master equations. We illustrate our method by calculating the waiting time distribution of electron transport through a dissipative double quantum dot, where memory effects are present due to a strongly coupled heat bath. We consider the influence of non-Markovian dephasing on the distribution of electron waiting times and discuss how spectral properties of the heat bath may be detected through measurements of the electron waiting time.

HL 37.10 Tue 12:15 H20

Coherence and indistinguishability of single electron wavepackets emitted by independent sources — Erwann Bocquillon[1], Vincent Freulon[1], Jean-Marc Berroir[1], Pascal Degiovanni[2], Bernard Plaçais[1], Antonella Cavanna[3], Yong Jin[3], and •Gwendal Feve[1] — [1]Laboratoire Pierre Aigrain, Ecole Normale Supérieure, Paris, France — [2]Laboratoire de Physique de l Ecole Normale Supérieure de Lyon, Lyon, France — [3]Laboratoire de Photonique et Nanostructures, Marcoussis, France

Using two independent on-demand electron sources [1], two single-electron wavepackets are emitted on one-dimensional chiral edge channel located at at different inputs of an electronic beamsplitter. Whereas classical particles would be randomly partitioned by the splitter, we observe two-particle interferences resulting from quantum exchange in this electronic analog [2,3] of the optical Hong-Ou-Mandel [4] experiment. Both electrons, emitted in indistinguishable wavepackets with synchronized arrival time on the splitter, exit in different outputs as recorded by the low frequency current noise. Full random partitioning is recovered when the arrival of one electron is delayed with respect to the other. This two-electron interference experiment demonstrates the possibility to generate on-demand coherent and indistinguishable single-electron wavepackets in a quantum conductor.

[1] G. Fève et al., Science 316, 1169 (2007)
[2] Ol'khovskaya et al., Phys. Rev. Lett. 101, 166802 (2008)
[3] T. Jonckheere et al., Phys. Rev. B 86, 125425 (2012)
[4] C. K. Hong et al., Phys. Rev. Lett. 59, 2044 (1987)

HL 38: Organic electronics and photovoltaics II (DS, jointly with CPP, HL, O)

Time: Tuesday 9:30–12:45 Location: H32

HL 38.1 Tue 9:30 H32

Influence of triplet excitons on the lifetime of polymer based organic light emitting diodes — •Oili Pekkola, Andrea Gassmann, Christian Melzer, and Heinz von Seggern — Electronic Materials Division, Institute of Materials Science, Technische Universität Darmstadt, Petersenstr. 23, 64287 Darmstadt, Germany

Despite the promising development of polymer based organic light emitting diodes (PLEDs), device lifetime and stability are still among the most critical issues. One of the lifetime-related factors investigated to a lesser extent is the influence of the high density of non-emissive triplet excitons which could be responsible for local heating or act as traps for charge carriers, leading to a degradation of the device.

This study utilizes PLEDs based on poly(p-phenylene vinylene) (PPV) derivatives to understand the influence of triplet excitons on the fatigue by increasing their amount in the PPV film. This increase is achieved by blending different concentrations of the triplet sensitizer platinum (II) octaethylporphine ketone (PtOEPK) into the PPV matrix in order to convert PPV singlet excitons to triplets. One observes that in PLEDs both the t50 and t90 lifetimes are drastically shortened in the presence of PtOEPK. To rule out a possible influence of the sole presence of PtOEPK on charge carrier transport, single carrier devices with different sensitizer contents were prepared. In these devices, no fatigue is observed regardless of the sensitizer concentration, suggesting that the decrease in the lifetimes of the bipolar diodes is indeed caused by the increased triplet population in the diodes with sensitized polymer films and not by the sensitizer additive as such.

HL 38.2 Tue 9:45 H32

Homogeneity of thin ZnTPP-films on silicon measured with reflectance anisotropy spectroscopy and Raman spectroscopy — •Stephan Peter Kate[1], Simona Pop[1], Jörg Rappich[2], and Karsten Hinrichs[1] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Albert-Einstein Str. 9, Berlin, 12489 Germany — [2]Helmholtz-Zentrum for Materials and Energy GmbH, Kekulestraße 5, Berlin, 12489, Germany

Organic devices for electronic applications are an important field of research. To improve the efficiency of those components, the analysis of structure and homogeneity of thin films is of crucial importance. In this study we demonstrate that Reflectance Anisotropy Spectroscopy (RAS) and Raman spectroscopy are useful to investigate the homogeneity of thin films of zinc-tetra-phenyl-porphyrin (ZnTPP) on silicon substrates. The RAS spectra of the thin films show an optical anisotropy in the visible spectral range. Analyzing the anisotropy, conclusions about the homogeneity of the thin films can be drawn. The vibrational modes of the molecules seen with resonant Raman spectroscopy are sensitive to the film structure. A pyrrole-bending mode in the region of 1075 cm-1 serves us as a marker for the film homogeneity. The RAS and Raman results are correlated with AFM measurements.

HL 38.3 Tue 10:00 H32

Morphology evolution of diblock copolymer based ZnO nanostructures upon solvent vapor treatment — •Kuhu Sarkar, Christoph Schaffer, Anna Naumann, Daniel Mosegui Gonzalez, and Peter Müller-Buschbaum — TU München, Physik Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany

Nanostructured inorganic metal oxides with tunable morphologies are desirable for optimizing many potential applications in the field of gas/chemical sensing, catalysis and energy storage. Zinc oxide (ZnO) is chosen in the present study owing to its outstanding optical and electrical properties. Different ZnO nanostructures are synthesized using a suitable diblock copolymer template via sol-gel chemistry. Zinc acetate dihydrate is used as the suitable commercial precursor for ZnO. There are several possibilities to tune the morphology as most of the diblock copolymers respond to the external fields such as temperature and solvent vapor. Hence, tetrahydrofuran solvent vapor treatment has been employed to the as-prepared thin films corresponding a grid-like morphology for different annealing times. Grazing incidence small angle X-ray scattering (GISAXS) has been performed to probe the structural order over the entire film volume. Evolution of the morphology has been followed by GISAXS studies as a function of different solvent treatment times. The annealed films are subsequently calcined at a higher temperature in order to understand the preservation of higher orders in the ZnO structure even after removal of the diblock copolymer.

HL 38.4 Tue 10:15 H32

Correlation of morphology and electronic properties of MoO_3 doped CBP layers I: TEM and electrical properties — •Daniela Donhauser[1,2], Levin Dieterle[1,2], Paul Heimel[3,2], Tobias Glaser[3,2], Maybritt Kühn[4,2], Mustapha Al-Helwi[5,2], Rasmus R. Schröder[6], Eric Mankel[4,2], Michael Kröger[1,2], and Wolfgang Kowalsky[1,2] — [1]Institut für Hochfrequenztechnik, TU Braunschweig, Braunschweig — [2]InnovationLab GmbH, Heidelberg — [3]Kirchhoff-Institut für Physik, Universität Heidelberg, Heidelberg — [4]Institut für Materialwissenschaft, TU Darmstadt, Darmstadt — [5]BASF SE, Ludwigshafen — [6]CellNetworks, Universität Heidelberg

Since electrochemical doping can significantly improve the performance of organic devices, the understanding of the fundamental properties of doped thin films is crucial. For a variety of different material systems a very low doping efficiency was observed, although from energetical considerations a very efficient charge transfer is expected. Using bright-field TEM and electron tomography we show for MoO_3-doped CBP ((4,4'-Bis(N-carbazolyl)-1,1'-biphenyl) thin films that this low doping efficiency is due to filament-like dopant agglomeration which can be controlled by changing the substrate temperature during the evaporation process [1]. The observed morphology is finally correlated with electrical properties like charge carrier density and mobility and depending on the dopant concentration an anisotropic charge trans-

port is observed.
[1] Donhauser et al., Adv. Funct. Mater., 2012, 10.1002/adfm.201202089

HL 38.5 Tue 10:30 H32

Correlation of morphology and electronic properties of MoO_3-doped CBP layers II: IR spectroscopic study — •Tobias Glaser[1,5], Sebastian Beck[1,5], Daniela Donhauser[2,5], Maybritt Kühn[3,5], Bernd Lunkenheimer[4,5], Andreas Köhn[4,5], Eric Mankel[3,5], and Annemarie Pucci[1,5] — [1]Universität Heidelberg, Kirchhoff-Institut für Physik — [2]Technische Universität Braunschweig, Institut für Hochfrequenztechnik — [3]Technische Universität Darmstadt, Fachbereich Materialwissenschaft, Fachgebiet Oberflächenforschung — [4]Universität Mainz, Institut für Physikalische Chemie — [5]InnovationLab GmbH, Heidelberg

In order to obtain a further understanding on the charge transfer process in p-type doping using transition metal oxides, we performed in-situ FTIR-spectroscopy on thin layers of 4,4'-Bis(N-carbazolyl)-1,1'-biphenyl (CBP) doped with MoO_3. In the doped layers, charge transfer complexes (CTCs) are formed, that exhibit a broad electronic excitation in the near IR region. These CTCs are located at the interface of the MoO_3 agglomerates and the organic matrix, inducing an interface dipole. The intensity of this electronic excitation in the spectra of layers with various doping concentrations indicates a linear increase of the agglomerates' surface area with MoO_3 concentration. The vibrational changes in the spectra of the doped layers indicate a charge transfer of Z=1e within the CTCs. By cooling the substrate during the deposition process, the agglomeration of the dopants can be suppressed.
Financial support by BMBF (project MESOMERIE) is gratefully acknowledged.

HL 38.6 Tue 10:45 H32

Correlation of morphology and electronic properties of MoO_3-doped CBP layers III: XPS and UPS study — •Maybritt Kühn[1,4], Eric Mankel[1,4], Daniela Donhauser[2,4], Tobias Glaser[3,4], Thomas Mayer[1,4], and Wolfram Jaegermann[1,4] — [1]Technische Universität Darmstadt, Fachgebiet Materialwissenschaft — [2]Technische Universität Braunschweig, Institut für Hochfrequenztechnik — [3]Universität Heidelberg, Kirchhoff-Institut für Physik — [4]InnovationLab GmbH, Heidelberg

Electro-chemical doping is a prerequisite to improve efficiency and conductivity of organic OLED materials. Here the p-type doping behavior of MoO_3 is analyzed using photoelectron spectroscopy (XPS/UPS). The doped CBP layers were evaporated and analyzed under UHV conditions. Concerning the Fermi level shift three different regimes can be distinguished: At low doping concentrations (< 9 mol%) a rapid shift towards the HOMO level of CBP can be observed, becoming less strong and finally saturating at a maximum shift of 1 eV at a doping concentration of 45 mol%. The electron transfer from CBP to MoO_3 leads to the formation of reduced MoO_3. Determining the amount of these species we get information of the surface to volume ratio of the MoO_3 clusters in dependence of the doping concentration. Also here three different regimes can be distinguished. The morphology and Fermi level shift regimes will be correlated discussing the dopant morphology as shown in Talk I. Finally the amount of transferred charges is calculated regarding the reduced MoO_3 species and is compared with the number of cations determined by IR-spectroscopy (Talk II).

Coffee break (15 min)

HL 38.7 Tue 11:15 H32

Organic semiconductor devices on fibre shaped structures for smart textile applications. — •Tobias Könyves-Toth, Andrea Gassmann, and Heinz von Seggern — Electronic Materials Department, Institute of Materials Science, Technische Universität Darmstadt, Petersenstraße 23, 64287 Darmstadt, Germany

In the development of smart textiles already realized prototypes utilize embedded LEDs, displays or interactive communication devices based on inorganic semiconductor technology. Yet, these wearable smart textiles are not always comfortable since inorganic devices are stiff and rigid. On the other hand, organic electronic devices can be realized on flexible substrates employing very thin active layers of only about 100 nm thickness. The aim of the present work is to process organic semiconductor based devices directly on fibre surfaces. This task is challenging as manufacturing related problems due to the cylindrical shape of the fibre substrates and their small diameter of about 200 nm have to be overcome. Here, we present our findings on functional OLEDs on fibre substrates. Also the choice of proper fibre materials, ways to acquire smooth fibre surfaces and the structuring and encapsulation of fibre-shaped devices will be discussed. Additionally, methods to characterize the functionality of the devices, like angle dependence emission, will be presented.

HL 38.8 Tue 11:30 H32

Doping of organic semiconductors in case of dopant precipitation: the internal interface charge transfer doping model — •Thomas Mayer[1,2], Eric Mankel[1,2], Corinna Hein[1], and Wolfram Jaegermann[1,2] — [1]Technische Universität Darmstadt, Institute of Materials Science, Surface Science Division — [2]Innovation Lab Heidelberg

Doping of organic semiconductors is of paramount interest for device optimization as in addition to improved conductivity, engineering of space charge regions at interfaces e.g. of donor acceptor heterojunction solar cells is achieved. Photoemission data taken at the synchrotron BESSY on co-sublimed and bilayer films of prototypical organic semiconductors as CuPc and spiro-MeoTAD and prototypical p-type organic and inorganic dopants as TCNQ and WO3 show similar electronic trends, which can be explained assuming phase separation of the dopants within the matrix material. For metal oxides the precipitation is directly observed using TEM. For the doping induced variations of the matrix Fermi level in such semiconductor-dopant composites we propose the internal interface charge transfer doping model. According to this model the doping limit can be predicted from pristine matrix and pristine dopant electronic band diagrams. The model also admits of deriving measures that can be taken to improve doping efficiency.

HL 38.9 Tue 11:45 H32

Molecular orientation at heterojunctions for organic photovoltaics studied by NEXAFS — •Andreas Opitz[1], Norbert Koch[1], Ulrich Hörmann[2], Wolfgang Brütting[2], Christopher Lorch[3], Alexander Hinderhofer[3], Frank Schreiber[3], and Ellen Moons[4] — [1]Inst. f. Physik, Humboldt-Universität zu Berlin, Germany — [2]Inst. of Physics, University of Augsburg, Germany — [3]Inst. of Applied Physics, University of Tübingen, Germany — [4]Dept. of Physics and Electrical Engineering, Karlstad University, Sweden

Organic/organic heterojunctions are widely used in organic photovoltaic cells. The morphology at the interface, where the charge carrier separation takes place, plays an important role. In this contribution the interfaces between sexithiophene (6T) as donor and the acceptor materials fullerene (C_{60}) and diindenoperylene (DIP) [1] were analysed by angle resolved near-edge X-ray absorption fine structure spectroscopy and the results were compared to X-ray scattering data.

Different orientations are observed for molecules in the bulk, at free surfaces and at buried interfaces. Here, the orientation at the free surfaces depends on the substrate temperature during deposition for 6T but not for DIP. Furthermore, the acceptor molecules influence the orientation of the underlying 6T molecules. An improved crystallization and pronounced upright standing of the molecules in the underlying 6T film was observed upon deposition of C_{60}. In contrast the deposition of DIP on top of 6T leads to an orientational relaxation of the 6T molecules to the bulk inclination angle.
[1] U. Hörmann et al., phys. stat. sol. RRL 5 (2011) 241.

HL 38.10 Tue 12:00 H32

Electronic interface properties of PCBM using photoelectron spectroscopy — •Julia Maibach[1,2], Eric Mankel[1,2], Thomas Mayer[1,2], and Wolfram Jaegermann[1,2] — [1]Technische Universität Darmstadt, Fachbereich Materialwissenschaft — [2]InnovationLab GmbH, Heidelberg

The electronic interface properties of wet processed organic materials are of current interest as many fabrication techniques for organic electronic devices are based on inks. Photoelectron spectroscopy (PES) has proven to be a powerful method to investigate the electronic structure at semiconductor contacts. Due to high surface sensitivity of PES, the interface is generally prepared step by step in UHV. For films deposited from solution we integrated a newly developed ultrasonic nebulizer unit to the UHV cluster-tool of the analytic competence center at the InnovationLab, Heidelberg. Dilute solutions of Phenyl-C61-butyric acid methyl ester (PCBM) in Chlorobenzene were used to deposit the material on ozone and polymer treated ITO as well as on gold to investigate the contact behavior of PCBM. With the nebulizer method layer thicknesses in the range of 10-20 Å can be achieved while repeated exposure to the nebulae increased step by step the emission

intensities of the PCBM. Furthermore drop-casting of thicker layers has been performed allowing in combination the thickness dependent determination of the electronic properties. In case of PCBM on ozone treated ITO the HOMO spectra shift 0.4 eV to higher binding energy with increasing thickness, indicating the formation of a space charge region in PCBM due to electron transfer from ozone treated ITO.

HL 38.11 Tue 12:15 H32

Carbon Nanotubes and Organic Solar Cells — •Gerhard Lackner[1], Richard Boucher[2], Vladimir Shvartsmann[1], Viktor Bezugly[2], Ingolf Endler[3], Mario Krug[3], Frank Meissner[3], Martin Mkandawire[4], and Doru C. Lupascu[1] — [1]Universität Duisburg-Essen, Essen, Germany — [2]Technische Universität Dresden, Dresden, Germany — [3]Fraunhofer-Institut für Keramische Technologien und Systeme IKTS, Dresden, Germany — [4]Verschuren Centre for Sustainabilty in Energy and the Environment, Cape Breton University, Canada

Materials like carbon nanotubes (CNT) attracted much attention by researchers all around the world due to their exceptional electrical, mechanical and chemical properties. Especially single-walled carbon nanotubes (SW-CNT) offer great opportunities in the field of new electrical devices, for instance field effect transistors based on their semiconductor properties. CNT are also used in organic photovoltaics (OPV) as acceptor material, to enhance charge carrier transport within organic layers or as transparent electrodes. The application of CNT as acceptor material and for charge carrier enhancement is the main topic of this work. Therefore, we studied the photovoltaic device performance of different material combinations of CNT, regio regular Poly(3-Hexylthiophen-2,5-diyl) (rr-P3HT), Phenyl-C61-butric acid methyl ester (PCBM) and copper phthalocyanine (CuPc). Furthermore, different device architectures were investigated and compared with each other.

HL 38.12 Tue 12:30 H32

n-channel percolation in a pentacene-C60 ambipolar organic thin film transistor — Simon Noever, Stefan Fischer, and •Bert Nickel — Ludwig-Maximilians-Universität, Fakultät für Physik & CENS, München, D

We present [1] a well balanced ambipolar organic field effect transistor with high hole and electron saturation mobilities of 0.28 cm*/Vs and 0.18 cm*/Vs, respectively. The structure and morphology of the respective films are analyzed using AFM and GIXS methods. Furthermore, we track the formation of a pentacene-C60 heterojunction by in-situ measurements during deposition of C60. Upon percolation of the n-channel, the heterojunction charges, acting as an additional top gate for the hole conducting channel. The fact that the p-channel threshold does not shift before the n-channel develops highlights two interesting findings for bilayer ambipolar TFTs. Apparently, before the C60 film percolates, the fullerene islands are electronically floating and the charging of the interface is confined to the pentacene-C60 contact area. Secondly, the threshold voltage shift of the p-channel upon fullerene percolation implicates the generation of a second hole conducting channel at the pentacene top surface. The introduced method demonstrates a way to evaluate the electrostatic situation in operating organic heterojunction devices. [1] S. Noever, S. Fischer, B. Nickel, Advanced Materials (in press)

HL 39: Optical properties

Time: Tuesday 10:15–12:45 Location: H13

HL 39.1 Tue 10:15 H13

Optical properties of $Ga_{1-x}Mn_xAs$ from large scale ab initio calculations — •Jerome Jackson, Ricardo Cárdenas, and Gabriel Bester — Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany.

The properties of Mn impurities in GaAs are revisited employing a new methodology based on atomic effective potentials (AEPs [1]) which yields LDA accuracy at considerably reduced computational expense. We consider the case of very low Mn concentrations that cannot be considered using conventional ab initio methods and discuss the metal/insulator transition in terms of the Mn-d band localisation and its interpretation as a shallow acceptor. We discuss practical methods to improve upon the LDA bandgap in GaAs together with the excessive delocalisation of the Mn states. Using a configuration-interaction technique we calculate the optical spectra of $Ga_{1-x}Mn_xAs$ including the fine-structure (FSS) splitting which is of importance to the development of quantum computing devices based upon magnetic impurities in semiconductors[2].
[1] J. R. Cárdenas and G. Bester, Phys. Rev. B **86**, 115332 (2012)
[2] D. E. Reiter, T. Kuhn and V.M. Axt, Phys. Rev. B **83**, 155322 (2011)

HL 39.2 Tue 10:30 H13

Raman scattering study of phonon-polaritons in wurtzite GaN — •Christian Röder, Gert Irmer, Cameliu Himcinschi, and Jens Kortus — TU Bergakademie Freiberg, Institute of Theoretical Physics, Leipziger Str. 23, D-09596 Freiberg, Germany

Reports on Raman measurements of polaritons in uniaxial semiconductors are scarce. However, the Raman scattering efficiency of polaritons can be described taking both into account, an atomic displacement term and an electro-optic contribution which depends very strongly on the polariton frequency. The relation between the atomic displacement tensor components and the electro-optic ones is expressed using the Faust-Henry coefficients. According to the symmetry of wurtzite GaN three different Faust-Henry coefficients are implied. In order to specify charge carrier concentration and mobility in GaN by Raman spectroscopy the values of these parameters are required but they are still debated. In this work we present Raman scattering results on phonon-polaritons in single crystals of wurtzite GaN. The experiments were conducted in near-forward scattering geometry. Measurements of ordinary and extraordinary polaritons with defined symmetry could be performed. The observed dispersion curves and scattering efficiency results are compared with theoretical ones. 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.

HL 39.3 Tue 10:45 H13

Intensity fluctuations of a semiconductor laser at threshold - accessing critical dynamics with higher order noise spectroscopy — Sebastian Starosielec, Jörg Rudolph, and •Daniel Hägele — AG Spektroskopie der kondensierten Materie, Ruhr-Universität Bochum, Bochum, Germany

We investigate the intensity fluctuations $I(t)$ of an electrically driven single mode vertical cavity emitting laser that serves as a model system for critical dynamics at a second order phase transition [1]. Simulations of the fourth order frequency resolved correlation spectrum $S^{(\mathrm{corr})}(\omega,\omega') = \langle I_\omega I_\omega I_{\omega'} I_{\omega'}\rangle - \langle I_\omega I_\omega\rangle\langle I_{\omega'} I_{\omega'}\rangle$ reveal a characteristic structure in the spectrum at threshold and almost no structure below and above threshold. Measurements of $S^{(\mathrm{corr})}(\omega,\omega')$ with a bandwidth of 90 MHz and real time data processing (see [2]) are in good agreement with theory for all investigated lasers. Making use of modern electronics and data processing, we resolve for the first time pump-dependent features in a fourth order spectrum that were inaccessible before. Our experimental approach may open new routes for investigating temporal fluctuations at phase transitions in many systems including magnets and superconductors.
[1] V. DeGirogio and M. O. Scully, Phys. Rev. A **2**, 1170 (1970)
[2] S. Starosielec *et al.*, Rev. Sci. Instrum. **81**, 125101 (2010)

HL 39.4 Tue 11:00 H13

Fabrication and characterization of GaAs-based Air-Bragg microcavity structures — •Jonas Gessler[1], Arkadiusz Piotr Mika[1,2], Julian Fischer[1], Matthias Amthor[1], Alfred Forchel[1], Jan Misiewicz[2], Sven Höfling[1], Christian Schneider[1], and Martin Kamp[1] — [1]Julius Maximilian Universität Würzburg — [2]Wroclaw University of Technology

The high index contrast between Air and Gallium-Arsenide (GaAs) can lead to an enhanced photon confinement compared to GaAs/ Aluminum-Arsenide Bragg microcavities. This can be used to reduce the effective mode volume and to enhance light matter coupling effects in a GaAs/Air Bragg system with active quantum well (QW) emitters. We will present the fabrication of freely suspended GaAs/Air structures with Q-factors exceeding 1000. Various strategies for in-

plane photon confinement are demonstrated experimentally, resulting in photonic structures with quasi 2D, 1D and 0D characteristics. We finally demonstrate laser emission from weakly coupled QW-GaAs/Air Bragg systems and discuss indications for the formation of QW-exciton polaritons in our novel system.

HL 39.5 Tue 11:15 H13

Investigation of the strong coupling regime in GaAs microcavities up to room temperature — •Sebastian Brodbeck[1], Jan-Philipp Jahn[1], Arash Rahimi-Iman[1], Julian Fischer[1], Matthias Amthor[1], Stephan Reitzenstein[1,2], Christian Schneider[1], Martin Kamp[1], and Sven Höfling[1] — [1]Technische Physik, Physikalisches Institut and Wilhelm Conrad Röntgen-Research Center for Complex Material Systems, Universität Würzburg, Am Hubland, 97074 Würzburg — [2]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin

We study the strong coupling regime in a microcavity with GaAs quantum wells in the full temperature region between 4K and room temperature. Pronounced anticrossing of the polariton branches in reflection measurements is observed for all investigated temperatures. The temperature dependence of the vacuum Rabi splitting is reproduced by a simple equation with one fitting parameter. At room temperature we measure a vacuum Rabi splitting of more than 6meV.

The strong coupling regime at room temperature is also observed in an electrically driven sample whose electroluminescence shows two well resolved polariton branches. This device features an innovative pumping scheme where a reversely biased Esaki diode is placed in the cavity region in order to improve the electric pumping of the spatially separated quantum well stacks. The mixed light-matter nature of the emitting states is confirmed in photoluminescence measurements with varying bias where a Stark shift of up to 4meV is observed for both polariton branches.

Coffee break

HL 39.6 Tue 11:45 H13

Rolled-up microtubes for light-matter interaction with colloidal quantum dots — •Stefanie Kietzmann[1], Christian Strelow[1], Andreas Schramm[2], Jussi-Pekka Penttinen[2], Alf Mews[1], and Tobias Kipp[1] — [1]Institute of Physical Chemistry, University of Hamburg, Germany — [2]Optoelectronics Research Centre, Tampere University of Technolgy, Tampere, Finland

We report on rolled-up AlInP microtube resonators that can be coupled to colloidal nanocrystals emitting in the visible spectral range. These emitters can couple to the evanescent fields of the modes propagating in the very thin microtube walls, leading to sharp optical modes in the emission spectra due to constructive interference. Microtubes are fabricated by utilizing the self-rolling mechanism of expitaxally grown strained layer systems induced by selective chemical undercutting. Three-dimensional light confinement by various axial structurings of the tube geometry allows for a full control over the optical eigenmodes. As the mode energies of the spectra sensitively depend on the refractive index of the tube's filling, microtube resonators can be used as refractive index sensors. We present a successful coupling of colloidal nanocrystals to the evanescent fields of AlInP microtubes shown by sharp resonances in the observed spectrum. Moreover, the refractometer properties of the microtubes are demonstrated by comparing the observed mode shift due to a well-known refractive index change to 2D FDTD simulations [1].

We acknowledge financial support by the DFG via Ki1257/1.

[1] Ch. Strelow et.al., Appl. Phys. Lett. 101, 113114 (2012)

HL 39.7 Tue 12:00 H13

Theory of Metal Nano-Particle Affected Optical Properties of Supramolecular Complexes — •Yaroslav Zelinskyy, Gerold Kyas, Yuan Zhang, and Volkhard May — Institut für Physik, Humboldt Universität zu Berlin, Newtonstrasse 15, D-12489 Berlin, Germany

Optical and transport properties of supramolecular complexes (SC) placed in the vicinity of a metal nanoparticle (MNP) are investigated by applying a density matrix approach. This enables a nonperturbative consideration of the excitation energy transfer coupling in the SC as well as between the SC and the MNP. The coupling can be described in terms of a shift and a broadening of all Frenkel exciton levels together with a remarkable oscillator strength change. In particular the latter effect becomes clearly observable in absorption and emission spectra and explains the MNP induced enhancement of molecular spectra. Resulting from the absorption enhancement sub-picosecond laser pulse induced spatio-temporal excitation energy localization in the SC near a MNP is predicted. The importance of MNP multipole excitations is underlined at several places. The exact description of the interacting SC MNP coupling is confronted with a mean–field approximation which directly leads to a local field description of the effect of the MNP on an individual molecule. (Y. Zelinskyy, Y. Zhang and V. May, J. Phys. Chem. A 116, 11330 (2012), G. Kyas, Y. Zelinskyy, Y. Zhang, V. May, Ann. Phys. (in press), Y. Zelinskyy, Y. Zhang and V. May, J. Chem. Phys. (submitted)).

HL 39.8 Tue 12:15 H13

Photoconductance properties of gold nanorod arrays — •Sandra Diefenbach[1], Daniela Iacopino[2], Johannes Schopka[1], and Alexander Holleitner[1] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, 85748 Garching b. München, Germany — [2]Tyndall National Institute, Lee Maltings, University of Cork, Ireland

Gold nanorods are fabricated by dielectrophoretic self-assembly [1] and contacted by gold contacts. Conductance measurements in the dark confirm thermally activated transport at room temperature. At low temperature, a dominating Coulomb blockade is observed [2]. The photoconductance of the nanorod arrays depends linearly on laser power and exponentially on temperature. The photoconductance experiments allow us to clarify the impact of the longitudinal plasmon frequency of the nanorods on the optoelectronic properties of the arrays. Financial support by the grant HYSENS is acknowledged.

[1] A. Pescaglini et al. J. of Phys. Conf. Ser., 307, 012051 (2011).

[2] M. Mangold, M. Calame, M. Mayor, A.W. Holleitner, ACS Nano 6, 4181 (2012).

HL 39.9 Tue 12:30 H13

Giant enhancement of Pentacene (PEN) Raman scattering and fluorescence emission induced by plasmonic properties of gold Fischer patterns — Jan Rogalski, Andreas Kolloch, Paul Leiderer, Katharina Broch, Frank Schreiber, Alfred J. Meixner, and •Dai Zhang — Institute of Physical and Theoretical Chemistry, Uni. Tübingen, Tübingen

Fischer patterns are metallic nanostructures composed of a network of hexagonal aligned triangles. We studied the plasmonic effects of gold Fischer patterns regarding the substrate and its polarization effects via monitoring the photoluminescence (PL) spectral profile and intensity. The excitation of the Fischer patterns shows strong substrate dependence. On silicon substrates, the PL of Fischer patterns is much weaker than on glass substrates. By using a radially or azimuthally polarized laser beam, we selectively excite the center or corner plasmonic modes of the nanotriangles that make up the Fischer patterns. PEN is a commonly studied optoelectronic material which has found wide-spread application in light emitting diodes or solar cell research. Our experiments clearly show a giant enhancement of the Raman scattering and PL signal from PEN deposited on a Fischer pattern surface. A detailed analysis, entailing the enhancement factor and the plasmon-polariton coupling between the Fischer pattern and the PEN thin film will be presented.

HL 40: Focus Session: Frontiers of electronic structure theory III (O, jointly with HL, TT)

Time: Tuesday 10:30–13:15 Location: H36

Topical Talk HL 40.1 Tue 10:30 H36

Materials for Alternative Energies: Computational Materials Discovery and Crystal Structure Prediction — •Chris Wolverton — Northwestern University, Evanston, IL, USA

Many of the key technological problems associated with alternative energies may be traced back to the lack of suitable materials. The materials discovery process may be greatly aided by the use of computational methods, particular those atomistic methods based on density functional theory. In this talk, we present an overview of recent work on energy-related materials from density-functional based approaches. We have developed novel computational tools which enable accurate prediction of crystal structures for new materials (using both Monte Carlo and Genetic Algorithm based approaches), materials discovery via high-throughput, data mining techniques, and automated phase diagram calculations. We highlight applications in the area of Li battery materials and hydrogen storage materials.

HL 40.2 Tue 11:00 H36

Doping at the Si-SiO2 interface — Fabiano Corsetti[1] and •Arash Mostofi[2] — [1]CIC nanoGUNE Consolider, Donostia-San Sebastian, Spain — [2]Dept. of Materials & the Thomas Young Centre for Theory and Simulation of Materials, Imperial College London, UK

The Si-SiO2 interface is a common feature in modern silicon-based CMOS technology for the fabrication of integrated circuits. The ongoing miniaturisation drive for such devices makes it increasingly important to understand the effect of the interface on the dopant distribution and properties. Indeed, in some cases channel lengths can be a few tens of nanometres, with the device properties being determined by only about 100 dopant atoms.

We have investigated the properties of arsenic dopants at the Si-SiO2 interface. We use a large supercell to simulate both ordered (α-cristobalite) and disordered silica interfaces with crystalline Si. The disordered interface is generated using a multiscale approach in which a Monte Carlo method, parametrised with density-functional theory (DFT) calculations, is used to access the long time scales required for amorphising the oxide. The segregation of arsenic dopants in silicon at the interface is then studied using DFT.

We are able to accurately characterise the long-range quantum confinement effect due to the interface, which is found to result in a small energy barrier for segregation. We also investigate the effect of the local stress at the defect site on its segregation energy, and show that a simple 'particle in a box' model can be used to explain the calculated segregation energies at all substitutional silicon sites.

HL 40.3 Tue 11:15 H36

Pressure-induced structural transformations in nanomaterials: a linear-scaling DFT investigation — •Niccolo Corsini[1], Peter Haynes[1], Carla Molteni[2], and Nicholas Hine[1] — [1]Imperial College, London, UK — [2]King's College, London, UK

Semiconductor nanomaterials, including nanocrystals, nanorods and tetrapods, display a number of peculiar and tunable properties that distinguish them from their bulk counterparts and make them versatile materials for use as e.g. effective optical probes in medical diagnostics or photovoltaic devices. Of particular interest is their response to applied pressure, as they transform from one crystalline or amorphous structure to another. Accurate simulations are important for understanding finite size effects in the atomistic mechanisms of phase transformations (difficult to observe clearly in macroscopic experiments), for the opportunity to uncover novel metastable phases stabilized in finite systems, and for potentially innovative applications of nanomaterials. First-principles methods are essential to accurately describe the bond breaking/making in phase transformations and the realistic description of surfaces (often covered by complex surfactants). However the computational cost limits both the length- and time-scales attainable. We have combined an order-N density functional theory code for large systems and an electronic-enthalpy method to apply pressure to finite systems to model with quantum mechanical precision processes induced by pressure in nanomaterials (including their surfaces) under realistic conditions. The focus is on Si, CdSe and CdS nanocrystals that are currently favoured for technological applications.

HL 40.4 Tue 11:30 H36

Density functional / molecular dynamics simulations of nucleus-driven crystallization of amorphous Ge2Sb2Te5 — •Jaakko Akola[1,2,3], Janne Kalikka[4], Julen Larrucea[4], and Robert O. Jones[3] — [1]Department of Physics, Tampere University of Technology, Finland — [2]COMP Centre of Excellence, Department of Applied Physics, Aalto University, Finland — [3]GRSS and PGI-1, Forschungszentrum Jülich, Germany — [4]Nanoscience Center, Department of Physics, University of Jyväskylä, Finland

Early stages of nucleus-driven crystallization of the prototype phase change material Ge2Sb2Te5 have been studied by massively-parallel density functional/molecular dynamics simulations for amorphous samples (460 and 648 atoms) at 500, 600, and 700 K [1]. All systems assumed a fixed cubic seed of 58 atoms and 6 vacancies in order to achieve sub-nanosecond phase transition. Crystallization occurs within 600 ps for the 460-atom system at 600 and 700 K, and signs of crystallization (nucleus growth, percolation) are present in the others. Crystallization is accompanied by an increase in the number of ABAB squares (A: Ge, Sb, B: Te) [2,3], and atoms of all elements move significantly. The evolution of cavities/vacancies is closely monitored. The existence of Te-Te, Ge-Ge, Ge-Sb, and Sb-Sb (wrong) bonds is an inevitable consequence of rapid crystallization.

[1] J. Kalikka, J. Akola, J. Larrucea, and R. O. Jones, Physical Review B 86, 144113 (2012). [2] J. Akola and R. O. Jones, Phys. Rev. B 76, 235201 (2007). [3] J. Akola and R. O. Jones, Phys. Rev. Lett. 100, 205502 (2008).

HL 40.5 Tue 11:45 H36

Large-Scale Moiré Patterns of hexagonal Boron Nitride on Cu(111): DFT Studies of Structural and Electronic Properties — •Ralph Koitz, Ari P Seitsonen, Marcella Iannuzzi, and Jürg Hutter — Institute of Physical Chemistry, University of Zurich, Switzerland

Hexagonal boron nitride (h-BN) adsorbed on metal surfaces shows great promise for applications in nanoscience. Interesting structural and electronic properties have been found, e.g. for h-BN on Rh(111) and Ru(0001), where the overlayer is strongly corrugated. Recent experiments with h-BN on Cu(111) indicate that the difference in lattice constants and a rotation of the monolayer lead to moiré patterns with periodicities greater than 5 nm. To thoroughly understand this system, however, further insight is needed at the atomic level.

In this contribution we present an in-depth DFT study of a moiré pattern of a rotated 24×24 h-BN sheet on a 23×23 Cu(111) slab. The periodic pattern extends over 6 nm, making this simulation the largest of its kind so far reported. We study the gradual change of adsorption registry of the monolayer, and its influence on the electronic structure. Both B and N occupy the entire range of *top, hcp, fcc*, and bridging positions. This modulation over the unit cell is reflected in the projected DOS, the electrostatic potential, and the contrast in simulated STM images. Contrary to other h-BN/metal systems, only minute structural changes occur upon adsorption. Our results show that the observed corrugation is chiefly electronic in nature and strongly related to the lateral variation of adsorption registries.

HL 40.6 Tue 12:00 H36

A computational perspective for the development of electronic excited-states calculations — •Xavier Andrade — Department of Chemistry and Chemical Biology, Harvard University, Cambridge, United States

In this talk I present different aspects of my work, focused on improving electronic structure theory for excited states with the aim of making it suitable for current computer architectures.

First, I will present an approach to approximate the exchange and correlation (XC) term in density functional theory. In this approach the XC potential is considered as an electrostatic potential. Based on this representation we develop a scheme that fixes the asymptotic behavior of an approximated XC potential. Additionally, from the procedure it is possible to extract the derivative discontinuity of the XC potential to directly obtain the gap of atoms and molecules.

Real-time methods like molecular dynamics and real-time time-dependent density functional theory are a good alternative for computing response properties. However, long propagation times are needed to obtain resolved properties. As a second topic of this talk, we ad-

dress this problem by using a state-of-the-art signal-analysis technique: compressed sensing. By using this method instead of a Fourier transform, we find that the total propagation time required for resolved spectra can be reduced by a factor of five.

Finally, I will discuss my work on electronic structure calculations on graphical processing units (GPU) and the strategies to profit from the data parallelism available in the density functional formalism.

HL 40.7 Tue 12:15 H36

Nuclear quantum effects in first principles molecular dynamics by colored-noise thermostats — •Michele Ceriotti — University of Oxford, United Kingdom

Oftentimes atomistic computer simulations treat atomic nuclei as purely classical particles, even when the electronic structure problem is treated quantum mechanically. This is a very good approximation when the system contains only heavy atoms. However, lighter nuclei such as hydrogen exhibit a strong quantum behavior, which manifests itself as sizable zero-point energy, tunnelling, isotope effects, etc.

Path integral methods are the state-of-the-art technique to model quantum nuclei, but they are computationally very demanding. Here I will discuss how a correlated-noise Langevin dynamics can be used to approximate nuclear quantum effects inexpensively, and how it can reduce by an order of magnitude the cost of quantitatively accurate path integral molecular dynamics. I will also present applications to the simulation of nuclear quantum effects in hydrogen-bonded materials by ab initio molecular dynamics.

HL 40.8 Tue 12:30 H36

Semiconductor and Metal-Oxide Nanocrystal Simulations with Linear-Scaling PAW DFT — •Nicholas Hine — Department of Materials, Imperial College London, Exhibition Road, London SW7 2AZ, United Kingdom — Cavendish Laboratory, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom

Nanocrystals enable tuning of material properties by varying attributes not available in bulk crystals, such as size, shape and surface termination, and such systems have innumerable applications in the field of energy materials, particularly in photovoltaics and photocatalysis. While whole nanocrystals are too large to be studied with traditional cubic-scaling first-principles methods, linear-scaling formulations of density functional theory (LS-DFT) enable the study of systems of many thousands of atoms. This allows nanocrystal simulations to make contact with the realistic size regime of 5-10nm, thus overlapping with the feasible scale of experimental characterisation and control. I will discuss recent developments in the ONETEP LS-DFT code that enable these large-scale, high-accuracy simulations, including the Projector Augmented Wave method, and recent applications to TiO2 nanocrystals, pressure-induced phase transformations in II-VI semiconductor nanocrystals, and wurtzite-structure III-V semiconductor nanorods. I will discuss the origin of the large dipole moments which can be observed in such structures, and show how an effect akin to Fermi-level pinning can have a determining influence on the overall polarisation, explaining its variation with size, shape, surface chemistry and composition.

HL 40.9 Tue 12:45 H36

Many-body effects on the carrier dynamics of graphene — •Cheol Hwan Park — Department of Physics and Astronomy, Seoul National University, Seoul, Korea

It is very important to understand how a charge carrier in real materials interacts with other charge carriers or with the lattice vibration. In this presentation, I will explain that the measured carrier scattering rate versus energy behavior in graphene can be quantitatively described from first-principles calculations considering electron-electron interactions within the GW approximation and electron-phonon interactions within the Migdal approximation [1]. Then, I will show that our calculation can also explain (i) the mismatch between the extrapolations of the upper and lower Dirac cones in heavily doped graphene [2] and (ii) the significant deviation from linear energy dispersion in extremely low-doped graphene [3]. Last, I will show that first-principles calculations on the intrinsic electrical resistivity of graphene arising from electron-phonon interactions [4] can quantitatively explain the transport experiments on heavily doped graphene [5].

[1] C.-H. Park, F. Giustino, M. L. Cohen, and S. G. Louie, Phys. Rev. Lett. 99, 086804 (2007).

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[5] D. K. Efetov and P. Kim, Phys. Rev. Lett. 105, 256805 (2010).

HL 40.10 Tue 13:00 H36

Theory of nanomagnetic and graphene hybrid systems: adatoms and multiorbital Kondo physics — •Tim Wehling — Institute for Theoretical Physics and BCCMS, University of Bremen, D-28359 Bremen, Germany

Graphene combines chemical inertness with a distinctly symmetric low energy electronic structure. Here, we show based on first-principles calculations that these two characteristics largely determine its interaction with adatoms. We find that covalent bonds to first row elements cause midgap states which can control electron transport [1] and the dielectric properties [2] of graphene based systems. The special nature of the Dirac electrons furthermore governs the coupling of magnetic adatoms to graphene by orbital selection rules and leads to peculiar multiorbital Kondo physics [3,4]. Finally, it is shown how multiorbital effects control the physics of magnetic transition metal atoms coupled to normal metals [5] and topological insulators [6].

[1] T. O. Wehling et al., Phys. Rev. Lett. 105, 056802 (2010).
[2] S. Yuan et al., Phys. Rev. Lett. 109, 156601 (2012).
[3] T. O. Wehling et al., Phys. Rev. B 84, 235110 (2011).
[4] T. O. Wehling et al., Phys. Rev. B 81, 115427 (2010).
[5] B. Surer et al., Phys. Rev. B 85, 085114 (2012).
[6] J. Honolka et al., Phys. Rev. Lett. 108, 256811 (2012).

HL 41: Quantum dots and wires: Preparation and characterization

Time: Tuesday 11:15–12:45 Location: H15

HL 41.1 Tue 11:15 H15

Towards III-V semiconductor nanowire field effect transistors: Atomic layer deposition of Al_2O_3 on InAs nanowires — •Torsten Jörres[1,2], Torsten Rieger[1,2], Detlev Grützmacher[1,2], and Mihail Ion Lepsa[1,2] — [1]Peter Grünberg Institut - 9, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology

Nanowire field effect transistors require thin gate dielectric films with a low density of interface states. Here, the use of Al_2O_3 prepared by atomic layer deposition (ALD) is promising due to a self-cleaning mechanism resulting in a reduction of the native oxides and a good thickness control. In this presentation, we demonstrate the processing of InAs nanowires covered homogeneously by amorphous Al_2O_3. The InAs nanowires are grown by a vapour-solid mechanism in a molecular beam epitaxy system. The Al_2O_3 is deposited ex-situ in the ALD machine. Trimethylaluminum and ozone are used as precursors. In advance, deposition experiments on silicon substrates were performed to optimise the Al_2O_3 layer using XRR, ellipsometry and CV measurements for characterisation. High resolution transmission electron microscopy investigations on nanowires covered with Al_2O_3 show the high uniformity of the deposition process even for high nanowire density. Further on, we demonstrate a process for contacting single nanowires with source, drain and gate contacts using only one metallization step. Preliminary DC measurement results on processed devices are presented and discussed.

HL 41.2 Tue 11:30 H15

Different Approaches for Uncovering InAs/AlAs Quantum Dots — •Evgeniya Sheremet[1], Raul D. Rodriguez[1], Torsten Jagemann[2], Wolfgang Grünewald[3], Doreen Dentel[2], Alexander Toropov[4], Alexander Milekhin[4], and Dietrich R.T. Zahn[1] — [1]Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany — [2]Solid Surfaces Analysis, Chemnitz University of Technology, D-09107 Chemnitz, Germany — [3]Leica Mikrosysteme GmbH, 1170 Vienna, Austria — [4]Institute of Semicon-

ductor Physics, 630090 Novosibirsk, Russia

The versatile capability of tuning energy band-gap by changing size, and composition makes quantum dot (QD) materials of significant technological impact. In this work, towards the study of electronic, structural and vibrational properties of a single QD, we performed experimental investigations of InAs (AlAs) QD in AlAs (InAs) matrix prepared by molecular beam epitaxy on GaAs substrates. We report on the systematic investigation of different surface preparation methods including crystal cleavage, ion milling, and mechanical polishing and their effect on the QD superlattice topography. We found that the less invasive sample processing method, namely crystal cleavage, provides very good surface structure but fails for the structures with growth defects. In this case the most optimal QD surface is achieved by ion milling at low temperature and low ion energy, what is revealed by atomic force microscopy. The structural defects introduced by preparation on QD superlattices, as well as degradation over time were investigated using Raman spectroscopy.

HL 41.3 Tue 11:45 H15

MOVPE growth of InGaAs quantum dots on GaP for nanomemory cells — •Gernot Stracke, Bertram Jaeger, Tobias Nowozin, Leo Bonato, Sven Rodt, Andrei Schliwa, Andre Strittmatter, Christopher Prohl, Andrea Lenz, Holger Eisele, Udo W. Pohl, and Dieter Bimberg — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

InGaAs quantum dots (QDs) are realized on GaP(001) substrates by metalorganic vapor phase epitaxy. A prospective application of such QDs is the fabrication of nanomemory cells. These QD memory cells promise to combine the fast write and erase times of a DRAM with the non-volatility of a Flash memory. By replacing GaAs with GaP as matrix material, an extension of the storage time of holes in InAs QDs at room temperature from 0.5 ns to 1 s can be expected. Additionally, GaP offers the potential of integration with Si, since GaP and Si have almost the same lattice constant. The growth of coherent InGaAs QDs on GaP is found to depend critically on the deposition of a thin layer of GaAs prior to QD growth. On a bare GaP substrate the growth proceeds purely two-dimensional even for high indium concentrations of up to 83%. In contrast, Stranski-Krastanow growth of InGaAs QDs is observed already for indium concentrations as low as 25% when the surface of the GaP substrate is covered by 3 monolayers (ML) of GaAs. $In_{0.25}Ga_{0.75}As$/3 ML GaAs/GaP QDs exhibit luminescence around 1.9 eV. The storage time of holes in $In_{0.25}Ga_{0.75}As$/3 ML GaAs/GaP QDs is estimated to 3 μs at room temperature.

HL 41.4 Tue 12:00 H15

High density (Ga,In)As/GaP self-assembled quantum dots — •Matthias Heidemann, Sven Höfling, and Martin Kamp — Technische Physik and Wilhelm-Conrad-Röntgen-Research Center for Complex Material Systems, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The large lattice mismatch between usual III/V materials and Si is one of the most important issues considering defect-free nucleation of layer structures for monolithic integration with Si CMOS technology. Among the III/V materials, GaP offers the lowest lattice mismatch to Si with only 0.37% at 300K and the incorporation of 2% nitrogen results in a perfect lattice match to Si. Since GaP has an indirect bandgap, a direct bandgap III/V material epitaxially grown on GaP is required and various materials and nanostructures have been proposed. Dilute Nitride Materials are used to enhance the direct bandgap character in GaAsPN/GaP and GaInPN/GaP quantum wells. By using quantum dots (QDs) the growth of larger lattice-mismatched nanostructures is possible, resulting in a direct bandgap without the incorporation of nitrogen.

In this work self-assembled InGaAs QDs embedded in GaP have been grown using molecular beam epitaxy. Based on these QDs, light emitting diodes and laser structures were fabricated and characterized. The latest results show QDs with a high density of $8.2 * 10^{10} cm^{-2}$ and photo-/electroluminescence signal up to room temperature.

HL 41.5 Tue 12:15 H15

Whispering gallery modes in zinc-blende AlN microdisks embedded with cubic GaN quantum dots — •Matthias Bürger, Marcel Ruth, Stefan Declair, Cedrik Meier, Jens Förstner, and Donat Josef As — Universität Paderborn, 33098 Paderborn, Deutschland

Optical microcavities, like semiconductor microdisks offer applications in quantum information technology as well as low threshold lasing devices. Microdisks support strong confined whispering gallery modes (WGM). In the case of group III-nitrides only microdisks of wurtzite AlN/InN/GaN have been fabricated up to now. However, piezoelectric and spontaneous polarization fields in the polar (0001) c-direction of hexagonal GaN induce a Quantum Confined Stark Effect. These built-in electric fields influence the behavior of optoelectronic devices containing quantum dots (QDs). The recombination probability of electrons and holes is reduced due to a spatial separation of electron and hole wave functions and limits the performance of photonic devices. Therefore, the fabrication of real non-polar metastable cubic GaN (c-GaN) and AlN (c-AlN) in (001) growth direction is very interesting for future applications. To improve the light extraction efficiency QDs can be integrated into microdisks. This work reports on the growth of c-AlN layers and c-GaN QDs on 3C-SiC substrate by means of molecular beam epitaxy. The freestanding microdisk located on a 3C-SiC pedestal were fabricated by reactive ion etching. Morphological investigations were realized by scanning electron microscopy. WGMs were observed in low temperature micro-photoluminescence measurements.

HL 41.6 Tue 12:30 H15

Confinement enhancement in InGaN quantum dots by AlGaN barriers — •Carsten Laurus, Timo Aschenbrenner, Stephan Figge, Marco Schowalter, Andreas Rosenauer, and Detlef Hommel — Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee, 28359 Bremen, Germany

InGaN quantum dots (QDs) are of great interest to realize single photon emitters for quantumcryptography. Single photon emission (SPE) up to 50 K was achieved utilizing spinodal phase decomposition for QD formation [S.Kremling, APL **100**, 061115 (2012)]. One approach reaching SPE at 300 K is the implementation of a barrier which improves the confinement of charge carriers and thus the temperature stability. Using InGaN as active layer, AlGaN is a promising barrier material because of its higher bandgap. Several sample series were grown by MOVPE with respect to diverse growth parameters e.g. growth temperature of the AlGaN barrier, barrier thickness and aluminum concentration of the barrier. For structural analysis by SEM samples without a GaN capping layer were used, whereby μ-PL investigations were made with capped samples. Based on SEM data the surface structures of the uncapped samples are divided in two phases with different indium concentration. The indium-rich phase consists mostly of islands and the indium-low is a meander-like structure which are QDs. On the basis of TEM data the quality of the AlGaN barrier in dependence of the aluminum concentration will be evaluated. Furthermore the capping of InGaN QDs with GaN or AlGaN and its problems will be discussed.

HL 42: Invited Talk: Gregor Mussler

Time: Tuesday 12:30–13:00 Location: H2

Invited Talk HL 42.1 Tue 12:30 H2

MBE growth of topological insulator films and ARPES measurements — •Gregor Mussler, Jörn Kampmeier, Svetlana Borisova, and Detlev Grützmacher — Peter Grünberg Institute 9, Research Center Jülich

In this talk, we will present our results on molecular-beam epitaxy (MBE) of three dimensional topological insulators (TI) Bi_2Te_3, Bi_2Se_3, and Sb_2Te_3, as well as the ternary and quaternary alloys. By choosing proper growth parameters, single crystal epilayers with smooth surfaces and interfaces at the atomic level are grown. ARPES scans show the Dirac cone for all three material systems, evidencing the TI behavior of the MBE-grown epilayers. Besides, we will also present results on transport experiments. Due to naturally occurring defects, Bi_2Te_3 and Bi_2Se_3 are n-type doped, whereas Sb_2Te_3 is p-type doped. The ternary $(Bi,Sb)_2Te_3$ alloys show a change from n- to p-

type doping for antimony concentrations between 25 - 40%. For these samples, we observed low bulk carrier concentrations, and features of surface carriers, such as weak antilocalization and Shubnikov-de Haas oscillations, were detected.

HL 43: Invited Talk: Stefan Ludwig

Time: Tuesday 15:00–15:30 Location: H2

Invited Talk HL 43.1 Tue 15:00 H2

Single phonon quantum interference and back-action in quantum-dot electrical circuits — Ghislain Granger[1], Daniela Taubert[2], Carolyn Young[3], L. Gaudreau[1], A. Kam[1], S. Studenikin[1], D. Harbusch[2], Dieter Schuh[4], Werner Wegscheider[4,5], Zbigniew Wasilew[2], Aashish Clerk[3], Andrew Sachrajda[1], and •Stefan Ludwig[2] — [1]NRC Canada — [2]Uni München — [3]McGill, Canada — [4]Uni Regensburg — [5]ETH Zürich

Lateral few-electron quantum-dot circuits are promising candidates for metrology and quantum information applications. Qubit readout typically involves a charge measurement made probing the current through a nearby biased quantum point contact (QPC). For quantum applications it is critical to understand the back-action disturbances resulting from such a measurement approach. It is well-established that QPC detectors emit phonons which are possibly reabsorbed by nearby qubits [1]. Here, we present the observation of a pronounced back-action effect in multiple dot circuits, where the absorption of detector-generated phonons is strongly modified by a quantum interference effect [2]. The reported phenomenon is well described by a theory incorporating both the QPC and coherent phonon absorption in coupled dots. It also promises applications: destructive interference allows strategies to suppress back-action during the qubit readout procedure. Furthermore, our experiments reveal the usability of coupled dots as a single phonon detector and spectrometer.

[1] D. Harbusch, et al., PRL **104**, 196801 (2010); [2] G. Granger, et al., Nat. Phys. **8**, 522 (2012).

HL 44: Photonic crystals

Time: Tuesday 15:00–16:15 Location: H3

HL 44.1 Tue 15:00 H3

Random Laser Theory - Coherence and Co-Existenze of Random Lasing Modes and Threshold Behavior — •Regine Frank — Instutut für Theoretische Physik, Universität Tübingen

In any quantum or wave system dissipation leads to decoherence. We demonstrate that the loss dynamics of random lasers imply a finite lasing mode volume, which explains the co-existence of random lasing modes. The coherence properties of the laser are dependent to the systems inherent parameters like scatterers' sizes and filling fraction. The modal behavior and the thresholds are derived 'ab initio' by considering quantum field theoretical scattering and transport in disordered granular systems.

HL 44.2 Tue 15:15 H3

Design, Fabrication and Characterization of High-Q Photonic Crystal Cavities in SiN — •Michael Adler[1], Carlo Barth[1], Jürgen Probst[2], Max Schoengen[2], Bernd Löchel[2], Janik Wolters[1], and Oliver Benson[1] — [1]Nano-Optics, Institute of Physics, Humboldt-Universität zu Berlin, Newtonstraße 15, D-12489 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Nanometeroptik und Technologie (G-INT), Albert-Einstein-Straße. 15, D-12489 Berlin

Two-dimensional photonic crystal (PC) cavities combine a high quality factor (Q) with a low mode volume. Recently heterostructure cavities with extremely high quality factors operating in the infrared have been realized based on silicon [1]. Our results from finite-difference time-domain (FDTD) simulations prove that high-Q PCs for the visible spectral range can be realized using silicon nitride. First experiments on the realization of such structures are presented.

[1] E. Kuramochi, M. Notomi, S. Mitsugi, A. Shinya, T. Tanabe, T. Watanabe . Ultrahigh-Q photonic crystal nanocavities realized by the local width modulation of a line defect. Applied Physics Letters **88**, 041112 (2006)

HL 44.3 Tue 15:30 H3

Fabrication of GaN photonic crystals using Surface Charge Lithography — •Olesea Volciuc[1], Timo Aschenbrenner[2], Detlef Hommel[2], Ion Tiginyanu[3], and Jürgen Gutowski[1] — [1]Institude of Solid State Physics, Semiconductor Optics, University of Bremen, 28334 Bremen — [2]Institude of Solid State Physics, Semiconductor Epitaxy, University of Bremen, 28334 Bremen — [3]National Center for Material Study and Testing, Technical University of Moldova, 2004 Chisinau

Two-dimensional photonic crystal (2D PhC) structures/slabs based on GaN have been fabricated by a maskless technological approach known as Surface Charge Lithography (SCL). The fabrication and processing techniques of PhCs require both high lithographic resolution and smooth etching of surfaces. The quality demand for spatial resolution is usually achieved by e-beam lithography and reactive ion etching (RIE). However, dry etching gives rise to damaged surfaces which are detrimental to the performance of optoelectronic devices. In addition, e-beam lithography and dry etching techniques involve complex and expensive equipment. SCL is an attractive alternative which avoids the problem of pronounced surface damage and represents an efficient and cost-effective fabrication procedure. This approach is based on a photoelectrochemical etching (PEC) of samples preliminarily treated by low-fluence focused ion beam (FIB). Results concerning the spatial nanoarchitecture of such developed 2D PhCs are presented.

HL 44.4 Tue 15:45 H3

Active focal volume modification for two-photon polymerization process studies — •Erik Waller, Michael Renner, and Georg von Freymann — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern

Direct-Laser-Writing (DLW) is used for the fabrication of almost arbitrary three-dimensional structures by focusing an intense laser beam into photo resists. In standard DLW systems the iso-intensity surfaces of the focal volume and therefore the obtainable feature sizes are defined by the numerical aperture of the focusing optics. The resolution is additionally limited by the proximity effect caused by accumulated intensity in the photo resist. Here, we spatially structure the incoming laser beam with a spatial light modulator to modify the focal volume. Polymer template structures written with these shaped focuses give insight in the formation of the proximity effect.

To evaluate the effect of the accumulated intensity we introduce shaded-ring filters (SRF) which reduce the axial elongation of the focal volume but cause sidelobes. Using SRFs with different sidelobe height and feedback from high resolution three-dimensional structures we find an acceptable sidelobe level for the serial writing process. The evolution of the proximity effect with time is tested using phase patterns that generate highly uniform high-resolution multi-focuses along a line in a parallel writing approach. The resulting obtainable resolution is compared to the obtainable resolution of a two-dimensional grating written in a serial process. The accumulated intensity is deduced from point-spread-function scans, the writing speed and the spot distance.

HL 44.5 Tue 16:00 H3

Angle-Resolved Spectroscopy of Opal Films and Higher Brillion Zones — •Frank Marlow[1,2], Mulda Muldarisnur[1], and Iulian Popa[1] — [1]MPI für Kohlenforschung, 45470 Mülheim an der Ruhr — [2]Center for Nanointegration Duisburg-Essen (CENIDE), University Duisburg-Essen

The angular behavior of light transmission through opal films over a

broad range of wavelengths and angles was investigated. The opal films were prepared using the capillary deposition method (CDM). Many well-defined diffraction peaks were detected and indicate that the CDM results in opal films with very high quality. Peaks coinciding at normal incidence split when the samples are rotated. The angular shift of these peaks was found to fit very well with the kinematical diffraction theory. Furthermore, the variation of intensity with incident angle can be interpreted in terms of a simplified dynamical diffraction theory considering the photonic bandstructure of the opals. The behavior at higher Brillion zones turns out to be the key for the interpretation.

HL 45: Transport in high magnetic fields / Quantum Hall effect

Time: Tuesday 15:00–16:15 Location: H13

HL 45.1 Tue 15:00 H13

Evidence of low-lying gapped excitations in the 5/2 quantum fluid — •Ursula Wurstbauer[1,2], Aron Pinczuk[1], Ken West[3], and Loren Pfeiffer[3] — [1]Columbia University, New York, USA — [2]Walter Schottky Institut and Physik-Department, Technische Universität München, Germany — [3]Princeton University, Princeton, USA

The competition between quantum phases that dictate the physics in the second Landau level (SLL) results in striking phenomena. A highly fascinating state is the even denominator fractional quantum Hall (FQHE) state at filling ν=5/2 that is widely believed to support non-Abelian quasi-particle excitations. Our work explores the low-lying neutral excitation modes in the SLL by resonant inelastic light scattering measurements. At 5/2 the spectra revealed a band of gapped modes with peak intensity at energy of 0.07meV. These modes are interpreted as a roton minimum in the wave vector dispersion of spin-conserving excitations. The intensity of the roton band significantly diminishes by increasing the temperature to 250mK and it fully collapses for T>250mK. A long wavelength spin wave mode (SW) is seen at the bare Zeeman energy, indicating non-zero spin-polarization. Both, roton and SW modes appear only in a very narrow filling factor range. A gapless continuum of low-lying excitations emerges at filling factors slightly away from 5/2 demonstrating demonstrates a transition from an incompressible quantum Hall fluid at exactly ν=5/2 to compressible states at very close filling factors. Supported by the U.S. NSF and the AvH.

HL 45.2 Tue 15:15 H13

Negative Magnetoresistance induced by the interplay of disorder in a High Mobility 2DEG — •Lina Bockhorn[1], Igor V. Gornyi[2], Alexander D. Mirlin[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover — [2]Institut für Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe

We study magneto transport in a high mobility two-dimensional electron gas (2DEG). Hall geometries are created by photolithography on a GaAs/AlGaAs quantum well containing a 2DEG. The 2DEG has an electron density of n_e=3.1*10^{11}cm^{-2} and a mobility of μ_e=11.9*10^{6}cm^2/Vs. We observe a strong negative magnetoresistance around zero magnetic field, which consists of a peak around zero magnetic field and of a huge magnetoresistance at larger fields. The peak around zero magnetic is a two-dimensional effect, as concluded from tilted magnetic field measurements. The huge magnetoresistance vanishes by increasing the temperature to 800 mK, while the peak is left unchanged [1]. At low temperature (T<600 mK) the peak is induced by the interplay of smooth disorder and rare strong scatteres [2]. For higher temperature the temperature dependence of the peak is more complex, which is the result of a crossover between different regimes. At low temperature the density of the strong scatterers n_S is determined by the peak. The quality of a high mobility sample can be characterized on the basis of such magnetotransport measurements.

[1] L. Bockhorn, et al., Phys. Rev. B 83, 113301 (2011)
[2] A. D. Mirlin, et al., Phys. Rev. Lett. 87, 126805 (2001)

HL 45.3 Tue 15:30 H13

Magnetoresistance studies on two-dimensional electron gases in GaAs/AlGaAs heterostructures as a tool for sample quality investigation — •Eddy P. Rugeramigabo[1,2], Lina Bockhorn[1], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Abteilung Nanostrukturen, Leibniz Universität Hannover, Deutschland — [2]QUEST Centre for Quantum Engineering and Space-Time Research, Leibniz Universität Hannover, Deutschland

Several GaAs/AlGaAs heterostructures of similar mobility have been grown by molecular beam epitaxy. The two-dimensional electron gases are located in single GaAs quantum wells. The samples were grown with the same layer sequence but under different growth conditions. Despite the similar mobility, we observed differences in the quantum Hall effect measurements. At small magnetic fields we found in all samples parabolic negative magnetoresistances. This is an indication for electron-electron interaction under influence of disorder. The curvatures of the parabolic magnetoresistance are different, as well as their temperature dependences. The parabolic magnetoresistance has been used as a tool to characterize the quality of the heterostructures.

HL 45.4 Tue 15:45 H13

Optically induced ballistic transport in edge channels — Christoph Kastl[1], Markus Stallhofer[1], •Christoph Karnetzky[1], Dieter Schuh[2], Werner Wegscheider[3], and Alexander Holleitner[1] — [1]Walter Schottky Institut and Physik-Department, TU München — [2]Institut für Experimentelle und Angewandte Physik, Universität Regensburg — [3]Laboratorium für Festkörperphysik, ETH Zürich, Switzerland

We use GaAs-based quantum point contacts as energy tunable and spin-sensitive detectors for an optically induced charge carrier ensemble in a two-dimensional electron gas. Using this technique, we recently investigated spatially resolved photocurrent flow patterns in a mesoscopic circuit with a moderate perpendicular magnetic field applied [1]. At high magnetic fields, where Landau-quantization applies, we find a substantially enhanced propagation length compared to zero field [2] along the boundary of the circuit. We explain the findings in the framework of charge carrier transport within one-dimensional quantum Hall edge states. The presented technique principally allows for the selective optical excitation and electronic detection of spin-degenerate edge channels [3].

[1] M. Stallhofer et al., Phys. Rev. B 86, 115315 (2012).
[2] M. Stallhofer et al., Phys. Rev. B 86, 115313 (2012).
[3] C. Kastl et al. (2013).

HL 45.5 Tue 16:00 H13

Modification to the central-cell correction of germanium acceptors — •Oleksiy Drachenko[1], Dmitry Kozlov[2], Anton Ikonnikov[2], Vladimir Gavrilenko[2], Harald Schneider[1], Manfred Helm[2], and Jochen Wosnitza[3] — [1]Helmholtz Zentrum Dresden Rossendorf, Inst Ion Beam Phys & Mat Res, D-01314 Dresden, Germany — [2]Russian Acad Sci, Inst Phys Microstruct, Nizhnii Novgorod 603950, Russia — [3]Helmholtz Zentrum Dresden Rossendorf, Dresden High Magnet Field Lab HLD, D-01314 Dresden, Germany

In this work, we report a correction to the model potential of the Ga acceptor in germanium, evidenced by high-magnetic-field photoconductivity measurements. We found that under high magnetic fields the chemical shift of the binding energy of Ga acceptors vanishes, contrary to the results given by the generally accepted theory. To fit our data, we found that the central-cell correction should contain a repulsive part (i.e., it must be bipolar), in contrast to the purely attractive screened point-charge potential widely used in the literature.

HL 46: III-V semiconductors: mainly wires and dots

Time: Tuesday 15:00–16:15 Location: H15

HL 46.1 Tue 15:00 H15

Cathodoluminescence spectroscopy of single GaN/AlN quantum dots directly performed in a scanning transmission electron microscope — •Frank Bertram[1], Gordon Schmidt[1], Markus Müller[1], Silke Petzold[1], Peter Veit[1], Jürgen Christen[1], Aparna Das[2], and Eva Monroy[2] — [1]Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Germany — [2]CEA/CNRS group Nanophysique et Semiconducteurs, INAC/SP2M, CEA-Grenoble, France

In this study we will present a nanoscale optical and structural characterization of a III-nitride based quantum dot (QD) heterostructure. A 1 μm thick AlN layer grown on a sapphire substrate using metal organic vapor phase epitaxy (MOVPE) serves as template for the further growth process. Subsequent, a stack of 10 GaN QD layers, each embedded in 50 nm thick AlN barrier, were grown under an optimized plasma-assisted molecular beam epitaxy process on an AlN-MOVPE/sapphire template. The cross-section high angle annular dark field image (HAADF) in a scanning transmission electron microscope (STEM) clearly reveals the GaN QD layers. The comparison of the HAADF image with the simultaneously recorded panchromatic cathodoluminescence mapping at 16 K exhibits a spot like luminescence distribution of the upper six QD layers solely, indicating no formation of the first four intentionally grown QD layers. Addressing a very few to single QDs we observe a broad luminescence between 3.0 eV and 4.0 eV originating from the superposition of the single emission lines.

HL 46.2 Tue 15:15 H15

Epitaxial Grown InP Quantum Dots on a GaAs Buffer Realized on GaP/Si(001) Templates — •Walter Hartwig, Michael Wiesner, Elisabeth Koroknay, Matthias Paul, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen and Research Center SCoPE, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

The increasing necessity of higher computational capacity and security in the information technology requires originally technical solutions, which today's standard microelectronics, as their technical limits are close, can't provide anymore. One way out offers the integration of III-V semiconductor photonics with low-dimensional structures in current CMOS technology, enabling on-chip quantum optical applications, like quantum cryptography or quantum computing. Challenges in the heteroepitaxy of III-V semiconductors and silicon are the mismatches in material properties of the both systems. Defects, like dislocations and anti-phase domains (APDs), inhibit the monolithic integration of III-V semiconductor on Si. We present the growth of a thin GaAs buffer on CMOS-compatible oriented Si(001) by metal-organic vapor-phase epitaxy. To circumvent the forming APDs in the GaAs buffer a GaP on Si template (provided by NAsP$_{III/V}$ GmbH) was used. The dislocation density was then reduced by integrating several layers of InAs quantum dots in the GaAs buffer to bend the threading misfit dislocations. On top of this structure we grew InP quantum dots embedded in a $Al_xGa_{1-x}InP$ composition and investigated the photoluminescence properties.

HL 46.3 Tue 15:30 H15

Measurement of Thermoelectric Properties of Indium Arsenide Nanowires — •Philipp Mensch[1], Siegfried Karg[1], Bernd Gotsmann[1], Heinz Schmid[1], Pratyush Das Kanungo[1], Volker Schmidt[1], Hesham Ghoneim[1], Mikael Björk[2], Valentina Troncale[1], and Heike Riel[1] — [1]IBM Research, Switzerland — [2]QuNano AB, Sweden

Low-dimensional semi-conducting nano-structures are promising systems to achieve a high figure of merit (ZT) for thermoelectric devices. We report on the thermoelectric properties of indium arsenide (InAs) nanowires (NWs). High ZT values for thin InAs and other III-V NWs are predicted from simulations [1]. We present temperature-dependent measurements of ZT - determining the electrical conductivity σ, the Seebeck coefficient S and the thermal conductivity κ using thermoelectric test structures for single NWs. NWs were grown by MOCVD and in-situ doped with sulfur. They were transferred to SiO_2 or Polyimide coated substrates. A resistive heater and four contacts to the NW, each of them serving as resistive thermometer, were structured by electron beam lithography, deposition of a nickel/platinum bilayer and lift-off technique. S and σ were measured for different doping levels with σ ranging from 30 S/cm to 2000 S/cm. S ranges from 10 μV/K for the highest doped NWs up to 180 μV/K for undoped NWs. Using a self-heating technique [2], a thermal conductivity of $\kappa = 1.8\,\mathrm{W/mK}$ was determined, being a factor of 30 lower than in bulk InAs.

[1] Mingo, Erratum APL 84, 2652 (2004)
[2] S. Karg, et al., J. Electron Mat. (2012) in press

HL 46.4 Tue 15:45 H15

The investigation of alloy formation during InAs nanowires growth on GaAs (111)B substrate — •Muhammad Saqib[1], Andreas Biermanns[1], Anton Davydok[1], Torsten Rieger[2], Thomas Grap[2], Mihail Lepsa[2], and Ullrich Pietsch[1] — [1]Feströrphysik, Universität Siegen, Walter-Flex-Str. 3, Siegen 57072, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungzentrum Jülich, Jülich 52425, Germany

A possible way to obtain nanowires is the growth in molecular beam epitaxy (MBE) on the (111) oriented surface of the desired substrate, covered by a thin oxide layer. A crucial parameter in this method is the initial thickness of the oxide layer, often determined by an etching procedure. In this contribution, we report on the structural investigation of two different series (etched and unetched) of NWs samples. Vertically aligned InAs nanowires (NWs) doped with Si were self-assisted grown by molecular beam epitaxy on GaAs [111]B substrates covered with a thin SiO_x layer. Using a combination of symmetric and asymmetric X-ray diffraction we study the influence of Si supply on the growth process and nanostructure formation. We find that the number of parasitic crystallites grown between the NWs increases with increasing Si flux. In addition, we observe the formation of a $Ga_{0.2}In_{0.8}As$ alloy if the growth is performed on samples covered by a defective (etched) oxide layer. This alloy formation is observed within the crystallites and not within the nanowires. The Gallium concentration is determined from the lattice mismatch of the crystallites relative to the InAs nanowires. No alloy formation is found for samples with faultless oxide layers.

HL 46.5 Tue 16:00 H15

Imaging the local density of free charge carriers in doped InAs nanowires — •Benedikt Hauer[1], Kamil Sladek[2], Fabian Haas[2], Thomas Schäpers[2], Hilde Hardtdegen[2], and Thomas Taubner[1] — [1]I. Institute of Physics (IA), RWTH Aachen Univerity, Sommerfeldstraße 14, 52074 Aachen, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany

Semiconductor nanowires are promising candidates for future nanoelectronic devices. While the bottom-up approach for their growth could simplify the device fabrication, their quantitative characterization remains challenging. We use scattering-type scanning near-field optical microscopy (s-SNOM) to investigate the local density of free electrons in Si-doped InAs nanowires grown by selective-area metalorganic vapor phase epitaxy (SA-MOVPE) [1].

In s-SNOM the evanescent electric field at the apex of an illuminated tip is used to probe a sample at a strongly sub-wavelength resolution. This method is highly sensitive to variations in the sample permittivity around $\mathrm{Re}(\varepsilon) \approx -2$ [2]. The use of tunable mid-infrared lasers therefore allows addressing the plasma frequency of free charge carriers in highly doped nanowires [3]. Here, we demonstrate that the sensitivity of s-SNOM is sufficient to detect a slight unintended variation in the carrier concentration during the growth process. Furthermore, using model calculations, we give an estimate of the local density of free electrons.

[1] S. Wirths *et al.*, J. Appl. Phys. 110, 053709 (2011).
[2] B. Hauer *et al.*, Opt. Express 20, 13173 (2012).
[3] J. Stiegler *et al.*, Nano Lett. 10, 1387 (2010).

HL 47: Invited Talk: Mitiko Miura-Mattausch

Time: Tuesday 15:30–16:00 Location: H2

Invited Talk HL 47.1 Tue 15:30 H2

Compact physics-based modeling of semiconductor devices for circuit — •Mitiko Miura-Mattausch — Hiroshima University, Higashi-Hiroshima, Japan

Compact models of semiconductor devices for circuit simulation bridge the gap between basic semiconductor R&D and real industrial applications. The characteristics of semiconductor devices are decribed with simple yet accurate equations of the essential physical device properties. The physical correctness and accuracy of a compact model is the key for further aggressive industial developments of product applications exploiting the unique semiconductor properties.

The development trend in compact modeling has gone in recent years towards simplifications of the drift-diffusion theory with surface-potential based approaches, following the electromagnetic theory and leading to compact semiconductor-device models with both high accuracy and high computational efficiency.

The field of compact models is an example for a merging between science and technology, clarifying the common tasks of the next application era to realize rapid technological progress for the benefit of the society. An important example is the task of more efficient energy consumption and larger energy savings, which will be addressed in the presentation.

HL 48: Topological insulators (HL, jointly with O, TT)

Time: Wednesday 9:15–13:00 Location: H16

HL 48.1 Wed 9:15 H16

Topological Excitonic Superfluids in Three Dimensions — •Ewelina M. Hankiewicz[1], Youngseok Kim[2], and Matthew Gilbert[2] — [1]Wuerzburg University — [2]University of Illinois, Urbana

We study the equilibrium and non-equilibrium properties of topological dipolar intersurface exciton condensates within time-reversal invariant topological insulators in three spatial dimensions without a magnetic field. We elucidate that, in order to correctly identify the proper pairing symmetry within the condensate order parameter, the full three-dimensional Hamiltonian must be considered. As a corollary, we demonstrate that only particles with similar chirality play a significant role in condensate formation. Furthermore, we find that the intersurface exciton condensation is not suppressed by the interconnection of surfaces in three-dimensional topological insulators as the intersurface polarizability vanishes in the condensed phase. This eliminates the surface current flow leaving only intersurface current flow through the bulk. We conclude by illustrating how the excitonic superfluidity may be identified through an examination of the terminal currents above and below the condensate critical current. Reference: Phys. Rev. B 86, 184504 (2012).

HL 48.2 Wed 9:30 H16

Bi_2Te_3: A dual topological insulator — •Tomáš Rauch[1], Markus Flieger[1], Arthur Ernst[2], Jürgen Henk[1], and Ingrid Mertig[1,2] — [1]Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

The class of $\mathcal{Z}_2$ topological insulators requires time reversal symmetry, while topological crystalline insulators require a mirror symmetry (an example is SnTe [1]).

We show that the well-known $\mathcal{Z}_2$ topological insulator Bi_2Te_3 with $\mathcal{Z}_2$ invariant $(1;000)$ is also a topological crystalline insulator with mirror Chern number -1. This dual topological character allows to dope Bi_2Te_3 magnetically, thereby breaking time-reversal symmetry, while keeping the topological crystalline character. As a consequence, magnetized Bi_2Te_3 shows a Dirac state at its (111) surface shifted off the time-reversal invariant momentum $\overline{\Gamma}$, provided the magnetization is perpendicular to a mirror plane.

These fundamental features are elaborated by means of tight-binding calculations of both the bulk and the surface electronic structure as well as of the topological invariants. $\vec{k} \cdot \vec{p}$ model calculations and *ab initio* KKR calculations complement and support these results.

Our findings open a new path toward device applications that rely on topological insulators with magnetically controllable topological character.

[1] L. Fu, Phys. Rev. Lett. **106** (2011) 106802; T. Hsieh *et alii*, Nature Comms. **3** (2012) 982.

HL 48.3 Wed 9:45 H16

Three-dimensional Models of Topological Insulator Films: Dirac Cone Engineering and Spin Texture Robustness — David Soriano[1], •Frank Ortmann[1], and Stephan Roche[1,2] — [1]Catalan Institute of Nanotechnology, Barcelona (Spain) — [2]ICREA, Barcelona (Spain)

Topological insulators feature surface states which exhibit certain robustness to disorder and which can be gapped due to inter-surface tunneling. By designing three-dimensional models of topological insulator thin films, we demonstrate a tunability of surface states and the odd number of Dirac cones on opposite surfaces by modifications of the atomic-scale geometry at the boundaries. [1,2] This enables the creation of a single Dirac cone at the Γ point as well as possible suppression of quantum tunneling between Dirac states at opposite surfaces. We further analyze the robustness of the spin texture to bulk disorder which may help in quantifying bulk disorder in materials with ultraclean surfaces. [2]

[1] L. Fu, C.L. Kane, and E.J. Mele, Phys. Rev. Lett. 98, 106803 (2007)

[2] D. Soriano, F. Ortmann, and S. Roche, Phys. Rev. Lett. (in press)

HL 48.4 Wed 10:00 H16

Transport properties of point contacts between helical edge states — •Christoph P. Orth and Thomas L. Schmidt — University of Basel, Switzerland

We study a 2D topological insulator with helical edges that are connected by local electron tunneling. The edges are in contact with four reservoirs held at different chemical potentials. In contrast to existing theories, we treat the tunneling exactly but apply perturbation theory for the electron-electron interactions to calculate the current. Furthermore, we allow for a slow momentum dependent spin-rotation of the helical fields which can be created, e.g., by Rashba spin-orbit coupling. This allows inelastic spin-flip tunneling processes between the edges. Our results help to understand the interplay between electron-electron and spin-orbit interactions in topological insulators.

HL 48.5 Wed 10:15 H16

Exotic magnetic properties of diluted magnetic binary chalcogenides — •Maia G. Vergniory[1], Xabier Zubizarreta[1], Mikhail M. Otrokov[2], Igor V. Maznichenko[3], Juergen Henk[3], Evgueni V. Chulkov[4], and Arthur Ernst[1] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Tomsk State University, Tomsk, Russia — [3]Martin-Luther-University, Halle-Wittenberg, Germany — [4]Donostia International Physics Center, Donostia-San Sebastian, Spain

Using first-principles Green function approach we studied electronic and magnetic properties of diluted magnetic binary chalcogenides A_2B_3, doped with transition metals substituing the A element. The electronic structure of the impurities in the chalcogenides is mainly featured by the crystal field splitting. We found that two main mechanisms are responsible for long-range magnetic order in these materials: hole mediated magnetism within the layer of A atoms and indirect interaction between magnetic moments via a B atom. We also estimated Curie temperature of these systems, which was found in good agreement with the available experimental data. Our results shed light on the understanding of magnetic interaction and control in toplogical insulators.

HL 48.6 Wed 10:30 H16

Quasiparticle study of the bulk topological insulators Bi_2Se_3, Bi_2Te_3, and Sb_2Te_3 including spin-orbit coupling. — •Irene Aguilera, Christoph Friedrich, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

We present *GW* calculations of the topological insulators Bi_2Se_3 and Bi_2Te_3 within the all-electron FLAPW formalism and compare them with previous calculations. We extend the study to the topological insulator Sb_2Te_3, which poses additional problems when studied with *GW* based on non-relativistic density functional theory (DFT) as it exhibits a negative DFT band gap. In contrast to the previous *GW* calculations, we fully take into account spin-orbit coupling (SOC) allowing spin-off-diagonal elements in the Green function and the self-energy, and we discuss the differences to a simpler perturbative approach (*i.e.*, treating SOC on DFT level *a posteriori*). Additionally, we show that the inclusion of SOC induces fundamental changes in the Green function G, whereas changes in the screened interaction W are negligible. We also discuss the influence of off-diagonal elements of the self-energy matrix.

After inclusion of quasiparticle effects, we observe a direct band gap at the Γ point for Bi_2Se_3, in disagreement with predictions from DFT but in accordance with experiment. For all compounds, in the most critical case of the band-inversion region around the Γ point, we show that the *GW* effective masses are significantly different from DFT ones.

Funding was provided by the Alexander von Humboldt Foundation.

HL 48.7 Wed 10:45 H16

Controllable magnetic doping of the surface state of a topological insulator — •A. Eich[1], T. Schlenk[1], M. Bianchi[2], M. Koleini[3], O. Pietzsch[1], T.O. Wehling[3], T. Frauenheim[3], A. Balatsky[4], J.-L. Mi[5], B. B. Iversen[5], J. Wiebe[1], A.A. Khajetoorians[1], Ph. Hofmann[2], and R. Wiesendanger[1] — [1]Institute for Applied Physics, Universität Hamburg, Germany — [2]iNano, Aarhus University, Denmark — [3]Bremen Center for Computational Materials Science, Universitiy of Bremen, Germany — [4]NORDITA, Stockholm, Sweden — [5]Center for Materials Crystallography, iNano, Aarhus University, Denmark

A combined experimental and theoretical study of doping individual Fe atoms into Bi_2Se_3 is presented. It is shown through a scanning tunneling microscopy study that single Fe atoms initially located at hollow sites on top of the surface (adatoms) can be incorporated into subsurface layers by thermally-activated diffusion. Angle-resolved photoemission spectroscopy in combination with ab-initio calculations within density functional theory suggest that the doping behavior changes from electron donation for the Fe adatom to neutral or electron acceptance for Fe incorporated into substitutional Bi sites. According to the calculations, these Fe substitutional impurities retain a large magnetic moment thus presenting an alternative scheme for magnetically doping the topological surface state. For both types of Fe doping, we see no indication of a gap at the Dirac point.

T. Schlenk et al., arXiv: 1211.2142v1 (2012) [cond-mat.mtrl-sci]
J. Honolka et al., PRL **108**, 256811 (2012)

Coffee break

HL 48.8 Wed 11:15 H16

Induced superconductivity in the topological surface state of mercury telluride (HgTe) — •Luis Maier, Manuel Grimm, Peter Schüffelgen, Daniel Knott, Christopher Ames, Christoph Brüne, Philipp Leubner, Jeroen Oostinga, Hartmut Buhmann, and Laurens W. Molenkamp — Physikalisches Institut (EP3), Universität Würzburg, 97074 Würzburg

It has been recently demonstrated, that a strained grown layer of of HgTe is a 3D topological insulator (TI) exhibiting a single family of Dirac cone states at its surface. Since the bulk has nearly no carriers left, the transport through these structures is strongly dominated by the surface states [1].

Because of the prediction of creation of Majorana bound states [2] we are looking at a superconductor-TI interface. This talk presents our results on highly transparent S-TI-S junctions where we observe unusual behaviour in the Josephson current.

Preliminary results of this project are published in [3].

[1] C. Brüne et al., Phys. Rev. Lett. 106, 126803 (2011)
[2] L. Fu and C. L. Kane, Phys. Rev. Lett. 100, 096407 (2008)
[3] L. Maier et al., Phys. Rev. Lett. 109, 186806 (2012)

HL 48.9 Wed 11:30 H16

Strained bulk HgTe as a 3D topological insulator — •Cornelius Thienel, Christopher Ames, Philipp Leubner, Christoph Brüne, Hartmut Buhmann, and Laurens W. Molenkamp — Universität Würzburg, Lehrstuhl für experimentelle Physik III

HgTe is a semimetal that has an inverted band structure. We show that strained on CdTe the HgTe opens a bandgap and becomes a 3D topological insulator (TI). By magnetotransport measurements we confirm the existence of a 2D topological state and observe QHE from the surface. An analysis of SdH oszillations allows us to distinguish between two TI surfaces perpendicular to the magnetic field that have different charge carrier densities due to different electrostatic environments. When structuring a top gate on the sample, we are able to match the carrier densities of the surface states and therefore see a sequence of odd integer Hall plateaus, as predicted by Dirac physics.

HL 48.10 Wed 11:45 H16

Comparing scattering processes in topological insulators and giant Rashba semiconductors — •Peter Lemmens[1], Vladimir Gnezdilov[2], Dirk Wulferding[1], Patrik Recher[3], Helmuth Berger[4], Yoichi Ando[5], Angela Möller[6], R. Sankar[7], and Fang-Cheng Chou[7] — [1]IPKM, TU-BS, Braunschweig — [2]ILTPE, Kharkov, Ukraine — [3]IMAPH, TU-BS, Braunschweig — [4]EPFL, Lausanne, Switzerland — [5]ISIR, Osaka, Japan — [6]Dept. of Chemistry, Univ. Houston, USA — [7]CCMS, National Taiwan Univ., Taipei, Taiwan

Using Raman scattering experiments we probe scattering processes in BiTeI and topological insulators. In the former systems the surface termination, either by Iodine - Bi or Tellur - Bi determines the low energy scattering properties. A comparison of these surface induced signals with effects seen in topological insulators leads to a considerable gain of understanding of scattering mechanisms and the respective role of symmetry. Work supported by DFG, B-IGSM and NTH School for Contacts in Nanosystems.

HL 48.11 Wed 12:00 H16

Local photocurrent generation in thin films of the topological insulator Bi_2Se_3 — •Christoph Kastl[1], Tong Guan[2], Xiaoyue He[2], Kehui Wu[2], Yongqing Li[2], and Alexander Holleitner[1] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, 85748 Garching, Germany — [2]Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

We report on the optoelectronic properties of thin films of the three-dimensional topological insulator Bi_2Se_3 grown by molecular beam epitaxy. In spatially resolved scanning photocurrent experiments, we observe submicron photocurrent patterns with positive and negative amplitude [1]. The patterns are independent of the applied bias voltage, but they depend on the width of the circuits. We interpret the patterns to originate from a local photocurrent generation [2] due to potential fluctuations [3]. Furthermore, we verify and discuss the impact of the circular photogalvanic effect in optoelectronic Bi_2Se_3-based circuits [4].

[1] C. Kastl et al., arxiv: 1210.4743 (2012).
[2] J. C. W. Song and L. S. Levitov, arxiv:1112.5654 (2011).
[3] H. Beidenkopf et al., Nat. Phys. 7, 939 (2011).
[4] C. Kastl et al. (2013).

HL 48.12 Wed 12:15 H16

$Bi_{1-x}Sb_x$(110): A non-closed packed surface of a topological insulator — Lucas Barreto, Wendell Simoes da Silva, Malthe Stensgaard, Søren Ulstrup, Marco Bianchi, •Xie-Gang Zhu, Matteo Michiardi, Maciej Dendzik, and Philip Hofmann — Department of Physics and Astronomy, Interdisciplinary Nanoscience Center Århus University, 8000 Århus C, Denmark

Topological insulators are characterised by an insulating bulk band structure, but topological considerations require their surfaces to support gap-less, metallic states. Meanwhile, many examples of such materials have been predicted and found experimentally, but work has concentrated on the closed-packed (111) surface of the topological insulators. Thus, the theoretical picture of an insulating bulk embedded in a metallic surface from all sides of a crystal still needs to be confirmed. Here we present angle-resolved photoemission spectroscopy results from the (110) surface of the topological insulator $Bi_{1-x}Sb_x$

($x \approx 0.15$). The observed band structure and Fermi contour is in excellent agreement with theoretical predictions and slightly different from the electronic structure of the parent surface Bi(110), in particular around the X_1 time-reversal invariant momentum. We argue that the preparation of surfaces different from (111) opens the possibility to tailor the detailed electronic structure and properties of the topological surface states.

HL 48.13 Wed 12:30 H16

Charge screening at the surface of a topological insulator: Rb on Bi_2Se_3 — •Peter Löptien, Lihui Zhou, Jens Wiebe, Alexander A. Khajetoorians, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Germany

Adsorption of Rb atoms on Bi_2Se_3 leads to the formation of a two-dimensional electron gas (2DEG) in the conduction band at the surface of the topological insulator [1]. We investigated the coverage dependent distribution of the singly charged Rb atoms by low temperature STM. By a statistical analysis of the interatomic distances between the adatoms we quantitatively derived the pair interaction [2], which fits a screened Coulomb potential. Interestingly, screening length and dielectric constant turn out to be rather small, due to the contribution of the 2DEG and topological surface state.

[1] M. Bianchi, R. C. Hatch, Z. Li, P. Hofmann, F. Song, J. Mi, B. B. Iversen, Z. M. Abd El-Fattah, P. Löptien, L. Zhou, A. A. Khajetoorians, J. Wiebe, R. Wiesendanger, and J. W. Wells, ACS Nano 6, 7009 (2012)
[2] J. Trost, T. Zambelli, J. Wintterlin, and G. Ertl, Phys. Rev. B 54, 17 850 (1996)

HL 48.14 Wed 12:45 H16

Fabrication and characterization of thin Bi_2Se_3 topological insulators — •Srujana Dusari[1], Philipp Meixner[1], Anna Mogilatenko[2], Saskia F. Fischer[1], Jaime Sanchez-Barriga[3], Lada V. Yashina[4], Florian Kronast[3], Sergio Valencia[3], Akin Ünal[3], and Oliver Rader[3] — [1]Novel Materials, Humboldt Universität zu Berlin, D-12489 Berlin — [2]Ferdinand Braun Institut, D-12489 Berlin — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, D-12489 Berlin — [4]Dep. Chemistry, Moscow State University, Russia

Topological insulators (TIs) have electrically insulating states in the bulk and robust conducting states along the edges [1, 2]. The real-life TI samples available today contain residual bulk charge carriers that hinder exploiting their surface properties in device form. The aim of our work is to investigate the controlled combination of dimensionality and designed impurity and metallic defect structures on the quantum transport properties of well known Bi_2Se_3 TIs, in particular with respect to the implications for devices. Here we report preparation and characterization of exfoliated Bi_2Se_3 flakes. The samples are characterized using atomic force microscopy, transmission electron microscopy, and energy-dispersive X-ray spectroscopy. Surface stability and composition are determined using photoemission electron microscopy. Low temperature transport measurements are presented.

[1] C. L. Kane, and E. J. Mele, Phys. Rev. Lett. 95, 226801 (2005).
[2] M. Z. Hasan and J. E. Moore, Annu. Rev. Condens. Matter. Phys. 2: 55-78 (2011).

HL 49: Molecular electronics (TT, jointly with CPP, HL, MA)

Time: Wednesday 9:30–12:45 Location: H2

HL 49.1 Wed 9:30 H2

Inelastic scattering effects and electronic shot noise — •Amin Karimi, Markus Herz, and Elke Scheer — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

The study of shot noise for junctions formed by single molecules offers interesting new information that cannot be easily obtained by other means. At low bias it allows determining the transmission probability and the number of current carrying conductance channels [1]. We investigate the effects of phonon scattering on the electronic current noise through nano junctions with mechanically controllable break junction (MCBJ). Equivalent measurements have recently been reported to be able to reveal inelastic transport contributions to the current through gold atomic contacts [2]. We developed a new and versatile measurement system enabling measurements of the noise in a rather broad range of conductance values from 0.01 G_0 to 1 G_0 without the necessity of double wiring. First results on gold atomic contacts and benzendithiol will be presented.

[1] D. Djukic and J. M. van Ruitenbeek, Nano Lett. 6, 789-793 (2006)
[2] M. Kumar, R. Avriller and J. M. van Ruitenbeek, Phys. Rev. Lett. 108, 146602 (2012)

HL 49.2 Wed 9:45 H2

Electrical Characterization of Single Molecules via MCBJ — •Matthias Wieser[1], Torsten Sendler[1], Shou-Peng Liu[2], Samuel Weisbrod[2], Zhuo Tang[2], Andreas Marx[2], Jannic Wolf[2], Elke Scheer[2], Francesca Moresco[3], Grebing Jochen[1], and Artur Erbe[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V., D-01328 Dresden — [2]Universität Konstanz, D-78457 Konstanz — [3]Max Bergmann Center of Biomaterials, D-01069 Dresden

For future molecular electronics applications the detailed knowledge about the electrical transport properties of single molecules is very important. To achieve this goal we are using the mechanical controllable break junction technique in liquid environments in combination with insulating substrates. We characterize the electrical conductance and I-V characteristics of single molecules which consist of three phenyl rings connected by triple carbon bonds with two oxygen sidegroups binding to the central ring. The I-V characteristics are further investigated by creating 2D histograms for hundreds of I-V curves and by fitting a single level model which provides us the metal-molecule junction coupling constants and the molecular energy level.

HL 49.3 Wed 10:00 H2

Charge transmission through a molecular junction driven by a time–dependent voltage — •Yaroslav Zelinskyy[1,2], Yoram Selzer[3], and Volkhard May[1] — [1]Institut für Physik, Humboldt Universität zu Berlin, Newtonstraße 15, D-12489 Berlin, Germany — [2]Bogolubov Institute for Theoretical Physics, National Academy of Science of Ukraine, 14-b Metrologichna str., UA-03683, Kiev, Ukraine — [3]School of Chemistry, Tel Aviv University, Ramat Aviv, 69978 Tel Aviv, Israel

Time-dependent electron transport through a molecular junction driven by voltage pulses with a duration even in the sub-ps region is investigated theoretically. The transient behavior of the current is analyzed in focusing on the sequential transport regime and in utilizing a density matrix approach. As a quantity detectable in the experiment the averaged dc-current resulting from a sequence of voltage pulses is also calculated. The obtained data are analyzed with respect to their dependence on the voltage pulse shape, the magnitude and asymmetry of the lead-molecule coupling, and the mechanism and strength of intramolecular relaxation. All the findings are confronted with recent computations on transient currents due to optical excitation of the junction [1,2].

[1] L. Wang and V. May, Phys.Chem.Chem.Phys. 13, 8755 (2011)
[2] Y. Zelinskyy and V. May, Nano Lett. 12, 446 (2012)).

HL 49.4 Wed 10:15 H2

Surface Plasmon Enhanced Electroluminescence of a Molecular Junction — •Yuan Zhang[1,2], Yaroslav Zhelinskyy[1], and Volkhard May[1] — [1]Institut für Physik, Humboldt Universität zu Berlin, Newtonstraße 15, D-12489 Berlin, Germany — [2]University of Science and Technology Beijing, XueYuan Road 30, 100083 Beijing, P. R. China

There are some first experiments indicating surface plasmon enhanced emission of a molecular junction. We present a coherent theory for this phenomenon, which is based on our previous work on molecule metal nanoparticle complexes [1,2,3,4]. Ultilizing a density matrix description our theory accounts for electron transfer in junction, photon emission and energy exchange coupling between the molecule and spherical leads. As a central result, we report on a three order of magnitude enhanced molecular photon emission, which dependence on molecular and junction parameters are also discussed.

[1] Y. Zelinskyi, Y. Zhang, and V. May, J. Phys. Chem. A, DOI: 10.1021/jp305505c
[2] Y. Zhang, Y. Zelinskyy, and V. May, J. Phys. Chem. C, accepted

[3] Y. Zhang, Y. Zelinskyy, and V. May, J. Nanophot., in press
[4] Y. Zelinskyy and V. May, Nano Lett. **12**, 446 (2012)

HL 49.5 Wed 10:30 H2

Dynamics of a nano-scale rotor driven by single-electron tunneling — Alexander Croy[2] and •Alexander Eisfeld[1] — [1]MPIPKS Dresden — [2]Chalmers University of Technology S-412 96 Göteborg, Sweden

We investigate theoretically the dynamics and the charge transport properties of a rod-shaped nano-scale rotor, which is driven by a similar mechanism as the *nanomechanical single-electron transistor (NEMSET)*. We show that a static electric potential gradient can lead to self-excitation of oscillatory or continuous rotational motion. We identify the relevant parameters of the device and study the dependence of the dynamics on these parameters. We discuss how the dynamics are related to the measured current through the device. Notably, in the oscillatory regime we find a negative differential conductance. The current-voltage characteristics can be used to infer details of the surrounding environment which is responsible for damping.

[1] A. Croy and A. Eisfeld, *EPL (Europhys Lett)* **98**, 68004

HL 49.6 Wed 10:45 H2

First-principles investigation of electron transport through molecular junctions in an STM configuration — •Shigeru Tsukamoto, Vasile Caciuc, Nicolae Atodiresei, and Stefan Blügel — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich

Molecular electronics is exciting by the perspective that various types of functionalities are potentially realized only by single molecules with unique electronic structures. A number of interesting experiments on the transport properties have been performed in an STM configuration, in which a probing tip approaches a molecule on a metal surface.

By means of first-principles methods, we report about a systematic series of calculations on electron transport through molecules in the STM configuration. The molecules to be investigated are a Terephthalic acid molecule and its derivatives, which chemisorb on Cu(110) surfaces.

Electron transmissions are investigated by varying the tip–molecule distance in an STM configuration, as well as by tuning molecular electronic structures. As approaching the tip toward the molecule, some of the transmission peaks originating from unoccupied states move to lower energy due to the hybridization of tip and molecular states. This peak-shift contributes to increasing the electron transmission around the Fermi energy, which is an essential property in molecular devices. This exhibits that in molecular electronics, not only the molecule itself but also the geometrical configuration between a molecule and the electrodes is an important parameter to determine the functionality.

15 min. break

HL 49.7 Wed 11:15 H2

STM theory for π-conjugated molecules on thin insulating films — •Benjamin Siegert, Andrea Donarini, Sandra Sobczyk, and Milena Grifoni — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg

We present a microscopic STM theory, based on the reduced density matrix formalism, which is able to describe transport and topographical properties of interacting π-conjugated molecules on thin insulating films. Simulated current-voltage characteristics and constant height and constant current STM images for a Cu-Phthalocyanine (CuPc) molecule are presented as experimentally relevant examples. We predict negative differential conductance resulting from interference between degenerate many-body states of CuPc [1]. Criteria are given to find and identify the interference blocking scenario in experimental measurements.

[1] A. Donarini, B. Siegert, S. Sobczyk, and M. Grifoni, PRB **86**, 155451 (2012).

HL 49.8 Wed 11:30 H2

Influence of Electronic Properties of Graphene on Current-Voltage Characteristics of Molecule-Graphene Nanojunctions — •Ivan A. Pshenichnyuk, Pedro B. Coto, André Erpenbeck, and Michael Thoss — Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany

Graphene, thanks to its peculiar mechanical and electronic properties, is today considered as a perspective material in future electronics. Its well-known band structure with "zero band-gap" as well as the existence of so-called edge states leads to a non-trivial density of states distribution in graphene-based devices. This causes, in particular, distinctive current-voltage characteristics of molecule-graphene nanojunctions, where a single molecule is connected to two graphene nanosized contacts. We study the transport characteristics of graphene-based nanojunctions using tight-binding models and first-principles DFT calculations combined with the Landauer transport formalism.

HL 49.9 Wed 11:45 H2

Electron Transport properties of metallic carbon nanotubes with metal contacts — •Andreas Zienert[1], Jörg Schuster[2], and Thomas Gessner[1,2] — [1]Center for Microtechnologies, Chemnitz University of Technology, Chemnitz, Germany — [2]Fraunhofer Institute for Electronic Nano Systems, Chemnitz, Germany

Metallic carbon nanotubes (CNTs) are quasi ballistic one-dimensional conductors capable to carry large current densities. This makes them ideal candidates for applications in future microelectronic devices, partially replacing state-of-the-art copper interconnect lines. The performance of such a system not only depends on intrinsic properties of the CNTs but is also strongly affected by its size and the contact.

We investigate the transport properties of metal–CNT–metal devices theoretically, applying semiempirical (extended Hückel theory) and ab initio (density functional theory) electronic structure methods, combined with a Green's function formalism for ballistic transport at low bias. The study focuses on $(6, 0)$ CNTs of different length comparing the metal contacts Al, Cu, Pd, Pt, Ag, Au in a highly symmetric end-to-end configuration.

It turns out that Al forms the most transparent contacts, followed by Pd, Pt and Cu. The noble metals Au and Ag perform worse. Results are visualized and discussed in terms of the local density of states of the combined metal–nanotube systems and its isolated parts, as well as their contact distances, binding energies, and work functions.

HL 49.10 Wed 12:00 H2

First principles study of charge and heat transport through π-stacked molecules — •Thomas Hellmuth[1], Marius Bürkle[2], Fabian Pauly[3], and Gerd Schön[1] — [1]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]Nanosystem Research Istitute, National Institute of Advanced Industrial Science and Technology, Japan — [3]Theorie der Nanostrukturen, Universität Konstanz, 78457 Konstanz, Germany

We analyze charge and heat transport properties of π-stacked, multilayered paracyclophane molecules using density functional theory combined with non-equilibrium Green's function techniques. The conductance of that class of molecules was measured in Ref. 1. Beside the elastic conductance we investigate the not yet measured thermopower and inelastic electron tunneling spectra (IETS). The transmission eigenchannels show that the current is mainly carried by the π system of the paracyclophane molecules and by taking into account different contact geometries, we find that this is independent of the binding motif. While the conductance decays exponentially with increasing molecular length, the thermopower increases linearly and may change its sign. Similarly, we analyze how the IETS and the heat transport depend on the molecular length and vibrational modes in the specific junction geometries.

[1] S. T. Schneebeli *et al.* J. Am. Chem. Soc. **133**, 2136 (2011)

HL 49.11 Wed 12:15 H2

Spin selective transport in chiral systems — •Rafael Gutierrez, Thomas Brumme, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany

Recent experiments have demonstrated that the transmission of electrons through layers of chiral molecules can be strongly spin-dependent [1,2]. Here, we extend a previous model [3] to discuss the interrelation between the observed effect and the presence of a spin-orbit coupling interaction induced by helical electrostatic fields. Hereby, we present a minimal model Hamiltonian based on a representation of the Schroedinger equation on a helical pathway and discuss the influence of several parameters on the spin polarization. Complementary to it, full 3D wave packet propagation is discussed in the presence of spin-orbit coupling. Our results suggest that a spin polarization can be induced as a result of the symmetry of the system. However, it appears that a

full 3D description of the problem may be necessary.

[1] B. Goehler, V. Hamelbeck, T. Z. Markus, M. Kettner, G. F. Hanne, Z. Vager, R. Naaman, H. Zacharias, Science **331**, 894 (2011)
[2] Z. Xie, T. Z. Markus, S. R. Cohen, Z. Vager, R. Gutierrez, R. Naaman, Nano Letters **11**, 4652 (2011)
[3] R. Gutierrez, E. Diaz, R. Naaman, G. Cuniberti, Phys. Rev. B **85**, 081404(R) (2012)

HL 49.12 Wed 12:30 H2

Full ab initio description of strong electronic correlations in molecular devices — •David Jacob — Max-Planck-Institut für Mikrostrukturphysik, Halle

In order to obtain a *full* first-principles description of the correlated electronic structure and transport properties of nanoscopic devices we combine the so-called Coulomb-Hole-Screened-Exchange (COHSEX) approximation with more sophisticated many-body techniques such as the Dynamical Mean-Field Theory (DMFT). While the former yields an effective mean-field description of the weakly correlated conduction electrons, the latter describes the dynamic correlations of the strongly interacting electrons in the $3d$- or $4f$-shells of transition metal atoms. The combination of DMFT with COHSEX instead of Density Functional Theory (DFT) improves upon our recently developed "Molecular DMFT" approach [1,2] in two important aspects: First, the COHSEX yields the effective Coulomb interaction U for the strongly interacting electrons. Second, unlike in DFT+DMFT calculations the double-counting correction for COHSEX+DMFT is exactly known and straight-forward to calculate. With this approach it is now possible to actually predict e.g. the occurance of the Kondo effect in magnetic atoms and molecules on metal surfaces and attached to metallic leads, and to investigate the complex nature of the Kondo effect in these sytems.

[1] D. Jacob *et al.*, PRL **103**, 016803 (2009); PRB **82**, 195115 (2010)
[2] M. Karolak *et al.*, PRL **107**, 146604 (2011)

HL 50: Organic semiconductors

Time: Wednesday 9:30–12:30 Location: H13

HL 50.1 Wed 9:30 H13

Strain derivatives for localized-orbital based electronic-structure theory and application to organic semiconductors — •Franz Knuth, Christian Carbogno, Volker Blum, Viktor Atalla, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

The carrier levels of semiconductor materials can depend sensitively on strain and pressure. Here, we discuss the analytical implementation of strain derivatives, i.e. the stress tensor, for first-principles calculations in the density-functional framework based on numeric atom-centered orbitals in the all-electron `FHI-aims` code [1]. Besides the contributions for calculations with LDA/GGA functionals, we include the components needed for non-local hybrid functionals and van der Waals effects [2]. The last two elements are critical ingredients especially for the accurate description of the electronic structure of organic semiconductor materials, their band gaps and deformation potentials. We present benchmark results for various test systems, in particular for crystalline models of polyacetylene.

[1] V. Blum *et al.*, Comp. Phys. Comm. **180**, 2175 (2009).
[2] A. Tkatchenko and M. Scheffler, PRL **102**, 073005 (2009).

HL 50.2 Wed 9:45 H13

Exploring molecular-scale structure formation of HIOS by all-atom Molecular Dynamics computer simulations — •Karol Palczynski[1] and Joachim Dzubiella[2] — [1]Institut für Physik, Humboldt Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany — [2]Institut für Physik, Humboldt Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

The optical and electronic properties of Hybrid Inorganic/Organic Semiconductor (HIOS) devices strongly depend on the molecular configuration of the conjugated organic molecules at the inorganic semiconductor surfaces. The goal of this work is to explore the structure formation of para-Sexiphenyl (6P) on a molecular level by applying atomistically resolved molecular dynamics (MD) computer simulations. The temperature dependent crystal structure of 6P has been analyzed by means of orientational and conformational order parameters. The sensitivity of the obtained structures to atomic partial charges and charge distributions has been studied and the calculated results have been compared with experimental x-ray data.

HL 50.3 Wed 10:00 H13

DFT study of vibronic properties of fluorinated nickel phthalocyanine — •Davoud Pouladsaz — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Due to their electronic, optical, and structural properties, metal–phthalocyanines, a class of organic semiconducting dye molecules, have attracted considerable attention for their wide range of application including chemical sensors and photovoltaic devices, for which fundamental understanding of charge transport properties of the molecules is crucial. In π-conjugated systems, the electronic transport properties are manipulated by the strong coupling between geometric and electronic structure. The electronic transport is efficient when the electronic coupling between adjacent molecules is maximized and the reorganization energy is minimized. On the other hand, fluorinated phthalocyanines are shown to be sensitive to reducing gases due to the withdrawing effect of fluorine atoms. Therefore, by means of density functional theory, we have calculated the intramolecular reorganization energy and vibronic couplings for single fluorinated nickel phthalocyanine, which originate from the change in optimized geometry of the molecule due to the ionization. The results reveal how the reorganization energy and the vibronic couplings change due to the fluorination of the molecule.

HL 50.4 Wed 10:15 H13

Trap passivation in organic semiconductors using ultra-low molecular doping — •Selina Olthof[1,2], Swagat Mohapatra[3], Sanjeev Singh[4], Stephen Barlow[3], Shafigh Mehraeen[3], Veaceslav Coropceanu[3], Jean-Luc Brédas[3], Seth Marder[3], Bernard Kippelen[4], and Antoine Kahn[2] — [1]Institut für Physikalische Chemie, Universität zu Köln, Germany — [2]Department of Electrical Engineering, Princeton University, USA — [3]Center for Organic Photonics and Electronics and School of Chemistry and Biochemistry, Georgia Tech, Atlanta, USA — [4]Center for Organic Photonics and Electronics and School of Electrical and Computer Engineering, Georgia Tech, Atlanta, USA

Trap states in the band gap of organic semiconductors play a detrimental role in the performance of devices. We use charge carriers released from ultra low amounts of a molecular n-dopant to gradually fill up and thereby passivate trap states in the matrix material C60. The changes in Fermi level position as well as charge carrier transport are investigated. Experiments and kinetic Monte Carlo simulations confirm a distinct change in electronic behavior for doping concentration below and above typical trap densities. After passivation, an increase in C60 electron mobility by more than three orders of magnitude is achieved. We show that in organic field effect transistors the device performance can be greatly improved by trap filling, with high current on/off ratios as long as the doping concentration is kept below the trap density of the matrix. Controlled ultra-low doping is shown to be an effective way to passivate unwanted traps in organic semiconductor films.

HL 50.5 Wed 10:30 H13

Polarization resolved carrier dynamics in crystalline perfluoropentacene films — •Kolja Kolata, Tobias Breuer, Gregor Witte, and Sangam Chatterjee — Philipps-Universität Marburg

Perfluoropentacene (PFP) is a promising n-type counterpart to the p-type pentacene (PEN) for possible future organic pn-junction applications. Since the synthesis of PFP only dates back to 2004 little is known about the electronic excitations and dynamics in this material system. We performed polarization resolved optical pump-probe spectroscopy on highly ordered, crystalline PFP-films epitaxially grown on NaF(100) in order to investigate its carrier dynamics. Due to the distinct crystal growth of PFP on NaF yielding single crystalline domains of 100 μm^2 the optical response along the c- and b-axis can be probed independently. Two distinct time-regimes are observed in both crystal

directions: an ultrafast decay (≈1ps) of the majority of the carriers followed by slower relaxation and recombination processes. Furthermore, a flat, broadband, induced absorption arises a few tens of femtoseconds after the excitation along the b-axis, where a pronounced π-stacking in the herringbone-structure exists. This induced absorption shifts towards higher energies during the following few tens of picoseconds indicating a relaxing carrier system. This confirms the different carrier dynamics and electronic properties along different directions within the PFP crystal.

Coffee break

HL 50.6 Wed 11:00 H13

The Effect of Confinement on the Exciton Dynamics in the Organic Semiconductor Rubrene — •B. Gieseking[1], T. Schmeiler[1], B. Müller[1], C. Deibel[1], V. Dyakonov[1,2], and J. Pflaum[1,2] — [1]Experimental Physics VI, Julius-Maximilian University of Würzburg, D-97074 Würzburg — [2]Bavarian Centre for Applied Energy Research (ZAE Bayern), D-97074 Würzburg

As for its inorganic counterpart the future developements in organic electronics are driven by the advancing device miniaturization. As a consequence the correlation between the opto-electronic properties and device dimensions has shifted continuously into the spotlight.

In this work we present a systematic investigation of the temperature dependent photoluminescence decay for well-defined structures of the organic semicondutor rubrene. The analysed samples exhibit an increasing degree of confinement and we confirm a direct influence on the PL spectra as well as on the excitation dynamics on ultrafast timescales already for a localization of excitation on the μm scale. Our results highlight the role of the local enviroment affecting the exciton dynamics in organic semiconductors which has to be taken into account for the design of future organic opto-electronic devices.

Financial support by the DFG (FOR 1809) is acknowledged.

HL 50.7 Wed 11:15 H13

Model-free mobility determination in thin films of organic semiconductors: potential mapping — •Johannes Widmer, Janine Fischer, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, TU Dresden, Germany

Mobility is the key parameter for charge transport characterization. In disordered systems, it is generally not a constant, but a function of the electric field and/or the charge carrier density.

In our work, we characterize the charge transport in thin films of organic semiconductors perpendicular to the surface, i.e. in the direction relevant for common device applications. The effective mobility is determined as a function of the electric field and charge carrier density $\mu(E, n)$. This is achieved by a potential mapping approach, analyzing a series of current-voltage characteristics of single carrier devices with varying intrinsic layer thicknesses. The evaluation is validated with simulation data, demonstrating that field dependence and charge density dependence can be resolved separately.

The technique is applied to well-established and state-of-the-art material systems. For example, in a blend of zinc phthalocyanine (ZnPc) and Fullerene C60, a field activated hole mobility of $7.9 \cdot 10^{-9}\,\mathrm{cm^2/Vs} \cdot \exp\left(0.01\sqrt{E \cdot \mathrm{cm/V}}\right)$ is measured.

With this method, the charge carrier mobility can be studied systematically, and the field and charge density dependence upon variations of the chemical composition or the processing conditions can be quantified.

HL 50.8 Wed 11:30 H13

Spectroscopic investigation of air induced charge trapping in n-type polymer semiconductors — •Riccardo Di Pietro[1], Tom B. Kehoe[2], and Henning Sirringhaus[2] — [1]Institut für Physik und Astronomie, Universität Potsdam, Germany — [2]Cavendish Laboratory, University of Cambridge, United Kingdom

We have performed an optical spectroscopy study of how the presence of oxygen and water affects the radical anion charge states in one of the most widely studied electron transporting conjugated polymers, poly{[N,N9-bis(2-octyldodecyl)-naphthalene-1,4,5,8-bis(dicarboximide)-2,6-diyl]-alt-5,59-(2,29-bisthiophene)} (P(NDI2OD-T2)). By combining the results obtained from Charge Accumulation Spectroscopy (CAS)[1], a technique which allows optical quantification of the concentration of charged species in the polymer film, with electrical characterization of P(NDI2OD-T2) organic field-effect transistors (OFETs) we have been able to study the mechanism for bias-stress degradation upon exposure to ambient atmosphere. Here we show that the stability of the polymer anion against water is limited by two competing reactions, one involving the well-known electrochemical oxidation of the polymer anion by water and the other involving a radical anion-catalyzed chemical reaction of the polymer with water leading to degradation of the polymer film.

[1] Di Pietro, R. and Sirringhaus, H. High Resolution Optical Spectroscopy of Air-Induced Electrical Instabilities in n-type Polymer Semiconductors. Adv. Mater. 24 (2012).

HL 50.9 Wed 11:45 H13

Comparing the transition dipole orientation of different phosphorescent emitters in organic light-emitting diodes under electrical excitation — •Philipp Liehm, Caroline Murawski, Mauro Furno, Björn Lüssem, Karl Leo, and Malte C. Gather — Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Str. 1, 01062 Dresden, Deutschland

We investigate the average transition dipole orientation of different phosphorescent matrix/emitter systems that are used in state-of-the-art highly efficient organic light-emitting diodes (OLED). The orientation is determined using two different methods: in-situ angle resolved electroluminescence spectroscopy and analysis of the exciton decay time under electrical excitation. Both methods are supported by optical simulations. We find that the dipoles of the green emitter $Ir(ppy)_3$ align nearly isotropically in the matrices of TCTA/TPBi and CBP. By contrast, we show evidence that the $Ir(MDQ)_2(acac)$ and the $Ir(ppy)_2(acac)$ dipoles are preferentially horizontal when embedded in a NPB and a CBP matrix, respectively. Within the range of experimental error, we obtain similar results for both investigated methods. Using optical simulations, we provide a quantitative estimate of how the difference in average orientation influences the external quantum efficiency of OLEDs based on $Ir(ppy)_3$ and $Ir(ppy)_2(acac)$ embedded in a CBP matrix and compare against experimental results.

HL 50.10 Wed 12:00 H13

Self-passivation of molecular n-type doping during air-exposure using a highly efficient air-instable dopant — •Max Tietze, Florian Wölzel, Torben Menke, Axel Fischer, Björn Lüssem, and Karl Leo — Institut für Angewandte Photophysik, TU Dresden

Since several process steps of organic field effect transistors like photo-lithography cannot be performed in vacuum or inert atmosphere, an application of n-doping with the most efficient molecular n-type dopants is hampered because they are prone to be air-instable due to their low ionization potentials. We study systematically the degradation of films of the n-dopant tetrakis(1,3,4,6,7,8-hexahydro-2H-pyrimido[1,2-a]pyrimidinato)ditungsten(II) ($W_2(hpp)_4$) on different substrates and doped into C_{60} films by conductivity measurements, photoelectron spectroscopy, and laser desorption/ionization time of flight mass spectrometry. We find that the conductivity of n-doped C_{60} layers is restored after air-exposure, if annealed in vacuum. Hereby, the majority of the dopant molecules decompose immediately after air-exposure, whereas the remaining $W_2(hpp)_4$ molecules stay intact and slowly degrade with an exponential decay time of ≈ 11 min. These findings are explained by passivation of $W_2(hpp)_4$ molecules, which are in a charge-transfer state and thus protected from further oxidation. Hence, the conservation of the conductivity can be understood in terms of a self-passivation of molecular n-doping and an application of highly efficient n-doped thin films in functional organic devices processed even under ambient conditions is feasible.

HL 50.11 Wed 12:15 H13

using STM/nc-AFM to discriminate adsorbed molecules and attachment geometries on Si(111)-7x7 — •Zsolt Majzik[1], Benedict Drevniok[2], Wojciech Kaminski[3], Martin Ondráček[1], Alastair B. McLean[2], and Pavel Jelínek[1] — [1]Institute of Physics, Academy of Science of the Czech Republic, Cukrovarnicka 10, 162 53, Prague, Czech Republic — [2]Queen*s University, Kingston, Ontario, Canada, K7L 3N6. — [3]University of Wroczaw, plac Maksa Borna 9, 50-204 Wroczaw, Poland

Scanning tunneling microscopy (STM) has been used to study surface reactions leading to an improved understanding of surface chemistry at the atomic length scale. However, by using a qPlus sensor, non-contact atomic force microscopy (nc-AFM) can be performed at the same time, allowing simultaneous measurement of the tip-surface conductance and tip-surface interaction. Here we present a joined experimental and

theoretical study of the adsorption of hydrogen, ethylene and benzene on the Si(111)-7x7. Based on force site spectroscopy combined with density functional theory (DFT) simulations we found that over the molecules and hydrogen only a very weak attractive force appear and mainly the repulsive interaction acts along tip approach. The position of the attractive force maxima on the Z scale and the magnitude of the attractive force can be well used as a fingerprint to discriminate between common defects, such as vacancies, and adsorbates. Moreover, using benzene and ethylene as model systems, we demonstrate that combined STM/AFM provides more information about attachment geometries than STM alone.

HL 51: Invited Talk: Jürgen Christen

Time: Wednesday 9:30–10:00 Location: H15

Invited Talk HL 51.1 Wed 9:30 H15

Nano-scale characterization of semiconductors using helium temperature scanning transmission electron microscopy cathodoluminescence — •Jürgen Christen, Gordon Schmidt, Peter Veit, Frank Bertram, and Marcus Müller — Institute of Experimental Physics, Otto-von-Guericke-University, Magdeburg

For a detailed understanding of complex semiconductor heterostructures and the physics of devices based on them, a systematic determination and correlation of the structural, chemical, electronic, and optical properties on a nanometer scale is essential. Luminescence techniques belong to the most sensitive, non-destructive methods of semiconductor research. The combination of luminescence spectroscopy - in particular at liquid He temperatures - with the high spatial resolution of a scanning transmission electron microscopy (STEM) (dx $<$ 1 nm at RT, dx $<$ 5 nm at 10 K), as realized by the technique of low temperature scanning transmission electron microscopy cathodoluminescence microscopy (STEM-CL), provides a unique, extremely powerful tool for the optical nano-characterization of semiconductors, their heterostructures as well as their interfaces. Our CL-detection unit is integrated in a FEI STEM Tecnai F20 equipped with a liquid helium stage and a light collecting parabolic mirror. Panchromatic as well as spectrally resolved CL imaging is used, both collected simultaneously with the STEM signal at each pixel. Typical results on challenging structures will be presented.

HL 52: Graphene: Characterization and devices (HL, jointly with MA, O, TT)

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

HL 52.1 Wed 9:30 H17

Polarization dependence of phonon modes in graphene nanoribbons — •Felix Kampmann[1], Nils Scheuschner[1], Bernat Terrés[2,3], Christoph Stampfer[2,3], and Janina Maultzsch[1] — [1]Institut für Festkörperphysik, TU Berlin, Hardenbergstraße 36, 10623 Berlin, Germany, EU — [2]JARA-FIT and II. Institute of Physics B, RWTH Aachen University, Aachen, Germany, EU — [3]Peter Grünberg Institute (PGI-6/8/9), Forschungszentrum Jülich, Jülich, Germany, EU

Polarization dependent Raman spectroscopy has lately been used to investigate the edge states of few layer graphene revealing insight into the selection rules of their Raman modes.

Here we report polarization dependent Raman measurements on single-layer graphene nanoribbons with varying width down to 30 nm.

We show that the $\cos^2(\theta)$ behavior of the intensity ratio I(D)/I(G) can be reproduced as it has already been known for the graphene edge states. Furthermore we found a similar behavior for I(D′)/I(G) and discuss the dependence on the nanoribbon width.

HL 52.2 Wed 9:45 H17

Manifestation of charged and strained graphene layers in the Raman response of graphite intercalation compounds — Julio Chacon-Torres[1], •Ludger Wirtz[2], and Thomas Pichler[1] — [1]Faculty of Physics, University of Vienna, Austria — [2]Physics and Material Sciences Unit, University of Luxembourg, Luxembourg

We present recent Raman measurements together with a detailed analysis of potassium graphite intercalation compounds (GICs): stage II to stage VI (where stage n means one intercalant layer after every nth graphene layer). By ab-initio calculations of the charge densities and the electronic band dispersions, we demonstrate that most (but not all) of the charge donated by the K atoms remains on the outer graphene layers, i.e., the once adjacent to the intercalant layer. This leads to an electronic decoupling of the inner (uncharged) from the outer (charged) layers and consequently also to a decoupling of the corresponding Raman spectra: The G-line splits into two peaks and the 2D line is entirely due to the uncharged inner layers while the 2D line of the outer layers is suppressed due to the strong charging. The quantitative interpretation of the peak positions requires that the internal strain of the graphene layers is taken into account. This allows to unambiguously identify the Raman response of strained charged and uncharged graphene layers and to correlate it to the in-plane lattice constant. Raman spectroscopy is thus a very powerful tool to identify internal strain in single and few-layer graphene as well as to to identify the strain in nanoelectronic and optoelectronic devices or the local interfacial strain in other graphene composites.

HL 52.3 Wed 10:00 H17

C–axis transport in graphite and few–layered–graphene — •Ole Pfoch, Yuri Koval, Michael Enzelberger, and Paul Müller — Department of Physics and Interdisciplinary Center for Molecular Materials, Universität Erlangen

Electrical transport in single or few layered graphene was intensively investigated during the last decade. However, most experiments were performed with electronic transport in the plane. Measurements in perpendicular direction are rare and the results are rather sensitive to materials properties. For instance, the literature data for the anisotropy of the electrical conductivity in plane and along the c–axis varies between 100 and 10 000. One of the reasons for the wide spread of anisotropy data might be a significant influence of structural defects. We reduce the influence of these defects by decreasing the cross section of the measured structures down to $2 \times 2\,\mu m^2$. Mesa type structures were prepared by e–beam lithography and O_2–plasma etching. The influence of the mesa size on the c–axis conductivity and its temperature dependence were investigated. We have found that the c–axis conductivity is rather sensitive to the prehistory of the sample and to the origin of the graphite material. We present our recent results and discuss the mechanism of c–axis electrical transport.

HL 52.4 Wed 10:15 H17

Electronic transport of metallic thin films and islands on graphene with scanning tunneling spectroscopy — •Anne Holtsch, Hussein Shanak, Haibin Gao, and Uwe Hartmann — Institute for Experimental Physics, Saarland University, P.O. Box 151150, 66041 Saarbrücken

Electronic properties of graphene without and with metallic thin films and islands on top are investigated. The graphene layers are epitaxially grown on rhodium using a chemical vapor deposition (CVD) method. In a second step, metallic thin films and islands (Au) are deposited onto the surface of the graphene layer. Investigations are performed by using scanning tunneling spectroscopy (STS). An introduction to a method for an automated comparison and characterization of different spectroscopic curves is the focus of this presentation. This method will be used to clarify which impact the metallic thin films and islands have on the electronic properties of graphene. Therefore a comparison between the results obtained from graphene samples without and with metalic thin films and islands is presented.

HL 52.5 Wed 10:30 H17

Fano-Profiles in HOPG and graphene flakes. — •Matthias Städter, Matthias Richter, and Dieter Schmeisser — Brandenburg University of Technology, Cottbus, Germany

We investigated the electronic structure of the valence and conduction band of HOPG by 2D resonant photoemission spectroscopy. Our aim is to understand the electronic structure of defects and inhomogeneities in graphene and related materials in more detail. From our measurements we find that the transition from the σ-band to the π^*-band at the M-point shows a characteristic Fano-Profile. A Fano-Profile occurs as the result of the interference of the band to band transition and a parallel transition to a discrete energy level within the band gap.The theory of Fano enables us to determine the energetic location of these discrete level. It is found to be several meV above the Fermi-Energy. Additional measurements on graphene flakes lead to similar results for the σ- to π^*-band transition and the location of the discrete energy state. With this we not only can determine the energetic states of defects but also get a better understanding of the origin of the Fano profile which is a particular detail of the resonant absorption process.

HL 52.6 Wed 10:45 H17

Multiple Auger Decay at resonant photo-excitation In carbon thin films — •Matthias Richter, Matthias Städter, Ioanna Paloumpa, and Dieter Schmeisser — Brandenburg University of Technology Cottbus, Applied Physics and Sensors, K.-Wachsmann-Allee 17, 03046 Cottbus, Germany

We use resonant photoemission at the C1s edge to study the electronic structure of HOPG, graphene flakes and monolayer graphene. We find remarkable differences in the profile of the Auger decay channels, which we attribute to an additional multiple-Auger with a three-hole final state. A prerequisite for the appearance of this decay mechanism is the existence of localized excitonic states, which cause the appearance of the multiple Auger decay. Defects (pits, holes, steps and kinks) can act as localized excitonic states. We use those effects to identify the existence and the quantity of such defect states within the π^*-band regime in carbon thin films, because the intensity of the three-hole Auger decay is varying with the defect density of the carbon films. The defect-excitonic states can be either localized in the band-gap at the M-point or in case of surface defects like steps, kinks or pits even at the K-point by losing the pure sp^2 character of the films. We find that the appearance of the multiple Auger decay is different for multilayer and monolayer graphene. In particular the interaction of impurities leads to broadening of the C1s core levels. The three-hole Auger decay spectroscopy is a new method to detect such contaminations with a high sensitivity.

HL 52.7 Wed 11:00 H17

Characterization of large-scale graphene CVD with far-infrared radiation — •Christian Cervetti[1], Boris Gorshunov[1,4,5], Elena Zhukova[1,4,5], Martin Dressel[1], Klaus Kern[2,3], Marko Burghard[2], and Lapo Bogani[1] — [1]1. Physikalisches Institut, Universität Stuttgart — [2]Max Planck Institut für Festkörperforschung — [3]Institute de Physique de la Matière Condensée, Ecole Polytechnique de Lausanne, Switzerland — [4]A.M.Prokhorov General Physics Institute, Russian Academy of Sciences, Russia — [5]Moscow Institute of Physics and Technology (State University), Russia

We use monochromatic terahertz (THz) spectrometer and standard Fourier-transform spectrometer to measure the conductance of large scale single layer graphene obtained by chemical vapor deposition. We demonstrate the extreme sensitivity of the THz conductance to copper particles produced on graphene during the transfer process, making THz spectroscopy a powerful tool for monitoring the removal of unwanted leftovers during the production of large scale graphene samples.

Coffee break

HL 52.8 Wed 11:30 H17

Terahertz generation in freely suspended graphene — •Andreas Brenneis[1], Leonhard Prechtel[1], Helmut Karl[2], Dieter Schuh[3], Werner Wegscheider[4], Li Song[5], Pulickel Ajayan[6], and Alexander W. Holleitner[1] — [1]Walter Schottky Institut and Physik-Department, TU München, Germany — [2]Institute of Physics, University of Augsburg, Germany — [3]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [4]Laboratorium für Festkörperphysik, ETH Zürich, Switzerland — [5]University of Science and Technology of China — [6]Rice University, Houston, Texas, USA

We report on THz generation and picosecond photocurrents in freely suspended bilayers of graphene [1]. The graphene layers are connected to coplanar strip lines which serve as source and drain contacts. A pump laser pulse excites charge carrier in the graphene. The resulting charge carrier dynamics couple to the strip line circuit and propagate along the strip line. With a probe laser pulse focused onto an on-chip photo switch, the propagating signal is read out via a third contact with a picosecond time resolution. By varying the delay of the probe pulse relative to the pump pulse, the optoelectronic signal can be measured time-resolved. We discuss the generation of THz radiation, ultrafast displacement currents, and thermoelectric currents within the optically excited graphene. Financial support by the ERC-grant NanoREAL is acknowledged.

References: [1] L. Prechtel, L. Song, D. Schuh, P. Ajayan, W. Wegscheider, A.W. Holleitner, Nature Comm. 3, 646 (2012).

HL 52.9 Wed 11:45 H17

Broadband THz detection with graphene flakes — •Martin Mittendorff[1,2], Stephan Winnerl[1], Josef Kamann[3], Jonathan Eroms[3], Harald Schneider[1], and Manfred Helm[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Universität Dresden, Germany — [3]Universität Regensburg, Germany

We demonstrate a broadband THz detector based on graphene flakes, which are produced by scotch-tape method on SiO_2/Si, combined with a logarithmic periodic antenna. The antenna is coupled to the graphene flake with an interdigitated comb-like structure in the center. The detectors were characterized at roomtemperature using the free-electron laser FELBE at the Helmholtz-Zentrum Dresden-Rossendorf. The responsivity is above 1 nA/W for wavelengths from $30\mu m$ to $220\mu m$. The rise time of the measured signals is below 100 ps and their length is in the range of 200 ps, while the pulse duration of the FEL pulses is around 20ps. The effect of the antenna coupling could be confirmed via polarization dependent measurements. Due to the spectral bandwidth combined with high temporal resolution and simple handling these detectors can be very useful for timing purposes of short laser pulses.

HL 52.10 Wed 12:00 H17

Electrostatic force and Raman spectroscopy measurements on graphene replicating water layers on mica — •Vitalij Scenev, Philipp Lange, Nikolai Severin, and Jürgen P. Rabe — Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Deutschland

Recently it has been argued that graphenes exfoliated onto mica become hole-doped by the substrate and that the doping level can be blocked by molecular water interlayers confined during sample preparation [1]. We use Scanning Probe Microscopy (SPM), Electrostatic Force Microscopy (EFM) and Raman Spectroscopy to investigate both the structure and the electronic properties of graphene conforming to molecular water layers on the mica surface. The layers are fluid, since variation of ambient humidity allows to control in-situ the layer thicknesses in the range of a monolayer [2]. Our data imply that graphene is hole-doped by the water layers with the doping level increasing with the water layer thickness.

1. Shim, J., et al., Water-Gated Charge Doping of Graphene Induced by Mica Substrates. Nano letters, 2012. 12(2): p. 648-654.

2. Severin, N., et al., Reversible dewetting of a molecularly thin fluid water film in a soft graphene-mica slit pore. Nano letters, 2012. 12(2): p. 774-779.

HL 52.11 Wed 12:15 H17

Tailoring the graphene/silicon carbide interface for monolithic wafer-scale electronics — •Stefan Hertel[1], Daniel Waldmann[1], Johannes Jobst[1], Andreas Albert[1], Matthäus Albrecht[1], Sergey Reshanov[2], Adolf Schöner[2], Michael Krieger[1], and Heiko B. Weber[1] — [1]Chair for Applied Physics, Erlangen, Germany — [2]ACREO AB, Kista, Sweden

The vision of graphene as future material for electronic devices is derived from impressive material parameters. However, it is evident that graphene will not readily take over the role of a semiconductor. In particular, an efficient switch is lacking due to graphene's missing bandgap.

By focusing not only on the graphene layer, but considering the silicon carbide (SiC) substrate as an essential part of the system, we developed an easy scheme to fabricate transistors with high ON/OFF

ratio - suited for logic - by tailoring the interface between SiC and the graphene layer [1]. Therefore we currently work with two graphene materials on SiC: as grown monolayer graphene (MLG) and hydrogen intercalated quasi-freestanding bilayer graphene (QFBLG). We proved the high-quality ohmic contact of MLG to n-type SiC and also characterized the Schottky-like behavior of QFBLG.

Using these components we are currently able to demonstrate transistors with ON/OFF ratios exceeding 104 at room temperature in normally-on and normally-off operation mode. We present a concept for inverters using a resistor-transistor logic scheme.

[1] S. Hertel *et al.*, Nature Communications **3**, 957 (2012)

HL 52.12 Wed 12:30 H17

Electrical interfacing of cells with graphene field effect transistors — •Felix Rolf, Lucas H. Hess, Tobias Schneider, Benno Blaschke, Moritz Hauf, and Jose A. Garrido — Walter Schottky Institut, TU München

The next generation of neuroprosthetic devices will need novel solid-state sensors with improved performance. Increased signal detection capability, better mechanical and physiological compatibility with living tissue, and in general a higher stability in biological environments are among the main requirements. Due to its electronic and electrochemical characteristics, as well as its physico-chemical properties, graphene is one of the most suitable candidates to meet these demanding requirements.

In this talk, we will report on arrays of graphene solution-gated field effect transistors (G-SGFETs) which are able to detect the electrical activity of electrogenic cells. It will be discussed how the combination of high carrier mobilities in graphene and the large interfacial capacitance at the graphene/electrolyte interface results in such high signal sensitivities. Thereby it is possible for instance, to show the generation and propagation of action potentials in cardiomyocyte-like HL-1 cell cultures. Another application is the single cell-transistor coupling using Human Embryonic Kidney (HEK293) cells. In the latter case the response of the G-SGFETs to electrical activity as well as the cell chemical activity will be discussed. Our results confirm that G-SGFETs are able to outperform state-of-the-art devices, suggesting that G-SGFETs can play an important role in future bioelectronic systems.

HL 52.13 Wed 12:45 H17

Exploring the electronic performance of graphene FETs for bio-sensing — •Lucas Hess, Benno Blaschke, Max Seifert, and Jose Garrido — Walter Schottky Institut, TU München

For medical applications such as neuroprostheses and for fundamental research on neuronal communication, it is of utmost importance to develop a new generation of electronic devices which can effectively detect the electrical activity of nerve cells. The outstanding electronic and electrochemical performance of graphene hold great promise for bioelectronic applications. For instance, we have reported on arrays of CVD-grown graphene solution-gated FETs (SGFETs) for cell interfacing, demonstrating their ability to transduce with high resolution the electrical activity of individual electrogenic cells.

In this contribution, we will present a detailed discussion on the suitability of CVD-grown graphene SGFETs for in-electrolyte operation, together with a study of the effect of electrolyte composition on the device performance. The sensitivity of SGFETs is dominated by two characteristic parameters: transconductance and electronic noise, which will be analyzed in this talk by in-electrolyte Hall-effect experiments and low-frequency noise characterization. Finally, we will briefly report on the pH and ion sensitivity of graphene devices, highlighting the influence of the chosen substrate for the device fabrication, as well as the effect of surface contamination from the fabrication technology.

This work demonstrates the potential of graphene to outperform state-of-the-art Si-based devices for biosensor and bioelectronic applications.

HL 53: GaN: Devices

Time: Wednesday 10:00–11:45 Location: H15

HL 53.1 Wed 10:00 H15

Magnetoresistance of GaN-based High Electron Mobility Transistors (HEMT) — •Sebastian Roensch[1], Victor Sizov[2], Takuma Yagi[2], Saad Murad[2], Lars Groh[2], Stephan Lutgen[2], Markus Sickmoeller[2], Michael Krieger[1], and Heiko B. Weber[1] — [1]University of Erlangen-Nuremberg, Erlangen, Germany — [2]AZZURRO Semiconductors AG

GaN-based heterostructures are well-suited for the application in high-power electronics. In particular, epitaxially grown AlGaN/GaN heterojunctions can be utilised in high electron mobility transistors (HEMT) targeted on high-power application. The intrinsic material properties of AlGaN and GaN generate a two dimensional electron gas with a high electron mobility at the interface of the heterojunction. In order to gain a comprehensive understanding of the two dimensional electron gas we carried out temperature dependent magnetoresistance measurements in the temperature range from 1.5 K to 300 K. We report on quantum correction to the classical conductance, in particular weak localization, electron-electron-interaction, and Shubnikov-de Haas oscillations.

HL 53.2 Wed 10:15 H15

Strukturelle Charakterisierung von AlInN/AlN/GaN FET Strukturen — •Andreas Lesnik, Jürgen Bläsing, Jonas Hennig, Armin Dadgar und Alois Krost — Institut für Experimentelle Physik, Otto-von-Guericke Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg

FETs auf Basis von AlInN/GaN Heterostrukturen weisen eine weitaus höhere Leitfähigkeit im Vergleich zu den üblichen FETs mit AlGaN/GaN auf. Wir haben daher Serien von AlInN(˜5nm)/AlN(˜1nm)/GaN FETs mittels MOCVD hergestellt und mit Hilfe der Röntgenreflektometrie (XRR), hochauflösenden Röntgenbeugung (HRXRD) und Röntgenfluoreszenzanalyse unter streifendem Einfall (GIXRF) untersucht. Durch die alleinige Untersuchung der Schichtstruktur mittels XRR und HRXRD konnte die Schichtstruktur nicht vollständig charakterisiert werden. Erst eine weitergehende Untersuchung der Proben durch GIXRF und der Kombination mit den anderen Messverfahren ermöglichte es, die Struktur quantitativ zu bestimmen. Insbesondere das Vorhandensein des AlN Spacers und dessen Komposition konnte erst durch weiterführende GIXRF Untersuchungen verifiziert werden.

HL 53.3 Wed 10:30 H15

AlInN/GaN based FETs with 3DEGs — •Jonas Hennig, Oliver Krumm, Hartmut Witte, Jürgen Bläsing, Peter Veit, Annette Diez, Armin Dadgar, and Alois Krost — Institut für Experimentelle Physik, Otto-von Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg

AlGaN/GaN heterostructures are the common active layer structure applied for FET devices. In contrast to AlGaN/GaN FETs a much higher conductivity can be achieved by AlInN/GaN. Common for both device types is high current operation, with higher values for AlInN/GaN, but a varying transconductance at different applied gate voltages originating in the 2DEG at the heterointerface. We have applied the concept of 3DEGs to AlInN/GaN FETs on Si to combine high conductivity with a plateau like transconductance behavior. To achieve this a GaN-AlGaN gradient was grown prior to the AlInN heterointerface. We will present calculations and first results on the structures and devices characterized by XRD, Hall-effect, C-V and I-V measurements.

HL 53.4 Wed 10:45 H15

Toward light-emitting diodes based on homogenous III-N nanowire ensembles on Si substrates — •Mattia Musolino, Christian Hauswald, Friederich Limbach, Martin Wölz, Tobias Gotschke, Oliver Brandt, Lutz Geelhaar, and Henning Riechert — Paul-Drude-Institut für Festkörperelektronik, Berlin

Light-emitting diodes (LEDs) based on III-N nanowires (NWs) are an attractive alternative to conventional planar layers, since the NW geometry enables the growth of (In,Ga)N/GaN heterostructures with high crystal quality on cost-effective Si substrates. However, (In,Ga)N/GaN NW ensembles grown by self-assembly processes suffer from multicolour emission. Homogeneous emission can be achieved by controlling the diameter of the NWs by selective-area growth (SAG).

LEDs based on such NW ensembles have so far been fabricated only on expensive and not very versatile GaN templates.

Our approach for the SAG of NWs on Si substrates by molecular beam epitaxy exploits the longer incubation time of GaN NWs on the patterned SiOx mask than in openings to an AlN buffer layer. We optimized the growth of the AlN buffer in order to attain a thickness low enough to allow LED operation and at the same time preserve the requirements necessary for SAG. In order to prove the feasibility of operating devices on such an AlN buffer we fabricated functional (In,Ga)N/GaN LEDs based on NWs grown by self-assembly processes on this thin buffer layer. In addition, we demonstrated the SAG of GaN NW on such buffers, thus paving the way towards homogeneous NW LEDs on Si substrates.

HL 53.5 Wed 11:00 H15

Influence of waveguide layer composition and doping on the performance of blue-violet laser diodes — •Martin Martens[1], Martin Frentrup[1], Luca Redaelli[2], Jörg Jeschke[2], Carsten Netzel[2], Mark-Antonius Rothe[1], Sven Einfeldt[2], Jens Rass[1], Tim Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, EW 6-1, 10623 Berlin — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Gustav-Kirchhoff-Str. 4, 12489 Berlin

A crucial aspect about designing highly efficient laser diodes is the mode guiding structure surrounding the multiple quantum well (MQW) active region. In order to investigate the impact of composition and doping of the waveguiding layers (WG) on the laser threshold of the devices, we have fabricated broad area laser diodes emitting at around 410 nm with AlGaN cladding layers, InGaN/InGaN MQWs and different WG structures consisting of GaN and $In_{0.02}Ga_{0.98}N$ layers grown by MOVPE on free standing (0001) GaN substrates. Vertical far-field measurements, electro- and photoluminescence measurements as well as device simulations were performed to investigate the effect of the WG design on the optical confinement, injection efficiency and internal quantum efficiency in the different device structures. The lowest threshold current density of $2.4\,kA/cm^2$ was achieved with a symmetric InGaN WG and additional Si-doping in the lower WG.

HL 53.6 Wed 11:15 H15

Comparison of different carrier injection mechanisms in 290 nm LEDs — •C. Kuhn[1], F. Mehnke[1], T. Wernicke[1], J. Stellmach[1], T. Kolbe[1], C. Reich[1], M. Guttmann[1], V. Kueller[2], A. Knauer[2], M. Weyers[2], and M. 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

To achieve high external quantum efficiency in UV-B LEDs a high injection efficiency for electrons and holes is necessary. The injection efficiency is reduced by electron leakage into the p-doped side of the LED. Previous examinations of LEDs with varied emission wavelength between 285 nm and 345 nm, including an $Al_{0.7}Ga_{0.3}N$:Mg electron blocking layer have shown a strong p-side luminescence which is dominating the emission especially at shorter wavelengths. To overcome this problem of electron leakage an additional interlayer consisting of undoped AlN or $Al_xGa_{1-x}N$ ($x > 0.8$) was introduced. This interlayer blocks electrons while allowing a hole current to the active region by tunneling. Electroluminescence spectra of 290 nm LEDs grown by MOVPE with AlN interlayers with a thickness from zero to 6 nm show reduced p-side luminescence due to reduced electron leakage. The optimal interlayer thickness was found to be 4 nm which is consistent with simulations. For thicker interlayers the hole injection is reduced. Further investigations of the influence of a varied aluminum content of an AlGaN interlayer will be presented.

HL 53.7 Wed 11:30 H15

Investigation of extraction efficiency and internal quantum efficiency of GaN-based LEDs — •Ailun Zhao, Uwe Rossow, Heiko Bremers, and Andreas Hangleiter — Institut für Angewandte Physik, TU Braunschweig

In order to better understand the real physical mechanism of efficiency droop for GaN-based light emitting diodes (LEDs), it is very important to know the internal quantum efficiency under electroluminescence conditions since it plays a crucial role. In our study, we calculate the extraction efficiency of our LEDs and subsequently calibrated the results using a systematic variation of the LED structure. In our calculation we consider polarization-dependent partial reflections at interfaces as well as reflections at the metal contact and their interface. Both the dispersion of the refractive indices as well as the complex refraction index of the metal mirror are taken into account. We compare the result of the calculation with experimental data from a series of LEDs with varied distance between the quantum well and the mirror. This procedure allows us to obtain an absolute calibration of the extraction efficiency. Using the result for the extraction efficiency we have determined the internal efficiency from the measured efficiencies for LEDs with various modifications of the active region in order to assess their impact on the droop.

HL 54: Focus Session: Frontiers of electronic structure theory IV (O, jointly with HL, TT)

Time: Wednesday 10:30–13:30 Location: H36

Topical Talk HL 54.1 Wed 10:30 H36

Challenges in data-intensive computational materials design: methodology and infrastructure. — •Boris Kozinsky — Robert Bosch Research and Technology Center, Cambidge, MA, USA

First-principles high-throughput screening of novel materials requires simultaneously inexpensive and accurate predictive computations of key properties. The first and most difficult challenge is the selection of the appropriate descriptors that are relevant to the material performance, and formulating the computational strategy. We will present examples of the computational design process in the fields of materials screening in batteries, catalysis and ferroelectrics. In each case, the critical issue is the selection of practical methods and validation using available data and higher-level models.

The second challenge is the need to establish a materials* informatics infrastructure able to automatically prepare and execute calculations on large classes of materials, to monitor calculations, and to store, retrieve and analyze complex data. We accomplish this by integrating storage databases with grid-enabled computational workflow into a powerful flexible environment adaptable to diverse purposes. We will discuss the requirements and possible use cases of such infrastructure elements. Together with collaborators, we are developing and making available this open-source software platform named AIDA (*Automated Infrastructure and Database for Atomistic design*) to make computational design efforts faster, easier, and fully integrated with automatic data collection and community sharing.

HL 54.2 Wed 11:00 H36

DFT+U(ω): A simplified approach for dynamical Hubbard corrections to DFT: — •David D. O'Regan and Nicola Marzari — Theory and Simulation of Materials, EPFL, Switzerland.

Numerous successful techniques have been developed to date, such as DFT+U, in which the screened Coulomb interactions, underestimated by approximate density functionals, are described more accurately via a mapping onto the Hubbard Hamiltonian. Charge screening is a dynamical process, generally, and so to fully realise the capability of such methods for improving optical and quasiparticle spectra, the Hubbard U describing these interactions must gain a frequency dependence.

We introduce a simple and inexpensive approach, named DFT+U(ω), and readily implementable within an existing DFT+U or constrained-DFT code, in which the dynamical U tensor appropriate to the rotationally-invariant DFT+U functional is computed and used to correct DFT or static DFT+U spectra perturbatively. The rotationally-invariant DFT+U(ω) self-energy interpolates between static DFT+U and GW. We recast the density-functional linear-response approach for the static U, where it is defined as an energy curvature, within the language of many-body perturbation theory. Here, its dynamical generalisation, and its relationship to methods such as constrained RPA, becomes readily apparent. A plasmon-pole type model is used for the inverse dielectric function, whereby low-energy parameters are computed using the appropriately renormalised density-functional linear-response, and high-energy parameters are inexpensively approximated via independent-particle RPA or ALDA.

HL 54.3 Wed 11:15 H36

Effective onsite interactions for materials with strong non-local Coulomb interactions — •Malte Schüler[1], Alexander Lichtenstein[2], Mikhail I. Katsnelson[3], and Tim Wehling[1] — [1]Institut für Theoretische Physik, Universität Bremen, D-28359 Bremen, Germany — [2]1. Institut für Theoretische Physik I, Universität Hamburg, D-20355 Hamburg, Germany — [3]Radboud University Nijmegen, NL-6525 AJ Nijmegen, The Netherlands

sp-Electron systems and low-dimensional materials often comprise strong local Coulomb interaction and non-local Coulomb interaction at the same time. Here we report on a method to map a generalized Hubbard model with non-local Coulomb interaction to an effective Hubbard model with strictly local Coulomb terms U^*. With the examples of graphene and silicene we show that the non-local Coulomb interaction can reduce the effective local interaction up to a factor of 2. The U^* model is defined by a variational principle with respect to the free energy. In this framework, obtaining the effective interaction requires non-local charge correlation functions for various parameters of the effective Hubbard model, which are calculated by the determinant quantum Monte Carlo method. The temperature dependence of the effective interaction is discussed.

HL 54.4 Wed 11:30 H36

First-principles calculation of Hubbard U parameters for half-metallic ferromagnets — •Ersoy Sasioglu, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Correlation effects play an important role in the electronic structure of half-metallic ferromagnets (HM-FMs). They give rise to non-quasiparticle states above (or below) the Fermi energy at high temperatures [1], which reduce the spin polarization and as a consequence the efficiency of the spintronics devices. Employing the constrained random-phase approximation (cRPA) [2] within the full-potential linearized augmented-plane-wave (FLAPW) method [3], we have calculated the strength of the effective Coulomb interaction (Hubbard U) between localized $3d$ electrons in a series of HM-FMs like zincblende MnAs, half- and full-Heusler alloys NiMnSb and Co_2MnSi, respectively. The obtained Hubbard U parameters lie between 2.5 and 4.5 eV, being smallest for MnAs (Mn-$3d$) and largest for Co_2MnSi (Co-$3d$). The small value of U in the former can be attributed to the efficient screening of the As p electrons. For HM full-Heusler compounds the obtained U values are comparable to the ones in elementary $3d$ transition metals, while for half-Heusler compounds the U is a bit smaller.

[1] M. I. Katsnelson *et al.*, Rev. Mod. Phys. **80**, 315 (2008).
[2] E. Şaşıoğlu *et al.*, Phys. Rev. B **83**, 121101(R) (2011).
[3] http://www.flapw.de

HL 54.5 Wed 11:45 H36

Magnetic Spectroscopies with DFT + Hubbard (U,V) — •Emine Kucukbenli[1], Davide Ceresoli[2], and Nicola Marzari[1] — [1]Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne (CH) — [2]CNR-ISTM Institute of Molecular Science and Technology, Milan (IT)

Hubbard U corrections to exchange-correlation functionals, introduced to deal with correlated electrons, have been shown to greatly improve the accuracy of DFT calculations of transition-metals, thanks to their ability to restore piecewise linearity of energy as a function of occupations and thus correct self-interaction errors. In addition, U is not a fitting parameter but can be calculated ab initio, using linear-response (LR) formulations.

Nevertheless, transition-metal complexes that display both covalent and ionic character are poorly described by DFT+U. Recently, the addition of an intersite Hubbard V is suggested to restore the accuracy of DFT+U for these cases, while V can be obtained ab initio as well.

In this study we combine DFT+U+V with the gauge-invariant projector augmented wave (GIPAW) method, and calculate magnetic spectroscopic properties of systems with transition metals. We have been implementing this combination in Quantum ESPRESSO package, both for LR and the recently introduced converse approach, that uses a much simpler Berry-phase calculation of the orbital magnetization. We then examine the performance of U+V corrections in determining the structural properties and hyperfine interaction parameters of small transition-metal molecules and complex organometallic systems.

HL 54.6 Wed 12:00 H36

The magnetization of periodic solids from time-dependent current-density-functional theory. — •Arjan Berger[1,4], Nathaniel Raimbault[1,2], Paul de Boeij[3], and Pina Romaniello[2,4] — [1]Laboratoire de Chimie et Physique Quantiques, Université Paul Sabatier, IRSAMC, CNRS, Toulouse, France — [2]Laboratoire de Physique Théorique, CNRS, Université Paul Sabatier, IRSAMC, Toulouse, France — [3]Scientific Computing and Modeling, Amsterdam, The Netherlands — [4]European Theoretical Spectroscopy Facility

The evaluation of the macroscopic magnetization of solids is problematic when periodic boundary conditions are used because surface effects are artificially removed. This poses a problem unless surface effects can be reformulated in terms of bulk quantities. For example, in case of the macroscopic polarization one can express the contribution of the charge density accumulated at the surface in terms of the bulk current density through the continuity equation. Therefore one can work in the framework of time-dependent current-density functional theory to efficiently calculate the macroscopic polarization [1,2]. In this presentation we will study how also the magnetization can be described within this framework.

[1] F. Kootstra, P. L. de Boeij, and J. G. Snijders, J. Chem. Phys. 112, 6517 (2000).
[2] J. A. Berger, P. Romaniello, R. van Leeuwen, and P. L. de Boeij, Phys. Rev. B 74, 245117 (2006)

HL 54.7 Wed 12:15 H36

Structure, charge order, phonons and IR spectra of magnetite — •Charles Patterson — School of Physics, Trinity College Dublin, Dublin 2, Ireland.

The structure and charge order of magnetite (Fe_3O_4) below the Verwey transition have been contentious issues for over 70 years. An x-ray refinement for the full 112 atom, Cc space group crystal structure of magnetite was reported only recently [1]. Previous refinements were hampered by multiple domain twinning in samples, whereas the recent study was performed on a micron-sized sample with two domains. Here we report hybrid density functional theory (DFT) calculations for the crystal structure, charge order, vibrations and IR spectra of magnetite in the Cc (112 atom) and $P2/c$ (56 atom) unit cells. Charge order in the Cc structure is found to consist of Fe trimerons, both in experiment [1] and calculations.

[1] M. S. Senn, J. P. Wright and J. P. Attfield, Nature 481, 173 (2012).

HL 54.8 Wed 12:30 H36

Crystalline and Magnetic Anisotropy of the 3d Transistion-Metal Oxides — •Andreas Schrön[1], Claudia Rödl[1,2], and Friedhelm Bechstedt[1] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-DSM, 91128 Palaiseau, France

The $3d$ transition-metal oxides (TMOs) are subject of debate since many decades due to their extraordinary properties, such as the formation of an antiferromagnetic ordering AFM2 below their Néel temperature. Many studies, both experimental and theoretical, focus only on MnO and NiO, where the crystalline anisotropy is solely driven by exchange striction along the unique symmetry axis in the [111] direction and where the magnetic anisotropy is explained in terms of magnetic dipole interactions. In the other TMOs, FeO and CoO, however, orbital magnetization and spin-orbit interaction play an additional, yet crucial role for both crystalline and magnetic anisotropy.

We present density-functional theory (DFT) studies including an on-site interaction U of the crystalline and magnetic anisotropy of the electronic systems with non-collinear spins. The influence of the (semi-)local description of exchange and correlation (XC) by means of the local density approximation (LDA) and generalized gradient approximation (GGA) on the orbital moments in FeO and CoO and the implications on the aforementioned properties is investigated. We discuss the quenching of the orbital magnetization due to the gradient corrections.

HL 54.9 Wed 12:45 H36

Electronic Structure and Magnetic interactions in $5d$ Ir oxide compounds — •Vamshi Mohan Katukuri[1], Viktor Yushankhai[2], Radu Coldea[3], Liviu Hozoi[1], and Jeroen van den Brink[1] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, Helmholtzstr. 20 01069 Dresden, Germany — [2]Joint Institute for Nuclear Research, Joliot-Curie 6, 141980 Dubna, Russia — [3]Clarendon Laboratory, University of Oxford, Parks Road, Oxford OX1 3PU,

United Kingdom

We investigate the correlated d-level electronic structure and magnetic interactions of 5d Ir oxide compounds by fully *ab initio* quantum-chemical many-body calculations on finite embedded clusters. The wave-function quantum-chemical methods provide a promising alternative to density-functional-based approaches to the electronic structure of solids. The computed d-d excitations in square-lattice, honeycomb, pyrochlore, and chain-like iridates compare well with recent RIXS (resonant inelastic x-ray scattering) data. We also perform a detailed analysis of the relativistic spin-orbit wave functions and compute observables such as the $\langle \mathbf{L}\cdot\mathbf{S}\rangle$ ground-state expectation value of the spin-orbit operator. The latter is in principle accessible from x-ray absorption and provides information on the role of t_{2g}–e_g couplings in the ground-state wave function and on the strength of non-cubic fields that lift the degeneracy of the t_{2g} levels. As concerns to the magnetic structure, we find, in honeycomb lattice structures, A_2IrO_3, the magnetic interactions strongly deviate from the proposed Kitaev-Heisenberg model, due to low-symmetry crystal fields.

HL 54.10 Wed 13:00 H36

Bulk electronic structure of the diluted magnetic semiconductor GaMnAs through hard x-ray angle resolved photoemission — •Jan Minar[1], Igor diMarco[2], J. Braun[1], H. Ebert[1], A.X. Gray[3], and Ch. Fadley[3] — [1]University of Munich, Munich, Germany — [2]University of Upsalla, Upsalla, Sweden — [3]UC Davis, Davis, USA

A detailed understanding of the origin of the magnetism in diluted magnetic semiconductors is crucial to their development for applications. Using hard X-ray angle-resolved photoemission [1] at 3.2 keV, we investigate the bulk electronic structure of the prototypical diluted magnetic semiconductor GaMnAs, and the undoped reference system GaAs [2]. The fully self-consistent combination of LSDA and dynamical mean field theory (DMFT) [3,4] and its combination with the one-step model of photoemission has been used to explain the experimental findings. Distinct differences are found between angle-resolved, as well as angle-integrated, valence spectra of GaMnAs and GaAs, in good agreement with theory. In addition to the standard LSDA based calculations the LSDA+DMFT approach shows an important effect of electronic correlations on the states close to the Fermi level. The combination of LSDA+DMFT and corresponding the Monte-Carlo simulations indicates an origin of ferromagnetism in GaMnAs and provides us a rather unifying picture of this controversial material.

[1]A. Gray et al., J. Minar et al., Nat. mat. 10, 759 (2011) [2] A. Gray, J. Minar et al., Nat. mat. 11, 957 (2012) [3] J. Minar, J. Phys.: Cond. Mat. (Topical Review) 23, 253201 (2011)

HL 54.11 Wed 13:15 H36

Magnetic state of pyrochlore $Cd_2Os_2O_7$ emerging from strong competition of ligand distortions and longer-range crystal anisotropy — •Nikolay Bogdanov[1], Remi Maurice[2], Ioannis Rousochatzakis[1], Jeroen van den Brink[1], and Liviu Hozoi[1] — [1]IFW Dresden, Germany — [2]Groningen University, The Netherlands

We investigate the correlated d-level electronic structure of $Cd_2Os_2O_7$, a spin $S=3/2$ pyrochlore, by fully *ab initio* quantum-chemical many-body calculations on finite embedded clusters. The wave-function quantum-chemical methods provide a promising alternative to density-functional-based approaches to the electronic structure of solids. We describe the local Os d^3 multiplet structure, the precise mechanism of second-order spin-orbit coupling and zero-field splitting (ZFS), and determine the parameters of the effective spin Hamiltonian, i.e., the single-ion anisotropy, nearest-neighbor Heisenberg exchange as well as the Dzyaloshinskii-Moriya interactions.

The results indicate that local ligand distortions and the anisotropic Cd-ion coordination strongly compete, rendering the magnetic interactions and ordering crucially depend on these geometrical features. Without trigonal distortions a large easy-plane magnetic anisotropy develops. Their presence, however, reverses the sign of the ZFS and causes a large easy-axis anisotropy ($D\simeq -6.8$ meV), which in conjunction with the antiferromagnetic exchange interaction ($J\simeq 6.4$ meV) stabilizes an all-in/all-out magnetic order. The competition uncovered here is a generic feature of 227 pyrochlore magnets and opens new perspectives on the basic magnetism in these materials.

HL 55: Focus Session: Functionalized semiconductor nanowires II (DS, jointly with HL)

Time: Wednesday 11:45–12:45 Location: H8

HL 55.1 Wed 11:45 H8

First-principles calculations of electronic and optical properties of ZnO nanowires — •Michael Lorke, Andreia Luisa da Rosa, and Thomas Frauenheim — Bremen Center for Computational Materials Science, University of Bremen, Germany

Semiconductor nanowires are promising candidates for the next generation of optoelectronic devices. In this work we have investigated the electronic and optical properties of bare and passivated ZnO nanowires with small diameter. We show that density-functional theory using the PBE0 functional can reproduce well the experimental ZnO band gap. Furthermore, by using the GW method in combination with the Bethe-Salpeter equation, we show that excitonic effects are strongly dependent on the nanowire size and surface termination.

HL 55.2 Wed 12:00 H8

BEC relaxation in a multimodal whispering-gallery exciton-polariton system — •Christof P. Dietrich, Tom Michalsky, Chris Sturm, Helena Franke, Martin Lange, Rüdiger Schmidt-Grund, and Marius Grundmann — Universität Leipzig, Inst. für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig

We present one-dimensional Bose-Einstein condensates (BEC) of whispering gallery mode (WGM) exciton-polaritons in ZnO-microwires up to room temperature. We show massive occupation of the bosonic ground state at condensation threshold, its blueshift and the condensate's one-dimensional extension and spatial coherence. We find that the condensation mechanism is different from that observed in common (two-dimensional) Fabry-Perot microcavities since the WGM system provides numerous photonic modes. Its ground state is energetically far below the exciton transition, so the system is multimodal without polariton ground state. This leads to two effects: 1.) At room temperature, the scattering of reservoir polaritons into zero-momentum states is strongly assisted by LO-phonons and very efficient because the energy-momentum conservation can be very easily fulfilled. 2.) At low temperature, a parametric relaxation process of polaritons into lower polariton branches is observed when an occupation of one is reached. States with a fixed energy difference ΔE_R are occupied. As the polariton-branch separation ΔE_P increases for lower mode numbers, the condensate gains kinetic energy when $\Delta E_P > \Delta E_R$. The lowermost state which can be reached is determined by the coupling strength and the lifetimes of exciton and WGM photon.

HL 55.3 Wed 12:15 H8

Oxygen-controlled electron-transfer dynamics under optical exitation in hybrid ZnO nano-/CdSe quantum dot structures — •Stephanie Bley[1], Dongchao Hou[1], Michael Diez[1], Sebastian Resch[2], Siegfried Waldvogel[2], Jürgen Gutowski[1], and Tobias Voss[1] — [1]Institute of Solid State Physics, Semiconductor Optics, University of Bremen, 28359 Bremen, Germany — [2]Institute of Organic Chemistry, Johannes Gutenberg University Mainz, 55128 Mainz, Germany

Due to their optoelectronic properties hybrid ZnO nano-/CdSe quantum dot structures possess a high potential for applications in photovoltaics and sensing. For this, the use of organic linker molecules to selectively attach the quantum dots to specific surfaces is a very versatile technique. We chemically synthesize colloidal CdSe quantum dots and attach them to the surface of ZnO nanostructures via different ω-mercapto alkanoic acids. The electron transfer dynamics of this hybrid systems are studied under illumination with a photon energy below the bandgap of ZnO (argon ion laser: λ=458 nm, E=2.7 eV). A strong enhancement of the photoconductivity has been found, and the experimental results demonstrate efficient electron tunneling from excited states of the quantum dots into the conduction band of the nanostructures. We discuss the influence of the length and electronic structure of the linker molecules on the electron transfer dynamics in the hybrid structures. Furthermore, we analyse the passivation of the ZnO nanostructure surfaces to reduce the influence of oxygen desorp-

tion for further studies of luminescence decay dynamics.

HL 55.4 Wed 12:30 H8

Polarization dependent CdS nanowire lasing — •Robert Röder[1], Sebastian Geburt[1], Robert Buschlinger[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, Haberstraße 9a, 91058 Erlangen

The forthcoming limitations of electronic integrated circuits cause reinforced work in nanophotonics for the development of on-chip optical components. Since semiconductor nanowires offer efficient waveguiding and mark the physical size limit of a photonic laser, they are promising candidates to overcome these limitations via optical data transmission and processing. High quality CdS NWs synthesized via VLS mechanism 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. Since optical processing is specified by the direct emission of the device, a "head-on" setup was developed for the investigation of the light output originating out of the facet end along the nanowire axis. The slope efficiency of the optically pumped CdS nanolaser was determined with a high value of 5-10 %. The lasing emission as well as the ASE is furthermore highly dependent on the polarization of the optical pumping with polarization ratios around 0.15 for the emission. FDTD simulations reveal, that the increased pumping efficiency for along the nanowire axis polarized excitation is more likely based on the absorption profile than on the absolute absorption.

HL 56: GaN: Optical characterization

Time: Wednesday 12:00–13:00 Location: H15

HL 56.1 Wed 12:00 H15

Influence of compositional variations of quaternary barrier layers on the optical properties of an InGaN SQW — •Christopher Karbaum[1], Frank Bertram[1], Thomas Hempel[1], Jürgen Christen[1], Jan Wagner[2], Michael Jetter[2], and Peter Michler[2] — [1]Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Germany — [2]Institut für Halbleiteroptik und Funktionelle Grenzflächen, University Stuttgart, Germany

The optical properties of c-plane oriented group III-nitride layers were investigated using spatially and spectrally-resolved cathodoluminescence (CL) at liquid helium temperature. The characterized set of samples was grown on sapphire substrates with Si-doped GaN buffer layers. A nominally 3 nm thick InGaN SQW was embedded into quaternary AlGaInN barriers of varying In content due to different TMIn-fluxes ranging from 3 sccm up to 50 sccm during the pulsed MOVPE growth and finally capped by a p-doped GaN layer. In all samples the NBE emission exhibits an inhomogeneous distribution with an emission line shifted to shorter wavelengths (354.4 nm). In absolute contrast to this, with increasing In content the CL from the quaternary layers is shifted from 330 nm to the spectral position of the broad DAP emission band (380 nm). For lower In content distinct luminescence contributions from the InGaN SQW which are evenly distributed between 440 nm and 480 nm were found, whereas with an increase of the In content in the barriers the emission behavior of the InGaN SQW merges into a monomodal distribution with an emission band centered at about 445 nm causing a reduction of FWHM from 333 meV down to 140 meV.

HL 56.2 Wed 12:15 H15

Band-gap renormalization versus Burstein-Moss shift in (0001) GaN investigated by spectroscopic ellipsometry — •Sarah Osterburg[1], Martin Feneberg[1], Eberhard Richter[2], Stephanie Fritze[1], Armin Dadgar[1], Alois Krost[1], and Rüdiger Goldhahn[1] — [1]Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Berlin

High free electron concentrations in semiconductors lead to enhanced electron-electron and electron-ion interactions decreasing the fundamental band-gap of the material. On the other hand, the simultaneous filling of the conduction band shifts the Fermi level and thus the absorption onset to higher energies, counteracting the band-gap renormalization. The interplay of both effects is investigated in this study experimentally. Spectroscopic ellipsometry was employed on c-plane free standing HVPE grown GaN:Si samples ($n \leq 1.4 \times 10^{19}\mathrm{cm}^{-3}$) and c-plane GaN:Ge thin films grown on sapphire (3.8×10^{19} $\mathrm{cm}^{-3} \leq n < 2 \times 10^{20}$ cm^{-3}). When taking into account the strain state, a complete picture is obtained which will be discussed

HL 56.3 Wed 12:30 H15

Temperature-dependent external quantum efficiencies of bulk ZnO and GaN — •Nils Rosemann[1], Melanie Pinnisch[2], Stefan Lautenschläger[2], Martin Eickhoff[2], Bruno K. Meyer[2], and Sangam Chatterjee[1] — [1]Fachbereich Physik, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]I. Physikalisches Institut, Justus-Liebig-University Gießen, Heinrich Buff-Ring 16, 35392 Gießen, Germany

The most promising candidates for efficient solid-state UV-emitters today are probably those based on GaN. Nevertheless, ZnO has to be taken into account as an alternative material as these two materials share many physical properties such as large band-gap, exciton binding energies and a wurtzite crystal structure. However, both of them have their respective down-sides. In case of GaN the realization of high power devices remains the largest challenge, whereas ZnO still lacks the possibility of efficient and controllable p-type doping. To quantify the potential of both materials we investigate two series of GaN and ZnO bulk layers by temperature-dependent absolute photoluminescence spectroscopy using an integrating sphere mounted inside a cryostat. All samples show a strong decrease of the overall external quantum efficiency (EQE) with increasing temperature. Their differences only unveil in the spectral dependence of the EQE. For the GaN samples the EQE at room temperature is dominated by PL from deep defects while the ZnO is still dominated by near-edge emission.

HL 56.4 Wed 12:45 H15

Two-electron transition of excitons bound to neutral Si donors in homoepitaxial AlN — •Benjamin Neuschl[1], Martin Feneberg[2], Rüdiger Goldhahn[2], Zhihong Yang[3], Thomas Wunderer[3], Jinqiao Xie[4], Seiji Mita[4], Rafael Dalmau[4], Ramón Collazo[5], Zlatko Sitar[5], and Klaus Thonke[1] — [1]Institute of Quantum Matter / Group Semiconductor Physics, University of Ulm — [2]Department of Experimental Physics / Material Physics, University of Magdeburg — [3]Palo Alto Research Center Inc., Palo Alto, USA — [4]HexaTech Inc., Morrisville, USA — [5]Department of Materials Science and Engineering, North Carolina State University, Raleigh, USA

We successfully detected the contribution of two-electron transitions of excitons bound to neutral silicon donors to the emission spectra of aluminum nitride. The sample under investigation was grown homoepitaxially by MOCVD on PVT grown bulk aluminum nitride substrate. Its outstanding crystal quality allows for a very detailed analysis by low-temperature photoluminescence spectroscopy with excellent spectral resolution. For a multitude of excitation spots, we correlated the emission intensities of all luminescence bands in the bandedge region. We found a clear dependency of one single band on the emission of excitons bound to neutral silicon. Temperature dependent studies on the according emission bands confirmed our interpretation of a two-electron transition. This allows for a direct calculation of the donor binding energy of silicon in aluminum nitride.

HL 57: Spintronics/Quantum information: Materials and methods (HL, jointly with TT)

Time: Wednesday 15:00–18:45 Location: H2

HL 57.1 Wed 15:00 H2

Onsager relations in a two-dimensional electron gas with spin-orbit coupling — •Cosimo Gorini[1,2], Roberto Raimondi[3], and Peter Schwab[1] — [1]Institut für Physik, Universität Augsburg — [2]CNRS and Université de Strasbourg — [3]Dipartimento di Fisica, Università di Roma Tre

Theory predicts for the two-dimensional electrons gas with only Rashba spin-orbit interaction a vanishing spin Hall conductivity and at the same time a finite inverse spin Hall effect. We show how these seemingly contradictory results are compatible with the Onsager relations: the latter do hold for spin and particle (charge) currents in the two-dimensional electron gas, although (i) their form depends on the experimental setup and (ii) a vanishing bulk spin Hall conductivity does not necessarily imply a vanishing spin Hall effect. We also discuss the situation in which extrinsic spin orbit from impurities is present and the bulk spin Hall conductivity can be different from zero.

[1] - C. Gorini, R. Raimondi, P. Schwab, arXiv:1207.1289 (to appear in PRL)

HL 57.2 Wed 15:15 H2

On the misinterpretation of the temperature dependence of T_2^* in time-resolved Faraday rotation — •Sebastian Kuhlen[1], Ralph Ledesch[1], Carla Schenk[1], Matthias Althammer[2], Sebastian T. B. Gönnenwein[2], Matthias Opel[2], Rudolf Gross[2], and Bernd Beschoten[1] — [1]II. Physikalisches Institut A, RWTH Aachen University, Aachen — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching

Time-resolved Faraday rotation (TRFR) is a well-established optical pump probe technique to generate and to probe spin coherence in semiconductors. Spin dephasing times T_2^* can easily be determined from TRFR if their values are comparable to the available pump-probe-delay. If, however, T_2^* exceeds the laser repetition time resonant spin amplification (RSA) can equally be used to extract T_2^*. We demonstrate that in ZnO these techniques have several tripping hazards resulting in deceptive results for T_2^*. We show that the temperature dependence of the amplitude ratio of two separate spin species can easily be misinterpreted as a strongly temperature dependent T_2^* of a single spin ensemble, while the two spin species have T_2^* values which are nearly independent of temperature. Additionally, consecutive pump pulses can significantly diminish the spin polarization, which remains from previous pump pulses. While this barely affects T_2^* values extracted from delay line scans, it results in seemingly shorter T_2^* values in RSA.

Work supported by DFG through SPP 1285.

HL 57.3 Wed 15:30 H2

All-electrical time-resolved spin generation and coherent spin manipulation in n-InGaAs — •Ivan Stepanov[1,2], Sebastian Kuhlen[1,2], Manfred Ersfeld[1,2], Stefan Göbbels[1,2], Mihail Lepsa[2,3], and Bernd Beschoten[1,2] — [1]II. Physikalisches Institut, RWTH Aachen University, 52056 Aachen, Germany — [2]JARA: Fundamentals of Future Information Technology, 52074 Aachen — [3]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich, 52425 Jülich

Creation and manipulation of coherent spin information by electrical means are key tasks in semiconductor spintronics.

Here we demonstrate that a coherent spin polarization can be created and manipulated by two successive electric field pulses in n- InGaAs epilayer at zero external magnetic field. The first electric pulse $\parallel [1\bar{1}0]$ creates a current induced spin polarization (CISP) which is oriented in the plane of the sample. The subsequent electric field pulse $\parallel [110]$ generates a perpendicular magnetic field pulse [1] leading to a coherent precession of this spin polarization with 2-dimensional electrical control over the final spin orientation. Spin precession is measured by time-resolved Faraday rotation. We determine the build-up time of CISP during the first field pulse and extract the spin dephasing time and internal magnetic field strength during the spin manipulation pulse. The results are in good agreement with optical pump-probe experiments on the same device.

Work supported by DFG through FOR 912.

[1] S. Kuhlen *et al.*, Phys. Rev. Lett. 109, 146603 (2012).

HL 57.4 Wed 15:45 H2

Long hole spin lifetime in InGaAs/GaAs quantum wells probed by high field cyclotron resonance spectroscopy — •Oleksiy Drachenko[1], Dmitry Kozlov[2], Anton Ikonnikov[2], Kirill Spirin[2], Vladimir Gavrilenko[2], Harald Schneider[1], Manfred Helm[1], and Jochen Wosnitza[3] — [1]Helmholtz Zentrum Dresden Rossendorf, Inst Ion Beam Phys & Mat Res, D-01314 Dresden, Germany — [2]Russian Acad Sci, Inst Phys Microstruct, Nizhnii Novgorod 603950, Russia — [3]Helmholtz Zentrum Dresden Rossendorf, Dresden High Magnet Field Lab HLD, D-01314 Dresden, Germany

In this paper, we report long, milli-second range, hole spin relaxation time in InGaAs/GaAs quantum wells probed by cyclotron resonance-spectroscopy in high pulsed magnetic fields. In our experiments, we found strong hysteresis in the spectral weights of cyclotron resonance absorption lines when rapidly changing magnetic field is used for the experiment. The hysteresis vanishes when a much slower changing magnetic field is used. We attribute this behavior to a long energy relaxation time between two lowest spin-split hole Landau levels, i.e. a long hole spin relaxation time. We also present transition frequencies calculated using a 4x4 Luttinger Hamiltonian, which confirm our findings.

HL 57.5 Wed 16:00 H2

Magneto-optical study of the sp-d exchange interaction on 1.4 nm diameter Mn^{2+} doped $(CdSe)_{13}$ clusters — Rachel Fainblat[1], •Dino Iavarone[1], Jiwoong Yang[2], Taeghwan Hyeon[2], and Gerd Bacher[1] — [1]Werkstoffe der Elektrotechnik and CeNIDE, Universität Duisburg-Essen, Germany — [2]Nanomaterials Laboratory, Seoul National University, Korea

Magnetical doping of chemically synthesized nanostructures combines the optical and electronic properties of the host semiconductor with the magnetic characteristics of the doping ions. The mechanism of colloidal nanocrystal doping can be classified into doping at the "growth" or at the "cluster" stage and, in particular, the doping efficiency in small nanocrystals is controversially discussed. On one hand, the statistical adsorption of an impurity is expected to decrease with decreasing nanocrystal size [1], whereas a recent model points out that the dopant adsorption onto the sites of small clusters ($d < 2$ nm) is more efficient than the adsorption on larger nanocrystals ($d > 5$ nm) [2].

Here, we report on low temperature ($T = 5$ K) magneto-optical effects in so-called "magic size" Mn^{2+} doped $(CdSe)_{13}$ clusters. Both absorption and magnetic circular dichroism (MCD) spectra are dominated by a resonance peak related to the heavy hole excitonic transition at 3.65 eV. From the pronounced MCD signal a giant Zeeman splitting of about 15 meV at 1.5 T is extracted supporting the theory that the Mn^{2+} ions are doped directly into the $(CdSe)_{13}$ clusters.

[1] S. Erwin et al., Nature 436, 91-4 (2005)
[2] T. Singh et al., Appl. Phys. Lett. 100, 053105 (2012)

HL 57.6 Wed 16:15 H2

Influence of strong quantum confinement on the magnetic dopant-carrier exchange coupling in Mn^{2+} doped CdSe nanoribbons — Rachel Fainblat[1], •Franziska Muckel[1], Julia Frohleiks[1], Jung Ho Yu[2], Jiwoong Yang[2], Taeghwan Hyeon[2], and Gerd Bacher[1] — [1]Werkstoffe der Elektrotechnik and CeNIDE, Universität Duisburg-Essen, Germany — [2]Nanomaterials Laboratory, Seoul National University, Korea

Key materials for future spintronic applications might be magnetically doped semiconductors with a substantial coupling between the dopants and charge carriers of the host semiconductor. This interaction is expected to be significantly altered by quantum confinement, an issue which is controversially discussed since more than a decade.

Here, we report on a clear evidence of a quantum confinement induced modification of both, s-d and s-p exchange interaction in two dimensional 1.4 nm thick Mn^{2+} doped CdSe quantum nanoribbons [1]. Both absorption and magnetic circular dichroism spectra are dominated by spectrally well-separated resonance peaks related to the heavy and the light hole excitonic transition. This allows a separate study of the s-d and the p-d exchange interaction constants. Taking into account the optical selection rules and the statistical orientation of the nanoribbons on the substrate, a remarkable change of the s-d exchange constant with respect to bulk is indicated. Room-temperature studies revealed an unusually high effective g-factor up to ∼13 encouraging

the implementation of the nanoribbons for spintronic applications.

[1] R. Fainblat et al., Nano Letters 12, 5311 (2012)

HL 57.7 Wed 16:30 H2

Electron spin-flip Raman scattering in a CdTe/(Cd,Mg)Te quantum well — •Dion Braukmann[1], J. Debus[1], D. Dunker[1], V. F. Sapega[2], D. R. Yakovlev[1,2], G. Karczewski[3], T. Wojtowicz[3], J. Kossut[3], and M. Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44227 Dortmund, Germany — [2]Ioffe Physical-Technical Institute, Russian Academy of Science, 194021 St. Petersburg, Russia — [3]Institute of Physics, Polish Academy of Sciences, 02668 Warsaw, Poland

The Raman scattering of the electron spin in a neutral exciton has been studied in a CdTe/(Cd,Mg)Te quantum well (QW). The mechanism of the electron spin-flip Raman scattering (SFRS) is experimentally evaluated from the circular polarization properties of the scattered light as well as dependence of the electron-SFRS line intensity on the magnetic field direction with respect to the QW growth axis. The spin-flip process is governed by acoustic phonon interaction and anisotropic electron-heavy-hole exchange interaction. The probability of the anisotropic exchange interaction depends on the g factors of the involved carriers. It shows a strong angular dependence due to the anisotropic heavy-hole g factor. Moreover, by application of above-barrier illumination in addition to the resonant excitation of the neutral QW excitons the intensity of the electron-SFRS line can be modulated significantly.

Coffee break

HL 57.8 Wed 17:00 H2

Ultrafast Spin Noise Spectroscopy — •Hendrik Kuhn, Fabian Berski, Jan G. Lonnemann, Petrissa Zell, Jens Hübner, and Michael Oestreich — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover

Spin Noise Spectroscopy (SNS) is a powerful experimental technique which explores the full dynamics of stochastically oriented carrier spins close to thermal equilibrium [1]. With the conventional spin noise probing scheme relying on continuous wave (cw) laser probing, the detectable temporal spin dynamic is limited by the electrical bandwidth of the photoreceiver. We advance all optical spin noise spectroscopy in semiconductors to detection bandwidths of several hundred gigahertz by employing an ingenious scheme of pulse trains from ultrafast laser oscillators as an optical probe [2]. As all SNS techniques, ultrafast SNS avoids the need for optical pumping. It enables nearly perturbation free measurements of extremely short spin dephasing times, e.g at high temperatures. We expand our measurements on highly n-doped (n = 8.2 x 10^{17} cm^3) bulk GaAs towards room temperature and demonstrate the feasibility of ultrafast SNS for spin lifetimes down to the order of a few ten picoseconds.

[1] G. M. Müller, M. Oestreich, M. Römer, and J. Hübner Physica 43, 569-587 (2010).
[2] F. Berski et al., arXiv:1207.0081v1 [cond-mat.mes-hall].

HL 57.9 Wed 17:15 H2

Spin Noise Spectroscopy: Towards Solid-State Entanglement — •Fabian Berski[1], Agnes Beichert[1], Jens Hübner[1], Andreas Wieck[2], and Michael Oestreich[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany — [2]Ruhr-Universität Bochum, Angewandte Festkörperphysik, Universitätsstr. 150, D-44780 Bochum, Germany

We study spin dynamics of naturally confined, non-interacting donor electrons in Gallium Arsenide at low temperatures by means of all optical spin noise spectroscopy [1]. The MBE grown sample shows the intriguing feature of localised spins in an environment of stochastically oriented magnetic moments: The orientation of the electron spin is lost on two different timescales which results from the interplay between the spin degree of freedom of the lattice and of the electron. The first timescale is attributed to the transversal component of the electron spin with respect to the nuclear magnetic field inside the donor volume and is determined to 4.5+-3ns. The second timescale is at least two orders of magnitude longer and is linked with the longitudinal component. An extension of the electron spin relaxation time would be possible via initilizing the surrounding spin bath by dynamic nuclear polarization which simplifies the generation and verification of entanglement [2].

[1] G. M. Müller, et al., Physica E: **43**, 569 (2010).
[2] S. Simmons, et al., Nature: **470**, 69 (2011).

HL 57.10 Wed 17:30 H2

Single Molecule Magnets meet Graphene — •Christian Cervetti[1], Andrea Cornia[4], Eberhard Ulrich Stützel[2], Stephan Rauschenbach[2], Fernando Luis[5], Martin Dressel[1], Marko Burghard[2], Klaus Kern[2,3], and Lapo Bogani[1] — [1]1. Physikalisches Institut, Universität Stuttgart — [2]Max Planck Institut für Festkörperforschung — [3]Institute de Physique de la Matière Condensée, Ecole Polytechnique de Lausanne, Switzerland — [4]Dipartimento di Chimica, Università di Modena e Reggio Emilia, Italy — [5]Instituto de Ciencia de Materiales de Aragón, Spain

Graphene has a strong potential as component of novel spintronics devices. Besides its use as conducting channel for coherent spin transport, graphene is furthermore of interest for the detection and manipulation of the spin within molecule magnets. This task requires an appropriate coupling between the sheets and the single molecular magnets. Here, we describe the assembly of a functionalized Fe4 cluster compound on graphene exploiting non-covalent π-stacking interaction. We demonstrate the control over the organization of the molecules by tuning the deposition parameters and the type of graphene. The graphene phononic environment is found to influence the magnetization dynamics of the molecular magnets as evidenced by μ-SQUID study at mK-temperatures. Finally, preliminary spin-transport experiments at low-temperature are presented.

HL 57.11 Wed 17:45 H2

Enhanced Infrared Magneto-Optical Response of the Nonmagnetic Semiconductor BiTeI Driven by Bulk Rashba Splitting — •L. Demko[1], G. A. H. Schober[3], V. Kocsis[4], M. S. Bahramy[5], H. Murakawa[5], J. S. Lee[2], I. Kezsmarki[4], R. Arita[2], N. Nagaosa[2], and Y. Tokura[1] — [1]Multiferroics Project, ERATO, JST, c/o Department of Applied Physics, University of Tokyo, Japan — [2]Department of Applied Physics, University of Tokyo, Japan — [3]Institute for Theoretical Physics, University of Heidelberg, Germany — [4]Department of Physics, Budapest University of Technology and Economics and Condensed Matter Research Group of the Hungarian Academy of Sciences, Hungary — [5]CMRG and CERG, RIKEN ASI, Japan

We study the magneto-optical (MO) response of the polar semiconducting BiTeI with giant bulk Rashba spin splitting at various carrier densities. Despite being nonmagnetic, the material is found to yield a huge MO activity in the infrared region under moderate magnetic fields (up to 3 T). Our first-principles calculations show that the enhanced MO response of BiTeI comes mainly from the intraband transitions between the Rashba-split bulk conduction bands. These transitions connecting electronic states with opposite spin directions become active due to the presence of strong spin-orbit interaction and give rise to distinct features in the MO spectra with a systematic doping dependence. We predict an even more pronounced enhancement in the low-energy MO response and dc Hall effect near the crossing (Dirac) point of the conduction bands.

HL 57.12 Wed 18:00 H2

Transport of dynamically generated pure spin current in single-layer graphene — •Masashi Shiraishi[1], Zhenyao Tang[1], Hiroki Ago[2], Kenji Kawahara[2], Yuichiro Ando[1], and Teruya Shinjo[1] — [1]Graduate School of Engineering Science, Osaka Univ., Japan — [2]Institute of Materials Chemistry and Engineering, Kyushu Univ., Japan

Electrical spin injection and generation of a pure spin current in graphene using non-local electrical technique has opened a new frontier in molecular spintronics [1-3], after the achievements, a number of interesting physics related with spin transport and spin relaxation have been studied. However, there are still many issues in spin transport in graphene that need to be clarified, and the establishment of a novel technique for spin injection and generation of a pure spin current in graphene is strongly desired for discussing spin transport phenomena in graphene. Here, we show a new approach for generating and transporting pure spin current in single-layer graphene at room temperature, the dynamical spin pumping method [4]. The dynamical spin transport was successfully demonstrated, and the estimated spin coherence in CVD-grown graphene at room temperature (RT) was 1.36 micrometers.This study is partly supported by JSPS "Nano Carbon Terahertz Science" program.

[1] M. Ohishi, M. Shiraishi et al., JJAP 46, L605 (2007). [2] N. Tombros et al., Nature 448, 571 (2007). [3] M. Shiraishi et al., Adv.

Func. Mat. 19, 3711 (2009). [4] Z. Tang, M. Shiraishi et al., Adv. Func. Mat. submitted.

HL 57.13 Wed 18:15 H2

Investigation of spin drift effect in highly doped Si — •Masashi Shiraishi[1], Makoto Kameno[1], Yuichiro Ando[1], Eiji Shikoh[1], Toshio Suzuki[2], Tohru Oikawa[3], and Tomoo Sasaki[3] — [1]Graduate School of Engineering Science, Osaka Univ., Japan — [2]AIT, Akita Industrial Technology Center, Japan — [3]TDK Corporation, Japan

Spin drift, which is usually negligible in spin transport in metallic systems, contributes significantly to spin transport and spin accumulation voltages in semiconductors like Si. Since an electric field gives rise to spin drift, investigating spin accumulation voltages as a function of the bias electric field (bias voltage) in Si spin devices can clarify how spin drift governs spin transport and accumulation properties. In this presentation, we report on quantitative analyses of spin drift effect and electric field dependence of spin injection signals in Si [1,2].

[1] M. Shiraishi et al., Phys. Rev. B83, 241204(R) (2011). [2] M. Kameno, M. Shiraishi et al., Appl. Phys. Lett. 101, 122413 (2012).

HL 57.14 Wed 18:30 H2

Investigation of ordinal and inverted Hanle spin signals in highly-doped Si — •Masashi Shiraishi[1], Makoto Kameno[1], Yasunori Aoki[1], Yuichiro Ando[1], Eiji Shikoh[1], Toshio Suzuki[2], Tohru Oikawa[3], and Tomoo Sasaki[3] — [1]Graduate School of Engineering Science, Osaka Univ., Japan — [2]AIT, Akita Industrial Technology Center, Japan — [3]TDK Corporation, Japan

Spin injection and spin transport in Si has been attracting much attention in recent several years, and spin physics in Si at room temperature is intensively argued. Whereas non-local 3-terminal method (NL3T) has been widely used for showing spin accumulation at room temperature (RT) [1], heated discussion is arising since the NL3T does not completely exclude spurious signals [2]. For proving spin injection and transport, observation of magnetoresistance in the NL-4T method (NL4T) and Hanle-type spin precession provide the most powerful evidence, and our group exhibited the first transport of pure spin current at RT [3]. In this presentation, we show the results of the detailed study on Hanle effects in NL3T by comparing that in NL4T, which strongly suggests that the results obtained by using NL3T has much room for discussion about their interpretations [4]. [1] S. Dash et al., Nature 462, 491 (2009). [2] M. Tran et al., 102, 036601 (2009). [3] T. Suzuki, M. Shiraishi et al., APEX4, 023003 (2011). [4] Y. Aoki, M. Shiraishi et al., Phys. Rev. B86, 081201(R) (2012).

HL 58: Focus Session: Copper oxide semiconductors – An attractive material for photovoltaics?

The p-type conducting copper-oxide compound semiconductors (Cu_2O, 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. By a pronounced non-stoichiometry the electronic properties may vary from insulating to metallic conduction. They appear to be an attractive alternative absorber material in terms of abundance, sustainability, non-toxicity of the elements, and numerous methods for thin film deposition that facilitate low cost production. The future and possible limitations of copper-oxide based thin-film solar-cells will be discussed by a critical look at their established physical properties and at those which need to be further investigated and improved (Organizers: Christian Heiliger, JLU Gießen, and Carsten Ronning, FSU Jena).

Time: Wednesday 15:00–18:00 Location: H13

Topical Talk HL 58.1 Wed 15:00 H13

Potential and possibilities of copper oxide compounds — •Bruno K. Meyer — 1. Physics Institute, Justus Liebig University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

Many current thin film materials used in photovoltaics have resource limitations e.g. $CdTe$, CIGS. Earth Abundant Semiconductors such as Cu_2O, Zn_3P_2, or FeS_2 are currently under investigations since apart from abundance, sustainability, non-toxicity of the elements, and numerous methods for thin film deposition that facilitate low cost production are equally important aspects. In the talk the synthesis and characterisation of Cu_2O thin films used as p-type absorbers in heterojunction solar cells will be reported. We discuss i) controlled p-type doping by nitrogen ii) the role of the possible n-type dopant Zn, and iii) tuning of the energy gap by alloy formation.

Topical Talk HL 58.2 Wed 15:30 H13

Intrinsic and hydrogen related impurities in Cu_2O — •Graeme Watson — School of Chemistry and CRANN, Trinity College Dublin, Dublin 2, Ireland

Cuprous oxide (Cu_2O) is a prototypical p-type conducting oxide with applications in dilute magnetic semiconductors, low cost solar cells, gas sensors and catalysis. It is also the parent compound of many p-type transparent conducting oxides (TCOs), which are thought to retain the valence band features and conduction mechanisms of Cu_2O. Understanding conduction in Cu_2O is therefore vital to the optimization of Cu-based materials for many applications. Calculation of the native defects in Cu_2O show that GGA and GGA+U are not capable of obtaining an accurate description of the polaronic nature of p-type defects in Cu_2O,[1] however, hybrid-DFT yields deep single-particle levels, consistent with experimentally observed activated, polaronic conduction. Our calculated transition levels for simple and split copper vacancies explain for the first time the source of the two distinct hole states seen in DLTS experiments [2] and demonstrate that Cu_2O can never be made n-type by native defects.[3] We also investigate the behaviour of hydrogen in Cu_2O,[4] and elucidate the "quasi-atomic" hydrogen site that Muon spectroscopy has been unable to identify. We discuss the impact of H on the electrical properties of Cu_2O-based materials, and propose methods to increase device performance.

[1] J. Chem. Phys., 131, 124703 (2009), [2] Phys. Rev. Lett., 103, 096405 (2009), [3] J. Phys. Chem. Lett. 1, 2582 (2010), [4] Phys. Rev. Lett., 106, 186403 (2011)

HL 58.3 Wed 16:00 H13

Molecular Beam Epitaxy of copper oxides (mainly cuprous oxide Cu_2O) — •Max Kracht, Jörg Schörmann, Thomas Sander, Peter J. Klar, and Martin Eickhoff — I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Germany

Semiconducting binary oxides (SBOs) are currently gaining intense research interest. Within this class of materials the copper oxide system (Cu-O) with the two stable phases cubic Cu_2O (cuprous oxide) and monoclinic CuO (cupric oxide) presents a fascinating exception both in terms of its electronic and its optical properties. The different Cu-O phases possess optical band gaps in the visible part of the spectrum ($E_g(Cu_2O) = 2.1\ eV$, $E_g(CuO) = 1.4\ eV$ at RT) which makes them suitable for application as absorber layers in photovoltaic devices. Cu-O thin films were grown by plasma assisted molecular beam epitaxy (PAMBE) on MgO substrates. An increase of flux ratio of Cu/O leads to a phase transition from CuO to Cu_2O which means that the phase can be controlled by the adjustment of stochiometrie of the deposited layer. Phase pure Cu_2O films were achieved at a substrate temperature of 700 $°C$, as demonstrated by high resolution x-ray diffraction and Raman spectroscopy. For the growth of $Cu_2O(001)$ on $MgO(001)$ substrates the appearance of (011) misorientations, i.e. the growth rate on the different facets, has been found to be sensitively controllable and supressed by the Cu/O ratio during PAMBE growth. Hall-Effect measurements reveal a p-type carrier concentration of $6.1 \cdot 10^{15}\ cm^{-3}$ and a mobility of 47.2 $\frac{cm^2}{Vs}$ for Cu_2O films.

Coffee break

Topical Talk HL 58.4 Wed 16:45 H13

Accelerating efficiency enhancements in cuprous oxide thin films by applying a structured approach — •Tonio Buonassisi — Massachusetts Institute of Technology, Cambridge, MA 02139, USA

With the exception of cuprous sulfide (Cu2S), binary Earth-abundant photovoltaic compounds (FeS2, Cu2O, SnS...) have record conversion efficiencies of a few percent or less, despite decades of research. It has recently been questioned whether these materials are intrinsically limited, or whether further efficiency improvements are possible with a structured scientific approach. In this presentation, we will present evidence supporting the latter hypothesis, demonstrating how a systematic approach to absorber and buffer layer development can accelerate efficiency improvements in certain Earth-abundant compounds. This systematic approach, mirroring the successes of more traditional semiconductor compounds, features multiscale modeling and interface engineering as cornerstones of a concerted effort to improve device performance. We postulate that this systematic approach to improving device performance may extend to a wider range of Earth-abundant absorber materials, potentially increasing the range of "serious" candidate solar cell materials at a historically high rate.

Topical Talk HL 58.5 Wed 17:15 H13

Photoemission Spectra of CuO from First Principles: Quasiparticle Excitations and Beyond — •Claudia Rödl, Francesco Sottile, and Lucia Reining — Laboratoire des Solides Irradiés, Ecole Polytechnique, CEA-DSM, CNRS, 91128 Palaiseau cedex, France and European Theoretical Spectroscopy Facility (ETSF)

The insulating transition-metal oxide CuO constitutes the crucial building block of the high-temperature superconducting cuprates. The almost square-planar coordination of Cu with O together with an electron-correlation-induced coupling of the Cu 3*d* orbitals is assumed to be responsible for high-temperature superconductivity. In order to shed light on the electron-correlation effects in CuO, we aim for the full *ab initio* description of its photoemission spectrum capturing both quasiparticle and satellite excitations. Photoemission satellites are due to a coupling of the one-particle excitations to other excitations in the system (e.g. plasmons) and, hence, a sign of correlation.

We calculate the photoemission spectrum of CuO in the *GW* approximation (GWA) of many-body perturbation theory. Besides studying quasiparticle excitations and their life times, we focus on satellite structures. The energy loss that is due to plasmon excitations is obtained from time-dependent density-functional theory (TDDFT). Further, we will explore a recently developed approach to plasmon satellites that is based on an electron-boson coupling model and has already been applied successfully to simple *sp* semiconductors.

HL 58.6 Wed 17:45 H13

Band Structure and Optical Properties of Copper Oxide Compounds from First Principles — •Markus Heinemann and Christian Heiliger — I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Germany

Prospective applications in the fields of optoelectronics and solar technology raise the interest in the p-type semiconductors cuprous oxide (Cu2O), cupric oxide (CuO), and paramelaconite (Cu4O3) and demand a profound knowledge of the electronic and optical properties of these materials. While the electronic and optical properties of Cu2O are well investigated theoretically, there are only a few studies on the remaining two compouds where traditional methods within density functional theory (DFT) fail to describe the semiconducting state [1]. We present the results of our first principles DFT calculations of the band structure for all three compounds using ab initio methods beyond the LDA. We compare the DFT+U approach to hybrid functionals and quasiparticle calculations within the framework of the GW approximation. Further we assess the optical properties of the three copper oxide phases by calculating the dielectric function.

[1] B. K. Meyer, A. Polity, D. Reppin, M. Becker, P. Hering, P. J. Klar, Th. Sander, C. Reindl, J. Benz, M. Eickhoff, C. Heiliger, M. Heinemann, J. Blasing, A. Krost, S. Shokovets, C. Müller, and C. Ronning, Phys. Status Solidi B, 249: 1487-1509 (2012)

HL 59: Goup IV elements and their compounds I

Time: Wednesday 15:00–16:45 Location: H15

HL 59.1 Wed 15:00 H15

Time-resolved electronic capture in germanium doped with hydrogen-like impurity centers — •Nils Dessmann[1], Sergey Pavlov[2], Valery Shastin[3], Roman Zhukavin[3], Stephan Winnerl[4], Martin Mittendorff[4], and Heinz-Wilhelm Hübers[1,2] — [1]Institut für Optik und Atomare Physik, Technische Universität Berlin, Deutschland — [2]Institut für Planetenforschung, DLR, Berlin, Deutschland — [3]Institute for Physics of Microstructures, Nizhny Novgorod, Russia — [4]Helmholtz-Zentrum Dresden-Rossendorf, Deutschland

The availability of intense short-pulsed THz radiation from sources such as free electron lasers (FELs) or synchrotrons demands broadband detectors with very short response times. This triggered a renewed interest in fast germanium (Ge) detectors. The fastest operation of Ge detectors demonstrated in the THz region of the electromagnetic spectrum so far showed an about 2-ns long decay time using highly compensated neutron transmutated p-Ge:Ga:As:Sb. The short-pulse narrow-band FEL radiation allows studying impurity photoconductivity kinetics and provides information important for optimizing the speed of response of extrinsic photoconductors. The capture of free holes and electrons in Ge doped by gallium (Ga) or antimony (Sb) has been studied by a time-resolved pump-probe experiment with the FEL FELBE at the HZDR. For Ga acceptors the relaxation times decrease with increasing pump power from approximately 3 ns to 1 ns (2 ns and 1 ns for Sb donors, respectively). The results support the development of fast photoconductive detectors in the THz region of the spectrum.

HL 59.2 Wed 15:15 H15

Photo-induced microwave emission of silicon vacancy defects in silicon carbide — •Stefan Väth[1], Daniel Riedel[1], Hannes Kraus[1], Franziska Fuchs[1], Andreas Sperlich[1], Vladimir Dyakonov[1,2], Victor Soltamov[3], Vladimir Ilyin[4], Pavel Baranov[3], and Georgy Astakhov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg — [3]Ioffe Physical-Technical Institute, St. Petersburg, RU-194021 Russia — [4]Saint Petersburg Electrotechnical University, St. Petersburg, RU-194021 Russia

Silicon vacancy defects in silicon carbide are a very promising candidate for a wide range of applications in quantum information processing, photonics and magnetometry. [1]
We have reconstructed the spin structure of silicon vacancy defects using the optically detected magnetic resonance (ODMR) technique. In particular, we have observed multi-quantum spin resonances, unambiguously indicating the high-spin ground state of these defects with $S = 3/2$, terminating an ongoing discussion about a triplet or quartet ground state. This ground state is energetically split due to the crystal field even without external magnetic field, and we were able to create an inverse population using optical spin pumping. This opens intriguing perspectives for the realization of tunable microwave amplification by stimulated emission of radiation (MASER) in a solid-state system.

[1] D. Riedel et al., Physical Review Letters 109, 226402 (2012)

HL 59.3 Wed 15:30 H15

Organophosphonate-Based PNA-Functionalization of Silicon Carbide — •Matthias Sachsenhauser[1], Dominik Weinbrenner[1], Matthias Moritz[1], Kung-Chiang Liao[2], Jeffrey Schwartz[2], Martin Stutzmann[1], Jose Garrido[1], and Anna Cattani-Scholz[1] — [1]Walter Schottky Institut, Technische Universität München, 85748 Garching, Germany — [2]Princeton University, USA

Inorganic semiconductors combined with bio-organic systems offer the potential for the development of a wide range of novel biohybrid devices. In this context, silicon carbide (SiC) is a particularly promising substrate material because it features a high chemical stability and biocompatibility, making it ideal for biomedical and biosensing applications. However, a fundamental requirement for using SiC in biosensing applications is the ability to immobilize tailored molecular and biomolecular layers on this semiconductor's surface. Re-

cently, we have demonstrated covalent functionalization of n-type 6H-SiC with organophosphonates. Structural and chemical properties of these monolayers were investigated through atomic force mircroscopy (AFM), X-ray photoelectron spectroscopy (XPS), contact potential difference (CPD) and Fourier-transform infrared spectroscopy (FTIR) measurements, revealing covalent bonding of the phosphonates to both (0001)- and (000-1)-oriented 6H-SiC crystal faces. Here we describe the potential of hydroxyl-terminated SAMs for the tailored biofunctionalization of (0001) 6H-SiC surfaces. In particular, we have focused our work on the covalent immobilization of peptide nucleic acid (PNA) oligonucleotides, which are receptors for DNA hybridization.

HL 59.4 Wed 15:45 H15

Formation of magnetic moments induced by annealing in epitaxial graphene on SiC detected by spin precession measurements — •Bastian Birkner[1], Daniel Pachniowski[1], Andreas Sandner[1], Markus Ostler[2], Thomas Seyller[2], Jaroslav Fabian[3], Mariusz Ciorga[1], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Lehrstuhl für Technische Physik, University of Erlangen-Nürnberg, 91058 Erlangen, Germany — [3]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

We present results of non-local and three terminal spin precession measurements on spin injection devices fabricated on epitaxial graphene on SiC. The measurements were performed before and after an annealing step at 150 °C for 15 minutes in vacuum. The values of spin relaxation length L_s and spin relaxation time τ_s obtained after annealing are reduced by a factor 2 and 4, respectively, compared to those before annealing. An apparent discrepancy between spin diffusion constant D_s and charge diffusion constant D_c can be resolved by investigating the temperature dependence of the effective g-factor, which is consistent with a model for paramagnetic magnetic moments.

HL 59.5 Wed 16:00 H15

Growth and bubbling transfer of graphene on recyclable copper substrates — •Simon Drieschner, Max Seifert, Lucas Hess, and José Antonio Garrido — Walter Schottky Institut, München, Deutschland

Chemical vapor deposition (CVD) is the most common method to synthesize large area high quality single layer graphene. Still, the commonly used copper foil substrate shows drawbacks in terms of surface roughness and crystal quality. We demonstrate the CVD growth of graphene in an induction heating setup, which enables the use of solid, polished copper blocks as well as copper single crystals as growth substrate. The parameter space for the growth process is explored, yielding single layer graphene of high crystal quality. A bubbling transfer method is employed to detach the graphene sheet from the copper substrate for electronic characterization. Such electrochemical transfer method allows the recycling of the catalyst substrate and a better control of the graphene crystal quality.

HL 59.6 Wed 16:15 H15

Tubes n' Triplets - On Excitation dynamics in (6,5)-single-wall carbon nanotubes — •Hannes Kraus[1], Florian Späth[2], Andreas Sperlich[1], Dominik Stich[2], Daniel Schilling[2], Tobias Hertel[2], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Institute of Physical and Theoretical Chemistry, Julius Maximilian University of Würzburg, 97074 Würzburg — [3]ZAE Bayern, 97074 Würzburg

Carbon nanotube research is picking up pace, as this material class provides a multitude of potential applications due to its intriguing structural, electrical and optical properties. Focusing on the latter, we present spin-sensitive photoluminescence and time-correlated single photon counting (TCSPC) studies on semiconducting (6,5)-single-wall carbon nanotubes (SWNT). For the first time, we can unambiguously identify the signatures of triplet-triplet interaction in SWNTs, using optically detected magnetic resonance (ODMR). Applying a 1D diffusion model to ODMR and TCSPC experimental data yields a triplet lifetime of (60 ± 30) μs. Additionally, the triplet diffusion constant was found to be very similar to the singlet excitons', i.e. on the order of 10 $\mathrm{cm^2 s^{-1}}$. The impact of the finding on the applications of carbon nanotubes in organic photovoltaics will be discussed.

HL 59.7 Wed 16:30 H15

Covalent functionalization of carbon nanotubes with tetramanganese complexes — •Robert Frielinghaus[1,5], Claire Besson[1,2,5], Anna-Katharina Saelhoff[1,5], Asmus Vierck[3], Marlou Slot[1,5], Lothar Houben[1,4,5], Janina Maultzsch[3], Paul Kögerler[1,2,5], Claus M. Schneider[1,5], and Carola Meyer[1,5] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institut für Anorganische Chemie, RWTH Aachen, 52074 Aachen, Germany — [3]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany — [4]Ernst Ruska Center for Microscopy and Spectroscopy with Electrons, 52425 Jülich, Germany — [5]JARA – Fundamentals of Future Information Technologies

We present first results on the covalent chemical functionalization of carbon nanotubes (CNTs) with tetramanganese coordination complexes. Raman spectra give indirect evidence of a successful reaction. It can only be achieved for tubes which contain defects with carboxylic groups. Changes in the magnetization behavior of the complexes due to the bonding to the CNTs are analyzed with temperature-dependent SQUID measurements. These results are correlated with bright and dark field high-resolution transmission electron microscopy (HR-TEM) measurements that show the repartition of the complex decoration on the CNTs. The TEM's elemental analysis capabilities, energy-dispersive X-ray and electron energy loss spectroscopy, prove the existence of Mn on the CNTs. We show that a mild oxidation, leaving the nanotubes conductive, is already sufficient for functionalization. This is important for the fabrication of transport devices.

HL 60: Focus Session: Coherent dynamics in semiconductor nanostructures and coupled devices

The further development of semiconductor nanophotonic devices such as high-speed lasers with bandwidths beyond 50 GHz requires a detailed understanding of the underlying nonlinear dynamical processes. Despite of severe conceptual and technological challenges in the study of associated ultra-fast phenomena, enormous progress has been achieved recently, e.g., coherent gain dynamics on a ps-timescale at room temperature. The study of ultrafast coherent processes is also vital for next generation quantum communication information systems. Here, dynamical and coherent aspects at the level of single emitters and photons are of crucial importance. This focus session will provide a platform for the presentation and discussion of state-of-the-art results, and will stimulate further research on ultra-fast and coherent nanophotonics. (Organizers: Stephan Reitzenstein and Eckehard Schöll, TU Berlin)

Time: Wednesday 15:00–18:30 Location: H16

Topical Talk HL 60.1 Wed 15:00 H16

Direct observation of coherent light matter interaction in room temperature semiconductor devices — •Gadi Eisenstein — EE Dept. Tedhnion, Haifa Israel

Direct observations of coherent light matter interactions requires that the electronic wave function dephases at a rate slower than the time of the measurement. In room temperature semiconductors, the dephasing time is 1-2 ps and therefore, experiments are traditionally performed at cryogenic temperatures so as to vastly increase the dephasing time.

An alternative approach is to shorten the observation time to well

below the 1-2 ps dephasing time but this requires a special characterization capability. A very good approach is to use FROG or X-FROG systems in which the complete complex electric field of a pulse after propagating through a nonlinear medium can be determined with high precision.

We will describe such experiments in which X-FROG was used to demonstrate Rabi oscillations and self induced transparency in a room temperature electrically driven laser amplifier. The X-FROG system has a temporal resolution of about 1 fs and is highly sensitive. The experiments are accompanied by a comprehensive model based on solving the Maxwell - Schrodinger equations using an FDTD code. The simulations confirm all the experimental observations.

Topical Talk HL 60.2 Wed 15:30 H16

Impact of coherent processes on the dynamics of quantum-dot lasers and amplifiers — •Kathy Lüdge — Institut für Theoretische Physik, Technische Universität Berlin, Deutschland

The coherent interaction between material polarization and light mode is discussed with respect to its impact on the dynamics of quantum-dot (QD) laser and amplifiers. We use a semiclassical Maxwell-Bloch approach to predict the dynamics of these devices and give further insights into the the interplay between structure and device performance. An essential part of the model is the systematic consideration of all Coulomb scattering processes. The predictive power of the model makes the results interesting for experimentalists as well as for the community engaged in QD modeling. It is found that the QD laser dynamics is considerably affected by the coherent processes if the laser is operated in a self pulsating regime, e.g., if subjected to optical injection or feedback. Further we show that the coherent interaction of the quantum dot states and the reservoir states has a huge impact on the phase dynamics and the chirp of ultrashort input pulses in amplifiers, making it important for high speed data transmission. For high input pulse intensities we observe a pulse breakup at the output facet of the amplifier that is due to pronounced Rabi oscillations of the QD polarization.

Topical Talk HL 60.3 Wed 16:00 H16

Ultrafast coherent exciton dynamics in individual quantum dots - phonons, coherent coupling, and CQED — •Wolfgang Langbein — School of Physics and Astronomy, Cardiff University, The Parade, Cardiff CF24 3AA, United Kingdom

Excitons are the fundamental optical excitations of semiconductors, determining their optoelectronic properties important for present devices such as light emitting diodes and semiconductor lasers. The coherent dynamics of the excitonic excitation is dominated by coupling to phonons and photons. The three-dimensional confinement in quantum dots (QDs) creates a finite excitation volume, yielding a discrete excitonic spectrum and phonon-assisted transitions which are enhanced with decreasing volume. The zero-phonon transition dynamics can be dominated by radiative coupling at low temperatures [10.1103/PhysRevB.70.033301], and inserting the QDs into an optical cavity the quantum strong coupling regime of CQED can be reached [10.1038/NMAT2717]. Spatially separated excitons can be coupled via an optical cavity [arXiv1206.0592], or for weakly confined excitons via a two-dimensional continuum [10.1038/NPHOTON.2010.284]. I will present measurements on QD ensembles and individual QDs using nonlinear optical spectroscopy[10.1393/ncr/i2010-10054-1], including using heterodyne detected photon echo and two-dimensional spectroscopy using heterodyne spectral interferometry [10.1364/OL.31.001151].

Coffee break

Topical Talk HL 60.4 Wed 16:45 H16

Optical Properties of coupled InAs submonolayer depositions in GaAs — •Udo W. Pohl[1], Thomas Switaiski[2], Ulrike Woggon[2], Jan-Hindrik Schulze[1], Tim D. Germann[1], and André Strittmatter[1] — [1]Inst. f. Festkörperphysik, TU Berlin, Germany — [2]Inst. f. Optik und Atomare Physik, TU Berlin, Germany

Localized states formed in a stack of InAs submonolayer depositions separated by few monolayer thick GaAs spacer layers recently received much advertence for optoelectronic applications. A high areal density [1] and direct relaxation into localized quantum dot (QD) states not coupled to a wetting layer are interesting for, e.g., direct modulated high-speed lasers [2]. On the other hand, coupling of stacked submonolayer depositions to a Stranski-Krastanow (SK) QD layer provides a tuning ability for the carrier dynamics and the transition energies.

The talk outlines the structural and optical properties of InAs/GaAs submonolayer stacks and reports on the carrier dynamics of such stacks coupled to a layer of SK QDs beneath. In the coupled system, the radiative recombination rate is controlled by the separation to the SK QDs. The measured dynamics is well described by a numerically simulated population of states localized in the submonolayer stack coupled to those of the SK QDs, taking Fermi blocking into account.

[1] A. Lenz et al., Atomic structure of buried InAs sub-monolayer depositions in GaAs, Appl. Phys. Express 3, 105602 (2010).

[2] F. Hopfer et al., 20 Gb/s 85°C error-free operation of VCSELs based on submonolayer deposition of quantum dots, IEEE J. Sel. Top. Quantum Electron. 13, 1302 (2007).

Topical Talk HL 60.5 Wed 17:15 H16

Coherent optical control of quantum dot spins and spin-photon entanglement — •Sven Höfling[1,2], Kristiaan De Greve[2], Peter L. McMahon[2], David Press[2], Leo Yu[2], Jason S. Pelc[2], Chandra M. Natarajan[2], Na Young Kim[2], Thaddeus Ladd[2], Eisuke Abe[2], Sebastian Maier[1], Dirk Bisping[1], Christian Schneider[1], Martin Kamp[1], Robert H. Hadfield[3], Alfred Forchel[2], M. M. Fejer[1], and Yoshihisa Yamamoto[1] — [1]Technische Physik, Universität Würzburg, Germany — [2]Ginzton Laboratory, Stanford University, USA — [3]Heriot-Watt University, Edinburgh, UK

Quantum computer and long-distance quantum communication technologies require robust qubits that can be coherently controlled, interfaced and entangled. Single III-V semiconductor quantum-dots in microcavities are ultra-bright emitters of indistinguishable single photons, and single electron and hole spins confined in them can serve as embedded quantum memories. In this contribution, coherent control experiments of single electron and hole qubits in a Voigt magnetic field will be summarized. By employing spin echo techniques we obtain coherence times of both qubit carrier types in the microsecond-range. Within this time scale about 10^5 complete single qubit rotations can be coherently performed with ultrafast optical pulses. Utilizing the Λ-type system of a single quantum-dot containing a single electron spin and ultrafast non-linear frequency conversion, quantum-dot spin-photon entanglement is demonstrated and presented.

HL 60.6 Wed 17:45 H16

Quantum statistical simulation of quantum-dot laser dynamics — •Jurijs Grecenkovs, Christian Otto, Franz Schulze, Andreas Knorr, Eckehard Schöll, and Kathy Lüdge — Institute of Theoretical Physics, Technical University Berlin, Berlin, Germany

Quantum dot lasers are optical devices that exploit quantum properties of specific nanostructures. These nanostructures consist of layers of nanoscale small heterogeneous material inclusions (quantum dots) in a semiconductur and are formed through a self-organizing growth process on the surface of this semiconductur. This laser type exhibits highly nonlinear dynamical behaviour.
Previous efforts in quantum dot laser decription were based on semiclassical rate equations for light intensity and carrier densities inside an optical cavity and provided some insights about behavior of this laser. The focus of this work is to explore the unusual features of the laser that are connected exclusively to its quantum-mechanical properties. To achieve this goal a fully quantum-mechanical description of the laser is considered and a numerical analysis is performed.

HL 60.7 Wed 18:00 H16

Ultrafast dynamics of 0D/2D transitions in semiconductor DWELL structures — •Mirco Kolarczik, Nina Owschimikow, Yücel Kaptan, and Ulrike Woggon — Institut für Optik und Atomare Physik, Technische Universität Berlin, Straße des 17. Juni 135, D-10623 Berlin, Germany

We investigate 0D/2D coupling in semiconductor quantum dot (QD) in a well (DWELL) structures using heterodyne two-color pump-probe spectroscopy. In our two color pump-probe experiments we vary the pump energy from the QD ground state transition to values exceeding the quantum well (QW) band gap. Depending on the carrier population in the 2D and 3D continua created by an injection current, multiple excitation pathways are possible at a given pump laser energy. These dynamics are modelled in a fully electronic rate equation system. Including direct optical interband transitions between quantum dot and quantum well states yields excellent agreement of observed traces and the numerical model. These transitions may affect the well known intradot dynamics, especially for transition energies near the

quantum well band edge, e.g. in cross gain and cross phase modulation.

To investigate coherent effects in the sub-picosecond time range, and thus obtain understanding of the complex interplay of energetically degenerate transitions, we extend the heterodyne setup to include pulse shape analysis.

HL 60.8 Wed 18:15 H16

Quantum optical approach towards quantum dot lasers with time-delayed optical self-feedback — Franz Schulze, Alexander Carmele, •Julia Kabuss, and Andreas Knorr — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany

Semiconductor lasers under the influence of time-delayed self-feedback show a large variety of dynamics which includes even chaotic behavior. The Lang-Kobayashi-model[1] (L-K-model) is widely used to study such systems. In contrast to the classical description of the light field within the L-K-model, we present in our contribution a quantum optical treatment of the time-delayed self-feedback. Our theoretical approach is based on a semiconductor quantum-dot laser model [2], which we extend to dynamically take into account photon-photon correlations between the quantized cavity and external photon field. Incorporating the interaction between the different photon modes significantly alters the light-statistics of the cavity field and yields additional insights into the dynamics of quantum-dot lasers with time-delayed self-feedback.

[1] R. Lang and K. Kobayashi, IEEE J. Quantum Electron. **16**, 347 (1980)

[2] C. Gies *et al.*, Phys. Rev. A **75**, 013803 (2007)

HL 61: Focused Session: Majorana fermions in condensed matter (TT, jointly with HL, MA, O)

Majorana fermions arise as quasi-particle excitations in condensed matter systems which exhibit non-Abelian exchange statistics. This property makes them a fundamentally new type of particles, and possibly allows topological quantum computing in this system. In the last few years, the study of Majorana fermions has rapidly evolved from being a mere theoretical concept to a practical realization: Following theoretical proposals involving hybrid nanosystems consisting of conventional superconductors and semiconducting nanowires, experiments have now found signatures of Majorana fermions. This Focused Session will discuss various aspects of Majorana fermions and the hybrid systems hosting them, including both theoretical and experimental contributions.

Organizers: Fabian Hassler (RWTH Aachen), Michael Wimmer (Leiden University)

Time: Wednesday 15:00–18:00 Location: H20

Invited Talk HL 61.1 Wed 15:00 H20

Subgap States in Majorana Wires — •Piet Brouwer — Freie Universität Berlin

A one-dimensional spin-orbit coupled nanowire with proximity-induced pairing from a nearby s-wave superconductor may be in a topological nontrivial state, in which it has a zero energy Majorana bound state at each end. In this talk, I will discuss how non-idealities in this proposal, such as potential disorder, deviations from a strict one-dimensional limit, or details concerning the termination of the wire, affect the topological phase and its signatures in a current-voltage measurement. In particular, I'll argue that the topological phase can persist at weak disorder or for multichannel wires, although some of the signatures of the presence of Majorana fermions are obscured.

Invited Talk HL 61.2 Wed 15:30 H20

New Measurements on Nanowire Majorana Systems — •Charles Marcus[1,3], Hugh Churchill[2,3], Mintang Deng[4], and Hongqi Xu[4] — [1]Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, Copenhagen, DK — [2]Department of Physics, MIT, Cambridge, MA USA — [3]Department of Physics, Harvard University, Cambridge, MA USA — [4]Division of Solid State Physics, Lund University, Lund, Sweden

This talk will present recent measurements on gated InSb nanowires coupled to a superconducting film. This set-up is one designed to detect Majorana end states. We show data similar to that seen in other groups recently, and also extend measurements in a number of directions, including higher field and higher conductance. Oscillatory structure suggesting interacting end-state Majoranas is found. We also identify transport regimes where even-odd Kondo-like features are evident, combined with Andreev bound states.

This research is sponsored by Microsoft Project Q, the Danish National Research Foundation, and Harvard University.

Topical Talk HL 61.3 Wed 16:00 H20

Adaptive Tuning of Majorana Fermions in a Quantum Dot Chain — •Anton Akhmerov — Harvard University, USA

I will explain how to overcome the obstacles that disorder and high density of states pose to the creation of unpaired Majorana fermions in one-dimensional systems. This is achieved by splitting the system into a chain of quantum dots, which are then tuned such that the chain can be viewed as an effective Kitaev chain with maximally localized Majorana fermions. Resonant Andreev spectroscopy allows us to make this tuning adaptive, so that each pair of dots may be tuned independently of the other. Our numerical simulations show that already in three quantum dots it is possible to have almost completely decoupled Majorana fermions.

15 min. break

Topical Talk HL 61.4 Wed 16:45 H20

Majorana Fermions in Disordered Quantum Wires — •Alexander Altland — Institute for Theoretical Physics, Zülpicher Str. 77, 50937 Köln

Proximity coupled spin-orbit quantum wires have recently been shown to support midgap Majorana states at critical points. We show that in the presence of disorder these systems are prone to the buildup of a second bandcenter anomaly, which is of different physical origin but shares key characteristics with the Majorana state: it is narrow in width, insensitive to magnetic fields, carries unit spectral weight, and is rigidly tied to the band center. Depending on the parity of the number of subgap quasiparticle states, a Majorana mode does or does not coexist with the impurity generated peak. The strong 'entanglement' between the two phenomena may hinder an unambiguous detection of the Majorana by spectroscopic techniques.

Topical Talk HL 61.5 Wed 17:15 H20

Parity Effects and Crossed Andreev Noise in Transport through Majorana Wires — •Bernd Rosenow[1], Björn Zocher[1,2], and Mats Horsdal[1] — [1]Institut für Theoretische Physik, Universität Leipzig, D-04009 Leipzig, Germany — [2]Max-Planck-Institute for Mathematics in the Sciences, D-04103 Leipzig, Germany

One of the defining properties of a topologically ordered state is the ground state degeneracy on surfaces with nonzero genus. In semiconductor-superconductor hybrid structures, a phase transition between regular and topologically nontrivial superconductivity is expected as a function of chemical potential or magnetic field strength. The difference in ground state degeneracies of the two phases is reflected in the parity and magnetic flux dependence of nonlinear Coulomb blockade transport through a ring shaped structure.

In nanowires of finite length, topologically non-trivial superconductivity is expected to give rise to Majorana bound states at the ends of the wire. The non-locality of Majorana bound states opens the pos-

sibility of crossed Andreev reflection with nonlocal shot noise, due to the injection of an electron into one end of the superconductor followed by the emission of a hole at the other end. When coupling the end states to leads via quantum dots with resonant levels, in the space of energies of the two resonant quantum dot levels we find a four peaked clover-like pattern for the strength of noise due to crossed Andreev reflection, distinct from the single ellipsoidal peak found in the absence of Majorana bound states.

HL 61.6 Wed 17:45 H20

Majorana qubit rotations in microwave cavities — •Thomas L. Schmidt, Andreas Nunnenkamp, and Christoph Bruder — Department of Physics, University of Basel, CH-4056 Basel, Switzerland

Majorana bound states have been proposed as building blocks for qubits on which certain operations can be performed in a topologically protected way using braiding. However, the set of these protected operations is not sufficient to realize universal quantum computing. We show that the electric field in a microwave cavity can induce Rabi oscillations between adjacent Majorana bound states. These oscillations can be used to implement an additional single-qubit gate. Supplemented with one braiding operation, this gate allows to perform arbitrary single-qubit operations.

HL 62: Graphene: SiC substrates and intercalation (O, jointly with HL, TT)

Time: Wednesday 16:00–19:15 Location: H17

HL 62.1 Wed 16:00 H17

Molecular Doping of Epitaxial Graphene on SiC with flouro-fullerenes — •Martina Wanke[1,2], Anton Tadich[3], Mark Edmonds[4], Yaou Smets[4], Chris Pakes[4], and Thomas Seyller[1,2] — [1]Institut für Physik, Technische Universität Chemnitz, Reichenhainer Strasse 70, 09126 Chemnitz, Germany — [2]LS Technische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erwin-Rommel-Strasse 1, 91058 Erlangen — [3]Soft-X-Ray-Beamline, Australian Synchrotron, 800 Blackburn Road, Clayton, VIC 3168, Australia — [4]Scholl of Physics, La Trobe University, Physical Sciences 1, Bundoora, VIC 3086, Australia

Epitaxial graphene (EG) on SiC(0001) is intrinsically n-type doped due to charge transfer from the substrate surface [1,2]. Charge transfer doping with F4-TCNQ reduces the carrier concentration and increases the carrier mobility [2], but the stability of the molecular layer in ambient conditions is not given [2]. Molecules with a sufficiently high electron affinity are needed in order to achieve a significant reduction of the electron concentration in EG by surface transfer doping. The mechanism of surface transfer doping of diamond with $C_{60}F_{48}$ is well understood [3]. Using ARPES we investigated the surface transfer doping of EG with $C_{60}F_{48}$. A net p-type doping of EG was observed for higher coverages of the $C_{60}F_{48}$.
[1] T.Ohta et al., Science **313** (2006) 951; [2] J.Jobst et al., PRB **81** (2010) 195434; W.Chen et al., JACS **129** (2007) 10418; C. Coletti et al., PRB **81** (2010) 235401. [3] M. T. Edmonds et al., JCP 136 (2012) 124701.

HL 62.2 Wed 16:15 H17

Transport properties of epitaxially grown graphene nanostructures — •Jens Baringhaus, Frederik Edler, Herbert Pfnür, and Christoph Tegenkamp — Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany

The patterning of graphene into small stripes, the so called graphene nanoribbons, is an essential task for the development of future graphene based electronic devices. For such ribbons with a well-ordered edge geometry the presence of one-dimensional edge states has been predicted. The fabrication of these well-defined structures requires the avoidance of any damaging post-processing. To overcome this obstacle we use a selective graphitization process on SiC-mesa structures, producing monolayer graphene nanoribbons of 40 nm to 100 nm in width and of several micrometers in length. The local electronic properties of the ribbons are investigated by means of a 4-tip STM. The self-assembled graphene nanoribbbons show metallic behavior and can be clearly distinguished from the non-metallic substrate. Conductances close to $G_0 = e^2/h$ are observed for a wide temperature range from 30 K up to room temperature. Description within the Landauer formalism is possible assuming ballistic transport dominated by a single ballistic channel. This is a strong indication for spin-polarized transport through the edge-states of the ribbons. These edge states also show up in scanning tunneling spectra. At higher temperatures the conductance increases due to the occupation of the next subband. Remarkably all investigated ribbons exhibit very large mean free paths up to 15 μm.

HL 62.3 Wed 16:30 H17

Local investigation of transport properties and morphology of epitaxially grown 2d graphene — •Frederik Edler, Jens Baringhaus, Herbert Pfnür, and Christoph Tegenkamp — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstraße 2, 30167 Hannover, Germany

Graphene has a peculiar band structure and special transport properties. The transport is strongly affected by imperfections of the graphene films, e.g atomic steps and impurities located at the interface between graphene and its support. A reliable control of these parameters is possible by epitaxial grown graphene on SiC. To characterize the epitaxial growth and correlate the structure with transport properties, the sheet resistance of graphene grown on SiC(0001) and SiC(000$\bar{1}$) have been studied via a 4-tip STM/SEM system. The SEM allows precise positioning of feedback controlled STM tips, enabling transport measurements on a nm-scale. While STM is used to characterize atomic size defect structures, step-bunches and nano-inhomogeneities can be identified in SEM. Sheet resistances were found to be independent from probe spacing indicating a 2d transport behavior but highly depending on ex-situ processing steps. Further in-situ annealing led to sheet resistances around $6 - 8$ k$\Omega/\square$. These values can be explained by diffusive transport theory [1] and correlate with the concentration of the nano-inhomogeneities. Structural defects induce a mobility gap as deduced from temperature-dependent transport measurements. The sheet resistance increased by a factor of three for elastically bend graphene layers across SiC step-bunches. [1] Adam *et al.*, PNAS, **104**, 18392 (2007)

HL 62.4 Wed 16:45 H17

Electronic structure of epitaxial graphene on 3C-SiC(111) — •Lydia Nemec, Volker Blum, Patrick Rinke, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, D-14195 Berlin

We present a study of the electronic structure of the carbon-rich surface phases on 3C-SiC(111), including quasi-freestanding graphene and intercalated phases. Our approach is based on density-functional theory (DFT) including van der Waals (vdW) dispersion terms in the Tkatchenko-Scheffler approach [1]. We use semilocal DFT (PBE+vdW functional) for our first-principles structure predictions. For the oxygen intercalated bilayer graphene, we consider an oxygen-rich interface passivating the Si dangling bonds [2]. Based on the predicted geometries, hybrid functionals (HSE06 and PBE0) are used to assess the electronic structure of: (1) the partially sigma-bonded "buffer layer" phase, (2) quasi-freestanding graphene up to three monolayers, and (3) hydrogen- and oxygen intercalated graphene phases. For the different phases, we discuss the changes of the electronic structure, addressing the influence of the intercalated material on the doping of the graphene and the charge transfer from the substrate to the graphene layer. We observe that in the intercalated phases graphene is decoupled from the substrate, making intercalation a promising approach for further studies.
[1] A. Tkatchenko, M. Scheffler, PRL **102**, 073005 (2009).
[2] M.H. Oliveira *et al.*; Carbon **52**, 83-89 (2013).

HL 62.5 Wed 17:00 H17

Graphene on cubic and hexagonal SiC: A comparative theoretical study — Oleg Pankratov, •Stephan Hensel, Paul Götzfried, and Michel Bockstedte — Theoretische Festkörperphysik, FAU Erlangen-Nürnberg, Staudstr. 7B2, D-91058 Erlangen

Epitaxial graphene grows on different SiC polytypes which possess distinct band gaps. We investigate the influence of polytypes on the graphene electronic spectrum employing density functional calcula-

tions with LDA and hybrid HSE functionals. We consider different buffer layer-graphene layer stackings as well as different substrate terminations.[1] We find a systematic displacement of the Dirac point relative to the valence-band edge as a function of the polytype hexagonality. The HSE values are in good agreement with available experimental results,[2,3] while LDA corroborates the trends. The Dirac point, the interface-related states, and the Fermi level follow similar polytype-dependent shifts, hence the graphene doping of the epilayer stays practically the same. For the AB stacked buffer and epilayer on Si-terminated SiC the Dirac spectrum exhibits an energy gap of 25-40 meV (depending on the polytype). On the contrary, for the AA stacking the Dirac cone remains intact. We suggest a symmetry-based analytical model which explains the origin of the gap and its absence for the AA geometry.

[1] Pankratov *et al.* Phys. Rev. B 86, 155432 (2012).
[2] Sonde *et al.*, Phys. Rev. B 80, 241406 (2009).
[3] Ristein *et al.*, Phys. Rev. Lett. 108, 246104 (2012).

HL 62.6 Wed 17:15 H17

Phonons of graphene on SiC(0001) — Stefan Fryska[1], Roland J. Koch[1], Felix Fromm[1], Alejandro Molina-Sánchez[2], •Ludger Wirtz[2], Martina Wanke[1,3], and Thomas Seyller[1,3] — [1]FAU Erlangen-Nürnberg — [2]University of Luxembourg — [3]TU Chemnitz

Epitaxial graphene (EG) on SiC(0001) can be grown on a wafer scale [1] but its charge carrier mobility is considerably lower than that of graphene flakes obstained by mechanical exfoliation. A previous study [2] of the temperature dependence of the mobility suggested that it is determined by remote phonon scattering with phonons of the buffer layer at the interface between EG and SiC(0001). The buffer layer, which is identical to the $(6\sqrt{3}\times 6\sqrt{3})R30°$ reconstruction of SiC(0001), consists of a monolayer of carbon atoms in a honeycomb structure. Due to a strong interaction with the substrate, the buffer layer has destorted π-bands and does not exhibit a Dirac cone [3]. In order to learn more about the phonons of the buffer layer we have carried out a study using high-resolution electron energy loss spectrscopy (HREELS) and Raman spectroscopy, accompanied by *ab-initio* calculations. We observe strong modifications of the phonons of the buffer layer with respect to weakly interacting, quasi-free standing graphene on SiC(0001). In particular, the Kohn anomaly is quenched, which agrees with the lack of a Dirac cone. [1] K. V. Emtsev et al., Nat. Mater. **8** (2009) 203. [2] F. Speck et al., Appl. Phys. Lett. **99** (2011) 122106. [3] K. V. Emtsev et al., Phys. Rev. B **77** (2008) 155303.

HL 62.7 Wed 17:30 H17

Intercalation of hydrogen at the graphene/Ir(111) interface — •Thorsten Balgar, Hyunil Kim, and Eckart Hasselbrink — Universität Duisburg-Essen, Universitätsstr. 5, D-45141 Essen

Epitaxially grown graphene on an iridium crystal exhibits a well known moire pattern due to the lattice mismatch of graphene and the Ir(111) surface. This leads to a buckling of the carbon layer and a lateral modulation of the chemical reactivity towards adsorbates [1,2]. Unlike intercalated metal atoms hydrogen cannot be directly detected with surface scientists' standard analysis tool box, namely XPS or AES. In our study we have used vibrational sum frequency generation (SFG) spectroscopy to monitor the stretching vibration of hydrogen chemisorbed on graphene [3]. The results are discussed in view of the intercalation of hydrogen and the local formation of graphane-like structures.

[1] C. Busse et al., Phys. Rev. Lett. 107 (2011) 036101 [2] J. Wintterlin et al., Surf. Sci. 603 (2009) 1841 [3] Kim et al., Chem. Phys. Lett. 546 (2012) 12

HL 62.8 Wed 17:45 H17

Decoupling of Epitaxial Graphene on Ir(111) by Oxygen Intercalation — •Søren Ulstrup[1], Rosanna Larciprete[2], Paolo Lacovig[3], Matteo Dalmiglio[3], Marco Bianchi[1], Jens Christian Johannsen[1], Federico Mazzola[1], Liv Hornekär[1], Fabrizio Orlando[4], Alessandro Baraldi[4], Silvano Lizzit[3], and Philip Hofmann[1] — [1]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, Denmark — [2]CNR-Institute for Complex Systems, Roma, Italy — [3]Sincrotrone Trieste, Trieste, Italy — [4]Physics Department and Center of Excellence for Nanostructured Materials, University of Trieste, and IOM-CNR Laboratorio TASC, Area Science Park, Trieste, Italy

Epitaxial growth of graphene on transition metal surfaces is now a well-established method for obtaining extended layers of high quality graphene. However, interactions between graphene and its metal substrate are unwanted in applications typically requiring a mechanical transfer of the graphene. Here we demonstrate a different strategy based on decoupling the graphene from an Ir(111) substrate by oxygen intercalation. More specifically, we present evidence using photoelectron spectroscopy techniques that the intercalation results in an extended layer of hole-doped quasi free-standing graphene (QFG). Analysis of the electronic self-energy near the Fermi level reveals an extremely weak electron-phonon coupling in QFG. Finally, we find that abrupt deintercalation of oxygen occurs at elevated temperatures, which is accompanied by a modest etching of the graphene lattice.

HL 62.9 Wed 18:00 H17

Transfer-free electrical insulation of epitaxial graphene from its metal substrate — Silvano Lizzit[1], Rosanna Larciprete[2], Paolo Lacovig[1], Matteo Dalmiglio[1], Fabrizio Orlando[3,4], Alessandro Baraldi[3,4], Lauge Gammelgaard[5], •Lucas Barreto[6], Marco Bianchi[6], Edward Perkins[6], and Philip Hofmann[6] — [1]Sincrotrone Trieste, Italy — [2]CNR-Institute for Complex Systems, Roma, Italy — [3]Physics Department and CENMAT, University of Trieste,Italy — [4]IOM-CNR Laboratorio TASC, Trieste, Italy — [5]Capres A/S, Lyngby, Denmark — [6]Institut for Fysik og Astronomi, Interdisciplinary Nanoscience Center (iNANO), Aarhus Universitet Denmark

High-quality, large-area epitaxial graphene can be grown on metal surfaces, but its transport properties cannot be exploited because the electrical conduction is dominated by the substrate. Here we show how to insulate epitaxial graphene from the Ru(0001) surface it is grown on by a step-wise intercalation of silicon and oxygen, and the eventual formation of a SiO_2 layer between the graphene and the metal. The reaction steps are followed by x-ray photoemission spectroscopy. The presence of a SiO_2 layer should insulate the metal from the substrate. In order to verify this, lateral transport measurements were performed using a nano-scale multipoint probe technique. The resistance obtained is substantially higher than expected for a clean ruthenium surface but consistent with that expected for graphene. Moreover, the data suggest two-dimensional electronic transport, as expected for graphene.

HL 62.10 Wed 18:15 H17

Intercalation as a route to atomically sharp graphene/ferromagnet interfaces: Structural and electronic investigations — •Philipp Leicht, Konstantin Krausert, Lukas Zielke, and Mikhail Fonin — Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

The interface between graphene (G) and the substrate plays a vital role for the electronic properties of G. Apart from direct growth of G on a small number of substrates, a variety of metals can be intercalated between G and the substrate interface [1,2] and allow for the production of G on a large number of materials. In this work, we present the investigation of Ni intercalation underneath G on Ir(111). The atomic structure and electronic properties were investigated for samples with intercalated Ni ranging from a submonolayer to few monolayers.

For Ni intercalation underneath G/Ir(111), scanning tunneling microscopy shows strongly increased moiré corrugation as well as a decreased average distance of G/Ni/Ir(111) compared to G/Ir(111). The stronger corrugation is accompanied by considerable changes in the electronic structure of the G layer. The intercalation channels including the influence of defects and diffusion of intercalants within the graphene-metal interface are discussed for the two regimes of submonolayer and multilayer intercalation.

[1] M. Sicot et al. ACS Nano 6, 151 (2012) [2] L. Huang et al. Appl. Phys. Lett. 99, 163107 (2011)

HL 62.11 Wed 18:30 H17

Magnetism of graphene/Ir(111) intercalation systems — •Régis Decker[1], Jens Brede[1], Nicolae Atodiresei[2], Vasile Caciuc[2], Stefan Blügel[2], and Roland Wiesendanger[1] — [1]Institute of Applied Physics, University of Hamburg, Jungiusstrasse 11, D-30355 Hamburg — [2]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungzentrum Jülich, D-52425 Jülich

The presence of intercalation compounds in graphite, i.e. impurities or layer(s) trapped between carbon sheets, can lead to changes in the transport, optical and catalytic properties compared to bulk graphite, or even to superconductivity. The intercalation of elements between graphene and its substrate can also influence the properties of graphene. Furthermore, this approach opens a new route to explore the behavior of graphene on a magnetic substrate.

Here, we present the local structure and magnetic properties of graphene on magnetic substrates, resolved by spin-polarized STM. The magnetic substrates are obtained by the intercalation of 3d elements (Co and Fe) between graphene and the Ir(111) surface [1]. In both cases, the atomic structure of the graphene layer is dominated by a highly corrugated Moiré pattern. Within the Moiré pattern different regions are identified. Interestingly, these regions show very different electronic and magnetic signatures in the experiments. The experimental observations are compared to state-of-the-art first principles density functional theory calculations.

[1] Atomic-scale magnetism of cobalt-intercalated graphene. R. Decker et al., accepted in Phys. Rev. B (Rapid Comm.).

HL 62.12 Wed 18:45 H17

Deuteration kinetics of the graphene — •Alexei Nefedov[1], Alessio Paris[2], Nikolay Verbitskiy[3,11], Ying Wang[4], Alexander Fedorov[5,6], Danny Haberer[5], Martin Oetzelt[7], Luca Petaccia[8], Dmitry Usachov[6], Denis Vyalikh[6,9], Hermann Sagdev[10], Christof Woell[1], Martin Knupfer[5], Berndt Buechner[5], Lucia Calliari[2], Lada Yashina[3], Stephan Irle[4], and Alexander Grüneis[5,11] — [1]KIT, Leopoldshafen, Germany — [2]FBK-CMM, Trento, Italy — [3]MSU, Moscow, Russia — [4]Nagoya University, Nagoya, Japan — [5]IFW Dresden, Dresden, Germany — [6]St. Petersburg University, St. Petersburg, Russia — [7]BESSY II, Berlin, Germany — [8]Elettra, Trieste, Italy — [9]TU Dresden, Dresden, Germany — [10]MPI für Polymerforschung, Mainz, Germany — [11]University of Vienna, Vienna, Austria

The kinetics of the hydrogenation/deuteration reaction of graphene was studied by time-dependent x-ray photoemission spectroscopy (XPS). The graphene layer was then exposed to hydrogen or deuterium atomic gas beams, obtained by thermal cracking in a tungsten capillary at T=3000 K. After each step XPS of the C1s line was performed in order to measure H/C and D/C ratios. We have observed a strong kinetic isotope effect for the hydrogenation/deuteration reaction leading to substantially faster adsorption and higher maximum D/C ratios as compared to H/C (D/C˜35% vs. H/C˜25%).

HL 62.13 Wed 19:00 H17

Intercalated thin films on Graphene/Ir(111) — •Hendrik Vita[1], Stefan Böttcher[1], Yuriy S Dedkov[2], and Karsten Horn[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin — [2]SPECS Surface Nano Analysis GmbH, Voltastr. 5, D-13355 Berlin

The investigation of graphene/metal systems is interesting from fundamental as well as applications-oriented point of view. Here we report on the interaction of weakly and strongly bound intercalated metals (Cu vs. Ni) with graphene grown on Ir(111), using core and valence level photoemission spectroscopy. Studying the electronic structure of graphene in these interfaces reveals the effect of weak and strong interaction between graphene and the underlying intercalated thin film. The graphene/Ni/Ir(111) system shows a strong hybridization between the graphene π-band and the Ni 3d valence bands, which leads to the destruction of the graphene Dirac cone. The graphene/Cu/Ir(111) system, on the other hand, shows at first glance the properties of weakly bonded graphene (Dirac cone with a linear dispersion of the π-band) but with additional doping due to the donation of electrons by the intercalated Cu. Contrary to the weakly bonded scenario we observe a hybridization between the distinct Cu3d states and the graphene π-band.

HL 63: Organic electronics and photovoltaics III (O, jointly with CPP, DS, HL)

Time: Wednesday 16:00–19:00 Location: H33

HL 63.1 Wed 16:00 H33

Effects of nuclear dynamics on light absorption, charge injection, recombination, and dye regeneration conditions in dye-sensitized solar cells — •Sergei Manzhos[1], Hiroshi Segawa[2], and Koichi Yamashita[3] — [1]Department of Mechanical Engineering, National University of Singapore, Blk EA #07-08, Singapore 117576 — [2]RCAST, University of Tokyo, 4-6-1, Komaba, Meguro-ku, Tokyo 153-8904, Japan — [3]Department of Chemical System Engineering, University of Tokyo, 7-3-1, Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

We present molecular dynamics studies of effects of nuclear motions on light absorption and charge injection, recombination, and dye regeneration conditions for two organic dyes adsorbed on anatase (101) surface of TiO2 in mono- and bi-dentate configurations. We studied the effects of temperature, deuteration, and co-adsorbed water. Averaged over nuclear motions driving forces for injection and regeneration can differ significantly from their static estimates computed in most works. As a result, injection rate could be different by orders of magnitude. As the expectation value of the ground state energy is higher than its optimum geometry value (by up to 0.1 eV), nuclear motions will affect dye regeneration by recently proposed redox shuttle-dye combinations operating at low driving forces. Dye orientation motions are predicted to increase back-donation rate by orders of magnitude. Dye structure, adsorption mode, and the presence of water affect strongly the dynamics of energy level matching. Temperature in the range of 300-350K and deuteration have little effect on driving forces but red-shift of the absorption spectrum by a few %.

HL 63.2 Wed 16:15 H33

Photoemission Studies of Highly Reactive Organic Photosensitizers — •Mathias Fingerle[1], Maximilian Hemgesberg[2], Yvonne Schmitt[2], Sebastian Schmitt[2], Dimitri Imanbaew[2], Harald Kelm[2], Eugen Risto[2], Stefan Lach[1], Markus Gerhards[2], Christoph van Wüllen[2], Werner Thiel[2], and Christiane Ziegler[1] — [1]Fachbereich Physik, Erwin-Schrödinger-Str. 56, D-67663 Kaiserslautern, Germany — [2]Fachbereich Chemie, Erwin-Schrödinger-Str. 52, D-67663 Kaiserslautern, Germany

Substituted phenothiazines (PTs) are promising candidates for applications in the field of organic electronics. Due to the fact, that the electronic, magnetic and geometrical properties of the phenothiazine compared to its radical cation differ substantially, PT redox couples are of great interest for organic devices like dye sensitized solar cells (DSSCs). Here, the electronic properties of N-substituted phenothiazine dyes derived from 3.8-dithien-2-ylphenothiazine (DTPT), among them the first PT containing an olefinic moiety with an electron withdrawing group close to the nitrogen atom, were probed via photoemission spectroscopy. The thin film growth of the dyes and their oxidized species after spin coating was analyzed by X-ray photoelectron spectroscopy (XPS) and qualitatively visualized by scanning force microscopy (SFM). Through UV-photoelectron spectroscopy (UPS) and inverse photoelectron spectroscopy (IPES), the occupied and unoccupied energy levels could be attained and compared to data acquired by UV/Vis spectroscopy and DFT calculations. It is shown, that chemical oxidation by NOBF4 leads to a dramatic decrease of the band gap.

HL 63.3 Wed 16:30 H33

Investigation of the electronic structure of phosphorescent Platinum(II) complexes on Au(111) by STM and STS — •Pascal Raphael Ewen, Hasmik Harutyunyan, Jan Sanning, Matteo Mauro, Cristian Alejandro Strassert, and Daniel Wegner — Physikalisches Institut - Westfälische Wilhelms Universität Münster

Quenching effects still limit the efficiency of state-of-the-art organic light emitting diodes (OLEDs) at higher doping concentrations of the triplet emitter molecules within the emission layer. A possible candidate for avoiding of the loss of luminescence are recently synthesized Pt(II) complexes that do not show quenching even when aggregated into fibers or gels. The efficient implementation of such complexes in electronic devices requires a fundamental understanding of the interaction of the molecules with the local environment. A systematic investigation of the adsorption and the electronic structure of slightly different phosphorescent Pt(II) complexes offers information about the influence of ligands and substituents on the complexes as well as their interactions with neighbours and the substrate. We have studied the impact of molecule-surface and intermolecular interactions on the self-assembly and electronic structure of Pt-complex monolayers on Au(111) using scanning tunneling microscopy (STM) and spectroscopy (STS) at low temperature. By determining energies and spatial distributions of several frontier orbitals, we are able to evaluate the impact of hybridization on the molecular electronic structure with important consequences

for the optical properties.

HL 63.4 Wed 16:45 H33

Overcoming the limitations of work-function modifications induced by adsorption of self-assembled monolayers — •Oliver T. Hofmann, Yong Xu, Patrick Rinke, and Matthias Scheffler — Fritz-Haber Institut der MPG, Berlin, Germany

Controlling the work function of electrodes critically determines charge-injection barriers and is of high importance for organic electronic devices. Such control can be easily achieved by adsorbing dipolar self-assembled monolayers. Despite the common application of this method, its limitations remain largely unexplored. It has, however, been demonstrated that charge-transfer occurs as soon as the molecular LUMO comes into resonance with the Fermi-energy when the molecular dipole moment is systematically increased by adding multiple repeat units. This Fermi-level pinning limits the achievable work-function modification. In turn, we argue that molecules with negative electron affinities never reach this limit and can reduce the work-function in principle all the way down to zero. As a proof of concept, we study the interaction between the ZnO($10\bar{1}0$) surface and pyridine using hybrid density functional theory with a variable fraction of exact exchange and a correction scheme for screened van-der-Waals forces. In agreement with experimental observations, we find an adsorption-induced work-function reduction of up to -2.9 eV. For a hypothetical ultra-dense pyridine monolayer the work-function reduction could even reach -4.3 eV for this surface.

HL 63.5 Wed 17:00 H33

Surface electronic structure and electron dynamics for pristine and adsorbate-covered ZnO($10\bar{1}0$) — •Jan-Christoph Deinert, Daniel Wegkamp, Michael Meyer, Julia Stähler, and Martin Wolf — Fritz-Haber-Institut der MPG, Abt. Physikalische Chemie, Faradayweg 4-6, 14195 Berlin

Zinc oxide is a promising electrode material for organic optoelectronics, because of its large optical band gap, possible n-type conductivity and its abundance. Despite many years of research, the electronic structure of interfaces between ZnO and - possibly functional - molecules or even its vacuum interface are not well understood. We use femtosecond time- and angle-resolved two-photon photoemission spectroscopy (2PPE) to analyze both the occupied and *un*occupied electronic states and dynamics at such interfaces. We show that hydrogen adsorption, even for very low coverage, leads to the formation of a surface electron accumulation layer and thus surface metallicity. Above band gap excitation with 3.8 eV fs laser pulses leads to ultrafast relaxation of hot electrons in the ZnO($10\bar{1}0$) conduction band and the alleged formation of an excitonic state with a lifetime in the 100 ps range. Furthermore, we demonstrate that molecules with negative electron affinity allow for massive work function reduction of ZnO($10\bar{1}0$), e. g. by $\Delta\Phi = -2.9$ eV in the case of a monolayer of pyridine. This opens a pathway to the design of cathodes with optimal electron injection barriers. We furthermore examine the changes in interfacial electronic structure upon biphenyl adsorption, which serves as a model system for optoelectronically functional poly(*p*-phenylene)-type molecules.

HL 63.6 Wed 17:15 H33

Defect-Driven Interfacial Electronic Structure at a Hybrid Organic / Inorganic Heterojunction — •Oliver Monti[1], Leah Kelly[1], Laura Schirra[1], Paul Winget[2], Hong Li[2], and Jean-Luc Bredas[2] — [1]The University of Arizona, Tucson, AZ, USA — [2]Georgia Institute of Technology, Atlanta, GA, USA

We present a combined experimental and theoretical study of the interfacial electronic structure of highly defined thin films of organic semiconductors on ZnO. We discuss the importance of shallow donor states in the near-surface region of ZnO in determining energy-level alignment and electronic structure at such interfaces. Using ultraviolet and x-ray photoelectron spectroscopy together with two-photon photoemission and first-principles calculations we investigate the nature of hybrid interface states inside the bandgap of ZnO. These states display strong charge-transfer character and may play an important role in charge-harvesting events in organic photovoltaic cells.

HL 63.7 Wed 17:30 H33

Electronic structure and excited states dynamics in polythiophene — •Lea Bogner[1], Gaurav Gupta[2], Michael Sommer[3], Mukundan Thelakkat[4], Thomas Thurn-Albrecht[2], and Petra Tegeder[1,5] — [1]Freie Universität Berlin, Fachbereich Physik — [2]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik — [3]Albert-Ludwigs-Universität Freiburg, Institut für Makromolekulare Chemie — [4]Universität Bayreuth, Makromolekulare Chemie I — [5]Rubrecht-Karls-Universität Heidelberg, Physikalisch-Chemisches Institut

Semiconducting conjugated polymers exhibit promising properties for applications in optoelectronic devices such as organic photovoltaic cells. Poly(3-hexylthiophene) (P3HT) and other poly- and oligothiophenes are auspicious electron donor materials due to their high charge carrier mobility. In this study thin films of semi crystalline P3HT with different degree of crystallinity [1] have been investigated by means of time- and angle-resolved two-photon photoemission (2PPE). We observed several unoccupied and occupied electronic states (bands) including the valence and conduction band. In addition two excited states are found which possess lifetimes in the order of hundred picoseconds.

Ref.: [1] Z. Wu, A. Petzold, T. Henze, T. Thurn-Albrecht, R. H. Lohwasser, M. Sommer, M. Thelakkat, Macromolecules, 2010, 43, 4646-4653.

HL 63.8 Wed 17:45 H33

Charge transfer at the interface between substituted pentacene nanorods and gold single crystals — •Sabine-Antonia Savu, Maria Benedetta Casu, and Thomas Chassé — Institute of Physical and Theoretical Chemistry, University of Tübingen, Tübingen, Germany

Pentacene is one of the most investigated organic molecules due to its successful application in organic electronics. Substitution in pentacene gives the opportunity to tailor the properties which are needed for applications; therefore it is necessary to investigate its influence on molecular aggregation and thin film formation. In particular, here we report our investigations on nanorods of three newly synthesized substituted pentacenes with different degrees of fluorination. We performed X-ray photoemission spectroscopy (XPS), near edge X-ray absorption fine structure (NEXAFS) spectroscopy, and atomic force microscopy (AFM) on nanorods deposited on Au(111) and Au(110) single crystals. XPS thickness dependent spectra in combination with NEXAFS investigations show that the screening of the core hole occurs via charge transfer from the metal to the molecule. In addition, the morphology of the nanorods has been investigated by using AFM, evaluating the nanorod characteristics also from a statistical point of view and taking the different degree of fluorination into account.

HL 63.9 Wed 18:00 H33

Photoemission Investigation of the Electronic Structure of P3HT:PCBM Bulk-Heterojunctions using a lift-off technique — •Angela Eckstein[1,2], Dirk Hauschild[1,2], Julia Kern[3], Markus Mingebach[3], Carsten Deibel[3], Vladimir Dyakonov[3], Achim Schöll[1,2], and Friedrich Reinert[1,2] — [1]Experimentelle Physik VII, Universität Würzburg, 97074 Würzburg — [2]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie KIT, 76021 Karlsruhe — [3]Experimentelle Physik VI, Universität Würzburg, 97074 Würzburg

Poly(3-hexylthiophene): phenyl-[6,6]-C61 butyric acid methyl ester (P3HT:PCBM) bulk heterojunctions (BHJ) are prototype active layers for organic solar cells. The electronic structure at the internal interface can be accessed by photoelectron spectroscopy (PES), thus providing insight into the alignment of the electronic levels and the occurrence of possible interface dipoles. However, the very surface sensitive PES investigation is complicated in case of P3HT:PCBM bulk heterojunctions since the film preparation by spin-coating creates a P3HT wetting layer on the film surface. In order to avoid this problem we used a lift-off technique to access the interface to the spin coating substrate (SiO2), which has shown to resemble the bulk situation [1]. P3HT:PCBM samples with different mixing ratio, which can be lift-off-prepared under UHV-condition thus avoiding contamination by ambient conditions, have been investigated by x-ray- and UV-PES as well as by inverse PES with particular respect to the influence of degradation and radiation damage. [1] Kahn et al. (Org. El. 11 (2010) 1779-1785)

HL 63.10 Wed 18:15 H33

Bottom-up synthesis of self-aligned conjugated polymers — Sören Krotzky[1], •Rico Gutzler[1], Vijay Vyas[1,2], Bettina Lotsch[1,2], and Klaus Kern[1,3] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Department of Chemistry, University of Munich (LMU), Munich, Germany — [3]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de

Lausanne, Switzerland

We investigate the synthesis of self-assembled organometallic structures and well-defined long 1D polymers by the surface-supported Ullmann reaction on an Ag(111) surface. The brominated semiconducting precursor molecule (2,7-dibromobenzothieno[3,2-b]benzothiophene) is sublimed under UHV conditions on the crystalline surface where a dehalogenation step is induced at room temperature. STM reveals self-assembly of the dehalogenated ditopic molecule into short organometallic coordination polymers that arrange in a ladder-like monolayer. Annealing to 420 K leads to C-C coupling of the molecules via ejection of the coordinated metal atom. At this temperature the newly formed 1D polymer strands align in a side-by-side manner with three preferred directions with respect to the high-symmetry directions of the surface. DFT calculations show that the length of the synthesized polymers is sufficient to reduce the HOMO-LUMO gap to its value at infinite length of the polymer. Together with the calculated band-structure this suggests possible unidirectional charge mobility within the well-ordered semiconducting polymeric monolayer.

HL 63.11 Wed 18:30 H33

How contact groups influence metal molecule hybrid structures under voltage — •Simon Liebing, Torsten Hahn, and Jens Kortus — TU Bergakademie Freiberg, Freiberg, Germany

In order to use molecules in electronics it is not only important to understand the properties of molecules themself but also properties of metal-molecule interfaces. Recent contributions discussed the behavior of thiole [1] and amino linker groups [2]. To get a more systematic understanding the authors have chosen a model system of benzene with variable linker groups between gold electrodes. Such groups can be thiole, amino, thiophen, nitrile, pyrol and cyanide. This allows for example to study the differences between σ- and π- like symmetry with respect to the individual interface geometry. The theoretical study combines the calculation of single molecule properties by density functional theory [3] with the nonequilibrium Greens functions technique [4] to calculate the transport properties [5] of the device. [1] Markussen, T. et al. JCP **132** , 224104 (2010)
[2] Angela, D. et. al. Nano Letters **10**, no. 7 (2010)
[3] Pederson, M. et. al. Phys. Status Solidi b **217**, 197. (2000)
[4] Datta, S. Nanotechnology **15**, 433. (2004)
[5] Brandbyge, M. Phys. Rev. B **65**, 165401 (2002)

HL 63.12 Wed 18:45 H33

Improving the contact materials of organic electronic devices: Polymeric dipole layers vs. self assembling monolayers — •Janusz Schinke[1,2], Julian Heusser[3,2], Marc Hänsel[3,2], Julia Maibach[4,2], Wolgang Kowalsky[1,2], Michael Kröger[1,2], Eric Mankel[4,2], and Wolfram Jaegermann[4,2] — [1]TU Braunschweig, Institut für Hochfrequenztechnik — [2]Innovation Lab GmbH — [3]Universität Heidelberg, Kirchhoff-Institut für Physik — [4]TU Darmstadt, Materials Science Institute, Surface Science Division

In organic electronic devices, charge injection at the contacts is crucial for high electrical performance. Most of these devices require at least one electrode with a sufficiently low work function (WF). Low-WF electrodes like alkaline earth metals are easily available; however, they are chemically very reactive and oxidize in ambient atmosphere. A smart way to overcome this problem is the use of molecular or polymeric dipole layers (PDLs). The use of PDLs to tune an electrodes work function can be advantageous over self assembled monolayers(SAMs) as the PDL concept can be applied to a wider range of electrode materials like ITO, Ag, Au or Al. We have used two different PDLs: branched polyethylenimine (PEI) and polyethyleneimine ethoxylate (PEIE). We studied the the properties of PDL treated substrates via AFM, ambient Kelvin probe and XPS/UPS. Both interlayers lower the metal substrate work function by approx. 1000meV. On ITO we reach absolute values of about 3.0eV which leads to strongly enhanced electron injection in model devices.

HL 64: Focus Session: Frontiers of electronic structure theory V (O, joinly with HL, TT)

Time: Wednesday 16:00–19:30 Location: H36

Topical Talk HL 64.1 Wed 16:00 H36

Screening high throughput density functional theory calculations using simplified models. — •Georg K. H. Madsen, Ingo Opahle, Alessandro Parma, Eunan J. McEniry, and Ralf Drautz — ICAMS, Ruhr Universität Bochum, Bochum, Germany

Thermoelectric materials can be utilized for an efficient conversion of waste heat to electric power. Thermoelectric properties of known compounds can be rationalized and predicted using only the structure as an input.[1] While this can used to discover potential thermoelectric materials by screening known structures[2], there remains a large challenge in discovering unknown phases computationally. Employing a newly developed high throughput environment we show how the stability of binary transition metal silicides can be reproduced using a systematic replacement technique.[3]

As ternary and higher compounds are considered, a combinatorial explosion of potential structures and combinations must be considered. We have therefore develop ed tight binding models of the electronic structure and datamining methods based on the calculation of binary compounds. It will be discussed how these simplified models can be interpreted and used to pre-screen the stability of higher compounds to limit the number of density functional calculations to be done.

HL 64.2 Wed 16:30 H36

Tight-binding scale-bridging calculations for steel research — •Nicholas Hatcher, Georg K H Madsen, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Universitätsstr. 150, 44780 Bochum, Germany

Parameterized methods to extend electronic structure calculations to large systems have recently garnered additional attention due to the limits of traditional DFT. The ability to model low carbon content in steel requires the accurate calculation of millions of atoms. However, interatomic potentials have been shown to be inconsistent with DFT in different environments and cannot give an accurate portrayal of chemical bonding or magnetism. Thus, a coherent transferable tight-binding (TB) parameterization was developed for Fe-C by extracting bonding interactions from DFT and finding a suitable interatomic repulsion. This model gives an accurate description of the energy hierarchy of relevant Fe-C structures, elastic properties, and defect energies. We apply this model to determine mechanisms of carbon segregation to grain boundaries and carbon diffusion in iron, including the interaction of multiple defects under tension and pressure. Furthermore, this intuitive energy functional forms the basis for bond order potentials, thereby extending system sizes to millions of atoms.

HL 64.3 Wed 16:45 H36

Local atomic energies from optimal atomic orbitals — •Björn Lange, Christoph Freysoldt, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Deutschland

Decomposing the energy of a condensed matter system into atomic contributions is of great use e.g. for understanding the physical origin of defect and surface energetics or for identifying chemically reactive regions in disordered systems. However, commonly employed energy calculations in the framework of density-functional theory (DFT) do not in general provide a natural decomposition into atoms. Here we propose a novel scheme to achieve this based on the recently introduced concept of atom-centered Quamols[1] that are variationally optimized to represent the electronic structure with a minimal basis set, which largely avoids local overcompleteness issues. The spillage resulting from the remaining small incompleteness is segmented according to a space separation derived from the Quamol atomic densities, maintaining the accuracy of the underlying DFT calculation. The total energy is then decomposed by combining this basis set with a local energy density treatment based on the ideas of Chetty and Martin[2]. We demonstrate the performance of our scheme by visualizing and analyzing the energy distribution at surfaces and in amorphous silicon.

[1] PRB 84, 085101, (2011)
[2] Chetty, N. and Martin, Richard M., PRB 45, 6074, (1992)

HL 64.4 Wed 17:00 H36

Environmental linear-scaling tight-binding for multicomponent metallic alloys — •Eunan J. McEniry, Georg K. H. Madsen, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum,

Bochum, Germany.

The development of accurate and transferable models to describe the behaviour of multicomponent systems is attracting considerable interest in materials modelling. Tight-binding models derived from density functional theory potentially provide an accurate and systematic approach to this problem. We introduce a methodology for environmental tight-binding (ETB) in which both the overlap and environmental contributions to the electronic structure are included. In order to implement the resulting ETB models within linear-scaling tight-binding approaches, a method for the evaluation of the screening matrix has been developed, based on a Chebyshev expansion of the inverse of the overlap matrix. The resultant linear-scaling environmental tight-binding framework has been applied to a number of relevant material systems, and the transferability and scalability of the approach is discussed. The present contribution outlines our attempts to extend the tight-binding approach towards larger-scale molecular dynamics simulations within a linear-scaling framework.

HL 64.5 Wed 17:15 H36

Spontaneous Electric Polarisation from a Classical Perspective. — •Paul Tangney — Imperial College London, London, UK

Spontaneous polarisation is a quantity attributed to noncentrosymmetric crystals and is often associated with a macroscopic electric field permeating the bulk of a sample. Its time derivative is measured as a current density during application of an external stimulus, such as temperature, strain, or an electric field. I will argue that such currents do not require the existence of a spontaneous polarisation field or a macroscopic electric field in the bulk of a polar material. They can be explained by symmetry arguments within a purely classical picture and should be calculable from the time dependence of the many-particle position probability density function of the material's constituent charges - a classical quantity. The only macroscopic electric field across any bulk crystal arises from the charges on its surfaces, which in most cases are strongly influenced by surface relaxation/reconstruction and chemical environment and unlikely to be determined by polarization currents. I will show how the classical picture of polarisation presented is consistent with the Modern Theory of Polarisation[1], in all but interpretation. I will illustrate my arguments with simulations of a toy system.

[1] R. Resta and D. Vanderbilt, "Theory of Polarization: A Modern Approach", in Physics of Ferroelectrics: a Modern Perspective C.H. Ahn, K.M. Rabe, and J.M. Triscone, Eds. Springer-Verlag, (2007).

HL 64.6 Wed 17:30 H36

Potential energy surface of $BaTiO_3$ explored with density-functional theory and classical force fields — •Joseph Fallon[1], David McComb[2], Arash Mostofi[1], and Paul Tangney[1] — [1]Imperial College London, London, UK — [2]The Ohio State University, Columbus, USA

Much is known about the electronic structure of $BaTiO_3$, its phonon dispersions, and the energetics of its long wavelength lattice distortions. However, there is much more to learn about the potential energy surface (PES) on which the atoms move. We study the PES using a combination of density functional-theory (DFT) and a polarisable ionic model of interatomic bonding. Our force field is in close agreement with DFT on structures, the PES, and phonon frequencies and allows accurate large scale atomistic simulations of domain structures and dynamics to be performed. A key advantage of an atomistic model over the coarse grained models that are often used to simulate domain dynamics is that it allows the simulation of heterogeneous materials (e.g. grain boundaries, point defects). However, we also point out some features of the PES, which may be important to domain dynamics, that effective Hamiltonians based on the transverse optic soft mode eigenvector and the local strain fail to capture.

HL 64.7 Wed 17:45 H36

Efficient Oscillator-Based Approach for Polarizability and van der Waals Interactions — •Vivekanand Gobre[1], Robert A. Distasio Jr.[2], Roberto Car[2], Matthias Scheffler[1], and Alexandre Tkatchenko[1] — [1]Fritz-Haber-Institut der MPG — [2]Princeton University, USA

The dynamic polarizability measures the response to an applied time-dependent electric field, and its accurate determination is crucial for van der Waals (vdW) interactions and other response properties. First-principles calculations of polarizabilities in principle require a computationally expensive explicit treatment of many-electron excitations, and are only applicable in practice to systems with less than about 100 atoms. In this work, we present an efficient parameter-free approach for calculating accurate frequency dependent polarizabilities for molecules with thousands of atoms, as well as periodic materials. This is achieved by the synergistic coupling of the Tkatchenko-Scheffler method [1], which accurately treats short-range hybridization effects, with the self-consistent screening equation from classical electrodynamics [2,3]. Using only the electron density and free atom reference, we obtain an accuracy of 7% for both static polarizabilities and vdW coefficients for an extensive database of gas-phase molecules and crystals. We analyze the interplay of hybridization and long-range screening effects on the polarizability. [1] Tkatchenko and Scheffler, PRL (2009), [2] Felderhof, Physica (1974), [3] Tkatchenko, DiStasio, Car, and Scheffler, PRL (2012).

HL 64.8 Wed 18:00 H36

Van der Waals interactions in Density Functional Theory and Linear-scaling Density Functional Theory — •Lampros Andrinopoulos, Nicholas D. M. Hine, and Arash A. Mostofi — Imperial College London, London, United Kingdom

Semilocal functionals in Density Functional Theory (DFT) achieve high accuracy simulating a wide range of systems, but miss the effect of dispersion (vdW) interactions, important in weakly bound systems. We study two different methods to include vdW in DFT: First, we investigate a recent approach [1] to evaluate the vdW contribution to the total energy using maximally-localized Wannier functions. Using a set of simple dimers, we show that it has a number of shortcomings that hamper its predictive power; we then develop and implement a series of improvements [2] and obtain binding energies and equilibrium geometries in closer agreement to quantum-chemical coupled-cluster calculations. Second, we implement the vdW-DF functional [3], using Soler's method [4], within ONETEP [5], a linear-scaling DFT code, and apply it to a range of systems. This method within a linear-scaling DFT code allows the simulation of weakly bound systems of larger scale, such as organic/inorganic interfaces, biological systems and implicit solvation models. [1] P. Silvestrelli, J.P.C. A 113, 5224 (2009). [2] L. Andrinopoulos et al, J.C.P. 135, 154105 (2011). [3] M. Dion et al, P.R.L. 92, 246401 (2004). [4] G. Roman-Perez, J.M. Soler, P.R.L. 103, 096102 (2009). [5] C. Skylaris et al, J.C.P. 122, 084119 (2005).

HL 64.9 Wed 18:15 H36

Microscopic van der Waals Interactions with Localized and Metallic States — •Victor Gonzalo Ruiz, Matthias Scheffler, and Alexandre Tkatchenko — Fritz-Haber-Institut der MPG

Several promising methods have been developed in recent years for an efficient modeling of van der Waals (vdW) interactions in molecules and solids. However, essentially all of these methods rely on an localized model for the polarizability, ignoring the rather strong interplay between localized and metallic electronic states. Such states are present in many relevant materials, including transition metals, hybrid organic/metal interfaces, and topological insulators. Here we show how to extend the Tkatchenko-Scheffler method [1] for vdW interactions to treat localized and itinerant electronic states on equal footing by using the gradient of the electron density. In our model, the vdW correction vanishes for the homogeneous electron gas as it should in density-functional theory built upon the local-density approximation. To illustrate the performance of the newly developed microscopic model, we study the cohesive properties of coinage metals and the binding of organic molecules on metals. [1] A. Tkatchenko and M. Scheffler, PRL 102, 073005 (2009).

HL 64.10 Wed 18:30 H36

Self-Consistent Density Functional Including Long-Range van der Waals Interactions — •Nicola Ferri[1], Robert A. Distasio JR.[2], Roberto Car[2], Matthias Scheffler[1], and Alexandre Tkatchenko[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Princeton University, USA

Van der Waals (vdW) interactions are significant for a wide variety of systems, from noble-gas dimers to complex organic/inorganic interfaces. The long-range vdW energy is a tiny fraction ($\sim$0.001%) of the total energy, hence it is typically assumed that vdW interactions do not change electronic properties. Although the vdW-DF functional self-consistently includes the effect of the vdW energy on electronic structure [1], the influence of "true" long-range vdW interactions is difficult to assess since a significant part of vdW-DF energy arises from short distances. Here, we present a self-consistent implementa-

tion of the long-range Tkatchenko-Scheffler (TS) density functional [2], including its extension to surfaces [3]. The analysis of self-consistency for rare-gas dimers allows us to reconcile two different views on vdW interactions: (i) Feynman's view that advocates changes in the electron density, and (ii) atoms separated by an infinite barrier. In agreement with previous work [1], we find the contribution from self-consistency to be negligible in the structure and stability of vdW-bound complexes. However, a closer look at complex organic/inorganic interfaces reveals notable modification of the energy levels when using the self-consistent TS vdW density functional. [1] Thonhauser *et al.*, PRB (2007), [2] Tkatchenko and Scheffler, PRL (2009), [3] Ruiz *et al.*, PRL (2012).

HL 64.11 Wed 18:45 H36

Many-Body van der Waals Interactions from Isotropically Damped Coupled Quantum Harmonic Oscillators — •Alberto Ambrosetti[1], Robert A. DiStasio Jr.[2], and Alexandre Tkatchenko[1] — [1]Fritz-Haber institut der MPG, Faradayweg 4-6 14195 Berlin, Germany — [2]Department of Chemistry, Princeton University, Princeton, NJ 08544, USA

The current interest in functional materials with increasing size and complexity demands high accuracy in first-principles calculations. In these systems, the collective many-body (MB) description of van der Waals (vdW) interactions is indispensable to reach the highly coveted "chemical accuracy". The recently introduced DFT+MBD method (PRL **108**, 236402 (2012); PNAS **109** 14791 (2012)) for the dispersion energy based on a coupled set of quantum harmonic oscillators (QHOs) was shown to reach chemical accuracy for gas-phase molecules and molecular solids. Its formulation, however, makes the derivation of interatomic forces and a fully self-consistent DFT+MBD implementation non-trivial. We propose here a simplified approach, making use of a set of QHOs with isotropically damped dipole–dipole coupling, which provides an effective random-phase approximation treatment of their vdW interaction (arXiv:1210.8343). This allows for a simple analytical treatment of interatomic forces, yet providing high efficiency and accuracy. Application over a wide range of systems shows a consistent improvement with respect to pairwise approximations, particularly for the most extended systems.

HL 64.12 Wed 19:00 H36

Interplay between H bond symmetrization and spin transition in ϵ-FeOOH: insights from first principles — •Carmen Quiroga and Rossitza Pentcheva — Dept. of Earth and Environmental Sciences, University of Munich

Structural and electronic spin transitions in high-pressure ϵ-FeOOH are studied using density functional theory calculations including an on-site Coulomb repulsion term. A high-spin to low-spin transition in trivalent iron is predicted at $\sim$ 58 GPa, in agreement with previous theoretical study [1] and experimental indications [2]. The spin transition is heralded by a second order $P2_1nm$ to $Pnnm$ phase transition at $\sim$ 43 GPa, driven by hydrogen bond symmetrization at the critical hydrogen bond O$\cdots$O limit of $\simeq$ 2.4 Å. Our results give indications of a possible connection between the symmetry of hydrogen bonds in ϵ-FeOOH and the spin state of Fe^{3+}, with important implications in disclosing the influence of water content in the mantle redox state.

Funding by DFG SPP1236 (PE883/8-1) is acknowledged.

[1] Otte et al. Phys. Rev. B **80**, 205116 (2009).
[2] Gleason et al. In preparation.

HL 64.13 Wed 19:15 H36

From spheres to iso: Implementing implicit solvation in FHI-aims — •Ran Jia, Chunsheng Liu, Daniel Berger, Harald Oberhofer, and Karsten Reuter — Department Chemie, Technische Universität München, Lichtenbergstr. 4, D-85747 Garching, Germany

At the cost of reduced accuracy, implicit solvation models yield strong speedups compared to explicit solvent simulations. Here, we report on the implementation of the multipole moment expansion (MPE) solvent continuum model into the density-functional theory (DFT) program package FHI-aims. Characterizing the surrounding solvent mainly by its dielectric constant and density, the form of the cavity employed for the solute and the description of the reaction field created by the polarized solvent are the two central characteristics of any implicit solvation approach. In MPE the reaction field is computed as a truncated multipolar expansion. In our implementation we discard the prevalent cavity representation in form of a set of overlapping spheres centered around the solute atoms in favor of an electron isodensity surface. This allows for more flexible shapes with increased physical meaning. In particular, it paves the way towards the description of one- or two-dimensional periodic systems, and therewith to complex solid-liquid interfaces.

HL 65: Poster: Organic electronics and photovoltaics (CPP; jointly with HL, O)

Time: Wednesday 16:30–18:30 Location: Poster C

HL 65.1 Wed 16:30 Poster C

Templating effects of 6T layers for organic DIP layers — •Christopher Lorch, Alexander Hinderhofer, Rupak Banerjee, Christian Frank, Johannes Dieterle, Alexander Gerlach, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

Recently, the donor-acceptor combination of the two compounds, α-sexithiophene (6T) [1] and diindenoperylene (DIP) [2], respectively, has shown an extraordinarily high open circuit voltage in organic solar cells with a planar heterojunction (PHJ) architecture [3].

Synchrotron based real-time *in situ* X-ray diffraction experiments were performed to study the temperature-dependent growth characteristics of 6T. Furthermore, the influence of the structural properties of the 6T layer on the top DIP layer were investigated. In this contribution, the following points are discussed: i) Dependence of the ratio of lying and standing domains in the top DIP layer on the corresponding ratio in the bottom 6T layer. ii) The thickness dependence of the DIP layer structure. iii) Possible reorganization effects in the bottom layer during the growth of the top layer. iv) The dependence of top layer structure on the temperature.

[1] W. Steinkopf *et al.*, Justus Liebigs Ann. Chem. 546, 180-199 (1941)
[2] A. C. Dürr *et al.*, Phys. Rev. Lett. 90, 016104 (2003)
[3] U. Hörmann *et al.*, Phys. Status Solidi RRL 5, 241-243 (2011)

HL 65.2 Wed 16:30 Poster C

Solution processing of self-assembled monolayers as charge injection layers in organic FETs. — •Milan Alt[1,4], Janusz Schinke[2,4], Kaja Deing[3,4], Uli Lemmer[1], and Norman Mechau[1,4] — [1]Karlsruher Institute of Technology — [2]TU Braunschweig — [3]Merck KGaA, Darmstadt — [4]InnovationLab, Heidelberg

All-solution processed organic field effect transistors (OFETs) are expected to play a key role in the mass production of organic electronic devices via high throughput printing techniques. In this study we focus on solution processing of self-assembled monolayers (SAMs) for enhancement of charge carrier injection at the metal-semiconductor interface. One necessity in order to make SAMs printable is an understanding of molecular assembly in dependency to process parameters like accumulation time and molecular concentration in the solution. We used well established benchmark materials to investigate the functionality of different benzyl-mercaptan and alkanethiol SAMs in OFETs. The methodic evaluation of OFET devices, in which the transistor effectively serves as a characterization tool, revealed an expected correlation between metal work function shift and device threshold voltage. More interestingly, an optimum ratio of accumulation time/SAM concentration has been identified. In contrast, investigations of SAM isle accumulation on crystalline Au 111 surfaces in literature reveal a saturation of work function shift when approaching a closed monolayer. This demonstrates that understanding of SAM growth mechanisms gained on single crystalline surfaces cannot naturally be transferred to assembly on printed or evaporated metal contacts.

HL 65.3 Wed 16:30 Poster C

Photophysical Processes in Polymer:PDI Solar Cells — •Dominik Gehrig, Valentin Kamm, Hannah Mangold, Ian Howard, Glauco Battagliarin, Chen Li, Klaus Müllen, and Frédéric Laquai — Max-Planck-Institute for Polymer Research, Mainz, Germany

We present the implementation of different polymers as donors in com-

bination with new PDI-based acceptors in organic solar cells. Increasing the absorption of the photoactive layer is a rational strategy that could give rise to an enhanced photon harvesting and hence an improvement of the photocurrent. The contribution of PDI to the photocurrent generation can be proved by EQE measurements. Additionally exciton and charge carrier dynamics as well as loss mechanisms are investigated by sub-picosecond to millisecond pump-probe transient absorption spectroscopy (TA) and time-resolved photoluminescence (TRPL) spectroscopy. The former tracks the dynamics of nonradiative species whereas the latter enables the observation of emissive decay channels. Supplementary experiments like the evaluation of the morphology by AFM and charge transport experiments by the time-of-flight (TOF) technique and space-charge-limited-current (SCLC) measurements deliver additional information which allow to derive meaningful structure-property-relations.

HL 65.4 Wed 16:30 Poster C

Increased conductivity of PEDOT:PSS for application in organic solar cells: electrical and morphological investigations — •Christoph Heller[1], Claudia M. Palumbiny[1], Volker Körstgens[1], Yuan Yao[1], Weijia Wang[1], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany — [2]HASYLAB at DESY, Notkestrasse 85, 22603 Hamburg, Germany

Poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate)(PEDOT:PSS) is commonly used as a transparent electrode for flexible electronic devices. Its conductivity plays a crucial role for the device performance.

In our study, the conductivity of PEDOT:PSS films has been increased via a post treatment method reaching the conductivity order of indium tin oxide (ITO) which is commonly used as an electrode in organic solar cells. Among other techniques the effect of the post treatment has been investigated using advanced scattering methods such as grazing incident small angle x-ray scattering (GISAXS). Furthermore, the influence of doping PEDOT:PSS, different post treatments, the treatment time and the effect of the number of post treatments have been investigated focusing on conductivity and morphological changes. The results are very promising for using post treated PEDOT:PSS as an electrode in ITO-free organic solar cells.

HL 65.5 Wed 16:30 Poster C

Low-bandgap DPP-type Polymers for OPVs: Relation between Device Performance and Photophysical Properties — •Julian Ochsmann[1], Mathieu Turbiez[2], Deepak Chandran[3], Ian Howard[1], Kwang-Sup Lee[3], and Frédéric Laquai[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]BASF, Basel, Switzerland — [3]Hannam University, Seoul, Korea

Low-bandgap polymers are promising materials to serve as electron donors in the photoactive layer of bulk heterojunction solar cells. In combination with a suitable electron acceptor such as PC70BM the photoactive layer covers a broad absorption range spanning from the visible to the near-infrared spectral region leading to increased photon harvesting and thus a higher photocurrent compared to mid-bandgap polymers such as P3HT.

In this study the photovoltaic performance of several low-bandgap polymers based on the diketopyrrolopyrrole (DPP) unit was evaluated in Organic Photovoltaic Cells (OPVs) prepared with different solvent mixtures. Depending on the polymer structure and preparation conditions maximum power conversion efficiencies between 1.6 and 5 % could be reached. The photophysical properties of the photoactive layers of the OPVs were investigated by steady-state photoinduced absorption and broadband transient absorption pump-probe spectroscopy (TA) to get further insight into the exciton and polaron dynamics as well as into the efficiency-limiting mechanisms of the devices.

HL 65.6 Wed 16:30 Poster C

Investigation of Polyethylenimine and Polyethylenimine-ethoxylated as electron injection layers in solution processed organic light-emitting diodes. — •Sebastian Stolz[1,4], Ingo Ringle[2], Eric Mankel[3,4], Janusz Schinke[4], Michaela Agari[2], Gerardo Hernandez-Sosa[1,4], Wolfram Jaegermann[3,4], Uli Lemmer[1], and Norman Mechau[1,4] — [1]Light Technology Institute, Karlsruhe Institute of Technology — [2]Pre-development, Heidelberger Druckmaschinen AG — [3]Materials Science Institute, Technische Universität Darmstadt — [4]InnovationLab GmbH, Heidelberg

One obstacle for inexpensive solution processed organic light-emitting diodes (OLEDs) is the current use of low work-function metals like calcium or barium as cathode materials. These metals are highly reactive, which is why they cannot be easily solution processed but have to be prepared in UHV. In this work, we investigate two organic polymers, Polyethylenimine (PEI) and Polyethylenimine-ethoxylated (PEIE), which are known to reduce the work-function of various metals, for their applicability as electron injection layers. Therefore, both polymers are dissolved in 2-Methoxyethanol with varying concentrations and are then spin coated on top of Aluminum substrates. The concentration dependent change in work-function is determined by kelvin probe measurements and ultraviolet photoemission spectroscopy. Furthermore, OLEDs using PEI, or PEIE respectively, as electron injection layer are prepared by spin coating. Compared to reference devices with calcium as electron injection material, these OLEDs show comparable turn on voltages and luminance values of more than 50%.

HL 65.7 Wed 16:30 Poster C

Surface morphology of P3HT, PCBM and blends of both — •Martin Dehnert[1], Mario Zerson[1], Sven Hüttner[2], Zhuxia Rong[2], Ullrich Steiner[2], and Robert Magerle[1] — [1]Fakultät für Naturwissenschaften, Technische Universität Chemnitz, Chemnitz, Germany — [2]Cavendish Laboratory, JJ Thomson Avenue,Cambridge,U.K.

We investigate the surface morphology of thin films of pure poly(3-hexylthiophene) (P3HT), [6,6]-phenyl C61-butyric acid methyl ester (PCBM) and blends of P3HT and PCBM using atomic force microscopy (AFM) operated in multi-set point intermittent contact (MUSIC) mode. This allows for depth-resolved mapping of the mechanical properties of the top surface layer of the specimen. AFM images of pure P3HT and PCBM before and after annealing show the crystallisation behaviour of the pure materials at the film surface. Blends of P3HT and PCBM with different composition were used for investigating the morphology, the nanomechanical properties, and the composition of the top surface layer. Our results indicate that for large range of blend compositions the volume ratio of P3HT and PCBM is constant within the top surface layer. Furthermore, we observe crystallisation of PCBM in films annealed at 175°C. We discuss the impact of the surface morphology of P3HT:PCBM blends and the crystallisation of PCBM on the efficiency and lifetime of organic solar cells.

HL 65.8 Wed 16:30 Poster C

Probing charge carrier dynamics in organic solar cells based on merocyanines — •Steven Graf[1], Martin Lenze[1], Julian Krumrain[1], Dirk Hertel[1], Klaus Meerholz[1], and Frank Würthner[2] — [1]Department für Chemie, Universität zu Köln, Luxemburger Straße 116, 50939 Köln — [2]Institut für Organische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg

Organic photovoltaics offer a very promising green energy alternative. Highly efficient organic solar cells can be produced by cost-effective methods such as coating from solution (SOL) or depositing under high vacuum conditions (VAC). In our approach we investigate merocyanines (MC), a class of low-molecular-weight colorants, as donor material in organic BHJ solar cells. These molecules are processable via both deposition techniques showing remarkable power conversion efficiencies (PCE) beyond 4% for SOL- and 6% for VAC-processed devices. Towards even higher PCEs it is mandatory to obtain a better insight into fundamental charge carrier processes such as generation, transport and recombination. We use steady state and time resolved photoluminescence spectroscopy to examine charge-transfer (CT) states in pure and blended merocyanine thin films. The role of these CT states in solar cells is further studied by field and temperature dependent measurements of the external quantum efficiency (EQE). By varying processing conditions as well as blend compositions the influence of morphology on the solar cells is illustrated. The investigations are supported by temperature and electric field dependent studies of charge recombination and transport via photo-CELIV technique.

HL 65.9 Wed 16:30 Poster C

Influence of different alkyl side chains on merocyanine dye performance in organic solar cells — •Julian Krumrain[1], Alhama Arjona Esteban[2], Steven Graf[1], Martin Lenze[1], Dirk Hertel[1], Frank Würthner[2], and Klaus Meerholz[1] — [1]Department für Chemie, Universität zu Köln, Luxemburger Straße 116, 50939 Köln (Germany) — [2]Institut für Organische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg (Germany)

In recent years, organic photovoltaics have attracted great attention as an alternative energy source due to their reduced cost and easier

proccessibility, compared to inorganic materials. Specifically, small-molecule dyes have achieved great strides in recent years reaching power conversion efficiencies up to 7%. These dyes have advantages over polymers, most notably their simplified, large-scale syntheses and purification. Furthermore small molecules can be processed either by solution or vapor-deposition processes. We have investigated organic solar cells based on merocyanine (MC) dyes as an electron donor material in vacuum-deposition processed bulk-heterojunctions (BHJ). In order to get a better understanding of the influence of side chains on the MC dyes in BHJ, we have synthesized MC dyes with different alkyl side chain lengths. We have carried out temperature and light intensity dependent current-voltage measurements as well as atomic force microscopy studies. It becomes apparent that the BHJ morphology is strongly influenced by the side chain length. The short-circuit current density degreases enormously for increasing side chain length in complete contrast to the solubility of the MC dyes.

HL 65.10 Wed 16:30 Poster C

Absorption and exciton management in DIP/C_{60} bilayer photovoltaic cells — •A. Steindamm[1,2], M. Brendel[1,2], K. Topczak[1], and J. Pflaum[1,2] — [1]Exp. Phys. VI, University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

The combination of the promising material Diindenoperylene (DIP) with the acceptor C_{60} has led to overall efficiencies up to 4 % in organic photovoltaic cells (OPVCs) [1]. A drawback in performance is found in the rather poor light absorption of the crystalline DIP layer due to its unfavorable orientation of transition dipoles perpendicular to the electric field vector of incident light. Therefore we pursued different approaches for increasing the current density. First, the orientation of the individual DIP molecules was altered by varying the growth conditions in order to increase light absorption. Second, the interface effects of an Bathophenanthroline (BPhen) exciton blocking layer (EBL) on the exciton management in DIP/C_{60} were investigated by a complementary study of current density, external quantum efficiency, and photoluminescence quenching for various EBL thicknesses. These investigations reveal exciton losses by contact metal quenching in both active layers if no EBL is applied. In contrast, an optimal trade-off between exciton blocking, suppression of metal penetration, and electron transport is achieved for a 5 nm thick BPhen layer yielding an improvement of power conversion efficiency by more than a factor of 2 [2]. Financial support by BMBF (GREKOS) and DFG (SPP1355) is acknowledged.

[1] A. Opitz, et al., IEEE J. Sel. Top. Quant. El. 16, 1707 (2010)
[2] A. Steindamm, et al., Appl. Phys. Lett. 101, 143302 (2012)

HL 65.11 Wed 16:30 Poster C

The effect of fluorination on the performance of F_nZnPc/C_{60} organic photovoltaic cells — •M. Brendel[1,2], A. Steindamm[1,2], F. Staub[1], and J. Pflaum[1,2] — [1]Exp. Phys. VI, University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

The material class of phthalocyanines has proven to be a suited donor material in small molecule organic photovoltaic cells (OPVCs). Planar heterojunctions based on zinc phthalocyanine (ZnPc) in combination with the acceptor C_{60} show high short circuit currents (j_{sc}) of 6.3 mA/cm^2 and fill factors (FF) of 51 % [1]. However, due to the small effective band gap $E_{g,eff}$ of only 1 eV between ionisation potential of the donor and electron affinity of the acceptor, the correlated open circuit voltage (V_{oc}) is limited to 0.5 V. As a possible approach energy levels of Pcs can be modified by substituting hydrogen atoms. With increasing degree of fluorination the position of the HOMO and LUMO levels are shifted to lower energies. In this contribution we investigated the impact of $E_{g,eff}$ on V_{oc} for a varying degree of fluorination (n = 0, 4, 8, 16) in F_nZnPc/C_{60} OPVCs. First results revealed a significant V_{oc} improvement of 20 % to 0.6 V for F_4ZnPc based cells compared to ZnPc, while j_{sc} and FF ideally remained unaffected. However, the gain in V_{oc} is smaller than expected by the difference in ionisation potential which accounts for 0.2 - 0.4 eV. This discrepancy will be analyzed in our studies and will lead to a deeper insight into the origins of V_{oc} and its correlation to the energetics on the molecular entities. Financial support by the BMBF (project GREKOS) and by the DFG (program SPP1355). [1] Z. R. Hong, et al., Appl. Phys. Lett. 2007, 90, 203505

HL 65.12 Wed 16:30 Poster C

Surface Structure of organic solar cells based on PBDTTT-C and PC70BM — •Mario Zerson[1], Andreas Zusan[2], Carsten Deibel[2], and Robert Magerle[1] — [1]Chemische Physik, Technische Universität Chemnitz, Chemnitz, Germany — [2]Experimental Physics VI, Julius-Maximilians-University of Würzburg, Würzburg, Germany

We study the surface structure of organic heterojunction solar cells based on blends of poly[4,8-bis-(2-ethylhexyloxy)-benzo[1,2-b:4,5-b']dithiophene-2,6-diyl-alt-(4-(2-ethylhexanoyl)-thieno[3, 4-b]thiophene))-2,6-diyl] (PBDTTT-C) and Phenyl-C70-butyric acid methyl ester (PC70BM) with a weight ratio of 1:1,5. The additive diiodooctane (DIO) is used with ratios between 0% and 10% to increase the compatibility of the two components. We investigate the surface structure of the devices with amplitude modulation atomic force microscopy (AFM). Conventional AFM height and phase images are complemented with data obtained from maps of amplitude-phase-distance (APD) curves. This allows us to determine the unperturbed (true) surface and the mechanical properties of the soft surface layer of the specimen. The AFM height and phase images of PBDTTT-C:PC70BM blends produced with different ratio of DIO indicate, that the additive plays a fundamental role in the structure formation process. Blends with DIO ratios between 1,8% and 5% show the best power conversion efficiency (PCE) up to 6,9%. We discuss the structure and the structure of the interface between donor and acceptor components in view of their impact on charge carrier dynamics and solar cell performance.

HL 65.13 Wed 16:30 Poster C

Triplet Excitons and Cations in DCV4T-Me:C_{60} blends with different mixing ratio — •Daniel Schütze[1], Christian Koerner[1], Roland Fitzner[2], Egon Reinold[2], Peter Bäuerle[2], Karl Leo[1], and Moritz Riede[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, Germany — [2]Institut für Organische Chemie II und Neue Materialien, Universität Ulm, Germany

Dicyanovinyl end-capped oligothiophenes (DCVnT) have demonstrated their ability of achieving high power conversion efficiencies of up to 6.9% in a bulk heterojunction solar cell[1]. Besides that, they act as a model system because of the possibility of changing properties by varying the length of backbone or side chains.

In this work, we use DCV4T with two methyl side chains at the first and the last thiophene ring. By photoinduced absorption spectroscopy (PIA) measurements we probe the long-living (μs-ms) excited states (triplet excitons, cations) after photoexcitation of our samples. With PIA, their generation and recombination behavior can be investigated. Here, we report our results obtained on a series of DCV4T-Me:C_{60} blends with varying mixing ratio from 3:1 to 1:2. We found strong influence of the mixing ratio on the generation rate of triplet excitons and also an influence in the generation rate and the activation energy of free charge carriers with increasing temperature. The results are compared to solar cells containing identical blend layers as active layer to investigate the dependence of the photo current on the mixing ratio.

[1] Fitzner et al., J. Am. Chem. Soc. 2012, 134, 11064 (2012)

HL 65.14 Wed 16:30 Poster C

Nucleation and Growth of Copper Phthalocyanine from Solution — •Fatemeh Ghani and Hans Riegler — Max Planck Institute f. Colloid & Interfaces, Potsdam-Golm, Germany

Silver nanoparticles are usually synthetized by physical vapor deposition or through compli-cated methods like ion implantation or wet chemistry. A self-assembly method is of interest due to its simplicity and cost-efficiency [202]. By combining physical vapor depo-sition and solvent treatment (spin casting), We applied a simple hybrid method to produce ap-propriate silver nanoclusters for organic solar cells. Through evaporation of the silver film (˜ 5 nm), nanoclusters (of ˜4 nm height and ˜ 25 nm widths) cover the surface. By spin casting the solvent, a thin liquid film covers the evaporated film. The silver clusters redistribute in the solution film and by evaporation of the solvent, they aggregate in larger clusters (˜20 nm height and ˜45 nm width). The process is influenced via physical parameters of growth from solution like evaporation rate and liquid film concentration. We show that the size of the clusters can be controlled by the thickness of the deposited film, type of solvent, and spin casting speed. We applied this method to increase the efficiency of a hybrid solution processed and vac-uum deposited unsubstituted copper phthalocyanine/fullerene organic solar cells.

HL 65.15 Wed 16:30 Poster C

Charge generation in solid-state dye-sensitized solar cells using peryleneimide sensitizers — •Yoojin Kim, Michael Meister, Ian Howard, Felix Hinkel, Glauco Battagliarin, Chen Li,

Klaus Müllen, and Frédéric Laquai — Max Planck Institute for Polymer, Mainz, Germany

Solid-state dye-sensitized solar cells (DSCs) have attracted a lot of attention owing to their advantages compared to liquid-electrolyte DSCs such as ease of fabrication and the absence of corrosive electrolytes that are typically used in liquid-electrolyte cells. However, fast charge recombination between electrons in the titania nanoparticle films and dye/hole conductor cations, incomplete pore-filling, and the decreased thickness of titania films necessary for efficient charge extraction currently limit the power conversion efficiency. In this contribution we compare the charge generation and recombination processes in a series of peryleneimide-sensitized DSCs studied by steady-state photoinduced absorption (PIA) and ultrafast broadband transient absorption spectroscopy (TAS) covering the sub-picosecond to millisecond timerange. By fitting the dynamics to a photophysical model we extract the parameters relevant for the photovoltaic efficiency such as the yield of electron injection and the recombination rate constants which allows us to derive meaningful structure-property relations.

HL 65.16 Wed 16:30 Poster C

Sequentially solution-processed bulk-heterojunction CuPc/PCBM - bilayer for organic solar cells — •Markus Regnat, Fatemeh Ghani, and Hans Riegler — Max Planck Institut of Colloids and Interfaces, Potsdam-Golm, Germany

Copper Phthalocyanine (CuPc) is a commonly used electron donor material in vacuum-processed organic solar cells (OSC) due to its suitable electronic properties, chemical stability and low material cost. Recent studies have revealed appropriate solvents for CuPc [1] and thus also opened a way for cost-efficient wet-deposition techniques, like spin casting or dip coating. Based on this, a working hybrid solution/vacuum processed OSC with a CuPc film prepared by wet-processing (spin cast) could be obtained [2]. The nanostructures of the CuPc film have an important influence on the efficiency of the OSC. A systematic study reveals the impact of various process parameters on nucleation and growth of wet-processed CuPc films and allows the optimization of the nanostructures. By using appropriate orthogonal solvents, even both essential optoelectronic layers (CuPc, PCBM) can now be sequentially wet-deposited for a bulk-heterojunction CuPc/PCBM - bilayer OSC.

[1] Ghani, F.; Kristen, J.; Riegler, H., Solubility properties of unsubstituted metal phthalocyanines in different types of solvents, J. Chem. (2012)

[2] Fatemeh Ghani; Ivelin Bochukov; Konstantinos Fostiropoulos; Hans Riegler, Hybrid solution/vacuum-processed bilayer heterojunction organic solar cells: Structural characterization and performance, Thin Solid Films (2012)

HL 65.17 Wed 16:30 Poster C

Preferential orientation of molecular dipoles in amorphous vacuum deposited films studied by surface potential measurements — •Christian Weigel, Sami Hamwi, and Wolfgang Kowalsky — Institut fuer Hochfrequenztechnik, TU Braunschweig

Amorphous thin films of semiconducting small molecules are commonly used in organic optoelectronic devices to avoid detrimental effects of grain boundaries in polycrystalline thin films. Studies of surface potential development with film thickness have shown that sublimation of common OLED molecules such as Tris(8-hydroxyquinolinato) aluminum (Alq3) or 1,3,5-tris(2-N-phenylbenzimidazolyl)benzene (TPBi) results in amorphous films with a preferential orientation of the molecular dipoles. Kelvin probe measurements provide a sensitive tool to detect a shift in the average molecular dipole orientation by as little as 5 degrees from the isotropic case. The detected shift in surface potential is characteristic for each molecules and is found in the order of several volts per 100 nm, comparable to operating voltages of organic electronic devices. The recorded increase in surface potential is largely independent of material or preparation of the substrate upon which the amorphous film is grown (barring the different interface dipoles between substrate and film), so that anisotropy at the organic film to vacuum interface drives the preferential orientation. Upon optical excitation, the measured potential vanishes, presumably due to mobile charges screening the dipole field.

HL 65.18 Wed 16:30 Poster C

Encapsulation of small molecule organic devices by a functional thin top layer of tetratetracontane — •Florian Staub[1], Andreas Steindamm[1,2], Michael Brendel[1,2], and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius-Maximilians-University, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

Providing long-term stability for organic devices is still a challenging task due to the sensitivity of molecular materials as well as organic/metal interfaces on water incorporation and oxidation processes. The straight-chain alkane tetratetracontane (TTC) is capable to protect organic devices from those degradation mechanisms by forming closely packed and highly crystalline films [1]. TTC is transparent in the visible range, highly hydrophobic and chemically inert and therefore suited to conserve the opto-electronic properties of the underlying films. In this contribution we apply nanometer thick top layers of TTC by thermal vacuum deposition onto planar heterojunction organic photovoltaic cells (OPVCs) based on zinc phthalocyanine (ZnPc) and diindenoperylene (DIP) in combination with the acceptor C_{60}, respectively. For ensuring best comparability, encapsulated and bare cells are prepared under identical conditions on the same substrate. We investigate the degradation mechanisms by measuring the external quantum efficiency and the IV-characteristics over time under exposure to various environmental conditions (vacuum, nitrogen, air). The occurring changes in the opto-electronic device performance will be discussed in relation with structural data obtained by AFM and X-ray diffraction. [1] M. Göllner et al., Adv. Mater. 2010, 22, 4350-4354

HL 65.19 Wed 16:30 Poster C

Brightly Blue and Green Emitting Copper Compounds for Singlet Harvesting in OLEDs — •Markus Leitl[1], Fritz-Robert Küchle[2], Lars Wesemann[2], and Hartmut Yersin[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Regensburg, D-93040, Germany — [2]Institut für Anorganische Chemie, Universität Tübingen, D-72076, Germany

In this contribution, a series of four Cu(I) complexes is presented. All substances exhibit high emission quantum yields of up to 65 % at relatively short emission decay times of several μs. The emission wavelength varies from the blue (460 nm) to the green (505 nm). This is induced by defined modifications of the chemical structure. Detailed photophysical investigations reveal that the energy separation $\Delta E(S_1 - T_1)$ between the triplet state T_1 and the singlet state S_1 is small and lies in the range of 500 cm^{-1}. As a consequence, emission at ambient temperature originates dominantly (> 99 %) from the S_1 state which is thermally populated from the energetically lower lying T_1 state. For this reason, the emission at ambient temperature represents a thermally activated delayed fluorescence (TADF). It is proposed to utilize this property for collecting both singlet and triplet excitons in the lowest excited singlet state for light generation in OLEDs. This effect represents the singlet harvesting mechanism.

HL 65.20 Wed 16:30 Poster C

Interface trap density investigation by impedance spectroscopy of MIS structures for different surface treatments — •Hippolyte Hirwa, Steve Pittner, and Veit Wagner — Jacobs University bremen,Campusring 1, D-28759 Bremen, Germany

For high performance electronic devices, reliability and stability are crucial parameters. Since reliabilities and stabilities issues in field effect transistors are mainly related to the semiconductor-gate insulator interface properties, a MIS (Metal-insulator-semiconductor) capacitor structure can be equally used for investigation of interface traps. We report on impedance measurements carried out on MIS capacitors fabricated using silicon oxide as insulator prepared under 3 different surface treatments and poly(3-hexylthiophene) as semiconductor. The conductance technique was used to extract the interface trap density. For this a proper equivalent circuit for our MIS structures had to be chosen. The results reveal first the formation of a double layer with 2 different conductivities in the semiconductor layer, secondly the presence of interface trap states and finally they show that the interface states density and energy distribution is related to the sample surface treatment.

HL 65.21 Wed 16:30 Poster C

Combined photoemission and X-ray absorption study of the 'rods-in-belt' supramolecular complexes containing gold-copper and gold-silver clusters — •Anna Makarova[1,2], Elena Grachova[2], Dmitry Krupenya[2], Julia Shakirova[2], Igor Koshevoy[3], Eckart Rühl[4], Clemens Laubschat[1], Sergey Tunik[2], and Denis Vyalikh[1] — [1]Technische Universität Dresden, Dresden, Germany — [2]St.-Petersburg State University, St.-Petersburg, Russia — [3]University of Joensuu, Joensuu, Finland — [4]Freie Universität Berlin, Berlin, Germany

Recently created self-assembled Au(I)-Cu(I) and Au(I)-Ag(I) 'rods-in-belt' supramolecular complexes display intriguing phosphorescence

properties. Another important issue is the tunability of their electronic structure, and consequently their photophysical properties through modification of the ligand environment that opens great perspectives for their implementation in light-emitting devices and in bio-imaging. It is believed that high structural ordering and self-assembling properties of such objects can open a new avenue for the design of artificial nanostructures that may potentially be ideal building blocks for next generation electronics. Nonetheless, the electronic structure of these materials has not been investigated experimentally by now. We have demonstrated that photoemission and X-ray absorption techniques can be successfully applied for systematic investigation of the series of these unique complexes. It has been shown that the all complexes inside the series exhibit similar electronic structures, however, the electronic states near the HOMO reveal notable differences.

HL 65.22 Wed 16:30 Poster C

A multiscale modeling study of loss processes in block-copolymer-based solar cell nanodevices — •Sergii Donets, Anton Pershin, and Stephan Baeurle — University of Regensburg, Institut of Physical and Theoretical Chemistry, D-93053

Flexible photovoltaic devices possess promising perspectives in optoelectronic technologies, where high mobility and/or large-scale applicability are important. However, their usefulness in such applications is currently still limited due to the low level of optimization of their performance and durability. For the improvement of these properties a better understanding and control of small-scale annihilation phenomena of the elementary particles involved in the photovoltaic process, such as exciton loss and charge carrier loss, are necessary. Here, we explore the causes for their occurrence with a novel field-based solar-cell algorithm on the example of self-organizing nanostructured block-copolymer systems, which possess a broad variability in their chemical and physical characteristics, and explore new routes to optimize their performance. From our calculations, we deduce that in the regime from low up to intermediate chi-parameters the charge transport efficiency (CTE) and internal quantum efficiency (IQE) of both block-copolymer systems increase up to a maximum, characterized by a minimum in the number of charge losses due to charge recombinations. In the regime of high chi-parameters they form nanostructures with a large number of bottlenecks and dead ends, leading to a large number of charge losses due to charge recombination, charge trapping and an impaired exciton dissociation.

HL 66: GaN: Preparation and characterization of rods and wires

Time: Wednesday 17:00–19:30 Location: H15

HL 66.1 Wed 17:00 H15

Hybrid inorganic/organic GaN-based nanowire structures for Förster resonant energy transfer — •Johannes Zettler, Sergio Fernández-Garrido, Oliver Brandt, Lutz Geelhaar, and Henning Riechert — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, D-10117 Berlin, Germany

The fabrication of hybrid GaN/organic semiconductor systems may facilitate combining the individual material's strength while compensating for their deficits. Förster resonant energy transfer (FRET) can be used to transfer energy from electrically injected carriers in GaN to an organic semiconductor overlayer, where light is generated more efficiently. Since FRET relies on dipole-dipole coupling, the separation between the GaN active region and the organic overlayer cannot be greater than a few nm. Thus, the use of GaN nanowires (NWs), where the side facets of the GaN active region can be covered with an organic semiconductor, may be an approach superior to planar structures as it permits both efficient electrical contacting and proximity of the GaN active region and the organic semiconductor. In this work, GaN and (Al,Ga)N/GaN NW heterostructures were grown by molecular beam epitaxy to study the FRET process in these hybrid systems. In a first stage, the growth and morphology of self-induced (Al,Ga)N NWs was optimized with respect to the FRET demands. Hence, thin, well separated NWs were grown with quantum disks extended over the whole diameter of the NWs. In a second stage, the spin-coating parameters for filling up the NWs with organic molecules were optimized to achieve a complete coverage of the GaN active region by organic molecules.

HL 66.2 Wed 17:15 H15

Investigation of the polarity of GaN nanowires grown by MBE on AlN/Si(111) with respect to substrate polarity — •Henning Hollermann, Joerg Malindretos, and Angela Rizzi — IV. Physikalisches Institut, Georg-August Universität Göttingen, Germany

III-V materials are most promising candidates for solid-state lighting devices. However, the problem of the green-gap, the drop of the external quantum efficiency at wavelengths around 550 nm, still remains unsolved. This could be overcome by InGaN/GaN quantum well structures grown in non-polar directions. But non-polar substrates are not available with sufficiently high quality at low prices, yet.

Here GaN-based nanowires could be an alternative. While self-organized GaN nanowires, grown on non-polar Si(111) substrates show N-polarity and flat c-plane top facets, we observed pyramidal semi-polar top facets in wires selectively grown on GaN/sapphire substrates with pre-structured molybdenum masks. Those facets could serve as a base for InGaN quantum well structures with strongly reduced quantum confined Stark effect.

Since simplification of the growth process is desirable for future applications we have investigated the influence of AlN buffer-layers on the morphology and polarity of GaN nanowires grown in a self-organized manner by plasma-assisted MBE on Si(111) substrates. The aim of this study is to produce wires with semi-polar top facets in a straightforward growth procedure. A detailed analysis of the structural properties is presented.

HL 66.3 Wed 17:30 H15

Nanometer scale correlation of optical and structural properties of individual InGaN/GaN nanorods by Scanning Transmission Electron Microscope Cathodoluminescence — •Marcus Müller[1], Gordon Schmidt[1], Peter Veit[1], Silke Petzold[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, Otto-von-Guericke-University Magdeburg, Magdeburg, Germany — [2]ISOM and Departamento de Ingeniería Electrónica, Universidad Politécnica de Madrid, Spain

A potential benefit of nanorods as light emitters, aside from their very high crystal quality, relies on better light extraction efficiency as compared to thin films, because of the high surface to volume ratio.
In this study we present a direct nano-scale correlation of the optical properties with the actual crystalline structure of ordered InGaN/GaN nanorods using low temperature cathodoluminescence spectroscopy in a scanning transmission electron microscope (STEM-CL). Direct comparison of the high-angle annular dark field image with the simultaneously recorded panchromatic CL mapping at 15 K reveals a weak luminescence from the bottom GaN layer. We observe the highest CL intensity in the middle of the InGaN region. The spectral position of the InGaN emission shifts continuously red from the GaN/InGaN interface (λ = 409 nm) to the NR top (λ = 446 nm) due to lattice pulling effects and InGaN partial decomposition. Additionally, optical active basal stacking faults in the GaN layer emitting at 366 nm can be found.

HL 66.4 Wed 17:45 H15

Optical and structural properties of InGaN/GaN multiple quantum wells grown on GaN nanorods by metal-organic vapor phase epitaxy — •Martin Heilmann[1], Christian Tessarek[1], Christel Dieker[2], Erdmann Spiecker[2], and Silke Christiansen[1] — [1]Max-Planck-Institute for the Science of Light, Günther-Scharowsky-Str. 1, 91058 Erlangen — [2]University Erlangen-Nuremberg, Center for Nanoanalysis and Electron Microscopy (CENEM), Cauerstraße 6, 91058 Erlangen

Hexagonally shaped GaN nanorods with varying aspect ratios were grown mask-free and uncatalyzed on c-sapphire substrates by metal-organic vapor phase epitaxy. The vertical nanorods consist of six non-polar sidewalls (m-plane) and one polar top facet (c-plane) which serve as growth surface for InGaN/GaN multiple quantum wells (MQWs). The influence of the growth temperature and growth time on the light

emission characteristics of the core-shell structures will be quantified.

The optical properties of the MQWs were investigated by room temperature cathodoluminescence. The emission wavelength could be adjusted between 420 and 460 nm by changing the growth conditions. Scanning transmission electron microscopy was used to evaluate the structural properties of the MQWs. The optical and structural differences between MQWs grown on the c- and m-planes of the GaN nanorods will be presented.

HL 66.5 Wed 18:00 H15

Impact of Structural Properties on the Internal Quantum efficiency of InGaN - GaN Core-Shell Nanorods — •Tilman Schimpke[1,2], Martin Mandl[1], Fabian Schuster[2], Gregor Koblmüller[2], Martin Stutzmann[2], Stephan Furthmeier[3], Dominique Bougeard[3], Elisabeth Reiger[3], Tobias Korn[3], Christian Schüller[3], Hans-Jürgen Lugauer[1], and Martin Strassburg[1] — [1]Osram Opto Semiconductors GmbH, Regensburg — [2]Walter Schottky Institut, Technische Universität München — [3]Institut für Exp. und Angew. Physik, Universität Regensburg

Core-shell III-nitride nanorods (NRs) have been proposed to solve a major issue in solid-state lighting, the so-called efficiency droop, by significantly increasing the active layer area scaling with the aspect ratio. However, the reported internal quantum efficiencies (IQE) in such core-shell structures are behind best planar LEDs.

To study the processes limiting the IQE, position-controlled GaN/InGaN core-shell NRs were grown by MOVPE with diameters between 300nm and 1.5μm and aspect ratios of >5. The recombination processes in the InGaN quantum wells were investigated by temperature-dependent and time-resolved PL measurements. In addition, microscopic resolution was applied to correlate the structural properties obtained by SEM and Raman spectroscopy with optical properties. E.g., a double peak emission observed in micro-PL could be related to the semi-polar and non-polar facets of the InGaN quantum wells, respectively. The IQE values were deduced by temperature-dependent and time-resolved PL measurements.

HL 66.6 Wed 18:15 H15

MOVPE Growth of Position-Controlled InGaN / GaN Core-Shell Nanorods — •Martin Mandl[1,2], Tilman Schimpke[1], Michael Binder[1], Bastian Galler[1], Xue Wang[2], Johannes Ledig[2], Milena Ehrenburg[2], Hergo-Heinrich Wehmann[2], Andreas Waag[2], Xiang Kong[3], Achim Trampert[3], Hans-Jürgen Lugauer[1], and Martin Strassburg[1] — [1]Osram Opto Semiconductors GmbH, Regensburg — [2]Institut für Halbleitertechnik, TU Braunschweig — [3]Paul-Drude-Institut für Festkörperelektronik, Berlin

Core-shell group III-nitride nano- and microrods (NAMs) enable a significant increase of the active layer area by exploiting the non-polar side facets (m-planes) and thus can potentially contribute to mitigating the so-called efficiency droop in LEDs.

GaN NAMs exhibiting high aspect ratios were grown in a production-type MOVPE system. Low V/III ratio, hydrogen-rich carrier gas mixture and surfactants supported the 3D growth of the pencil-shape n-type GaN core. Desired narrow distributions of shape, diameter and height were achieved. The arrangement of the NAMs was controlled by patterns etched into SiO_2 masks deposited on GaN templates. The active layer (InGaN/GaN SQW and MQWs) and the layer for the p-side were deposited with 2D-like conditions wrapped around the core. The crystalline quality of the NAMs, shell growth rates and the Indium distribution were investigated by high resolution transmission electron microscopy. Furthermore, optical emission was studied using density-dependent photoluminescence spectroscopy.

HL 66.7 Wed 18:30 H15

Catalyst-free, self-organized growth of GaN nanorods on r-plane and c-plane sapphire with MBE and MOVPE — •Julian Stöver, Timo Aschenbrenner, Stephan Figge, Gerd Kunert, and Detlef Hommel — Institute of Solid State Physics, Epitaxy, University of Bremen, Otto-Hahn-Allee NW1, 28359 Bremen

High-quality GaN nanorods can be grown on r-plane sapphire by a combination of MOVPE and MBE. The r-plane sapphire was nitridated in a MOVPE reactor at 1050 °C, which leads to a change in surface morphology, e.g. small AlN islands are visible. The nanorod growth is carried out in MBE, in which the AlN islands act as nucleation centers. The nanorod density can be controlled by GaN overgrowth in MOVPE after the nitridation process. A sharp D_0X emission in μ-PL measurements indicates the high crystalline quality [Aschenbrenner et al., Nanotechnology **20**(7), 075604 (2009)]. Assigning the growth parameters on c-plane sapphire will not provide changes in the morphology. Due to the missing nucleation centers, nanorod growth did not take place. With a higher growth temperature of 1270 °C, changes in the surface morphology are achieved. AlN islands with a diameter of 35 nm and a density of 50 islands/μm^2 are provided. Similar to the growth on r-plane sapphire, GaN is deposited after the nitridation. The GaN provides a partial coverage with hexagonal structures. The structures itself and the space in between have diameters of $450 - 500$ nm.

Differences in the growth on r-plane and c-plane sapphire will be presented as well as detailed analyses of the structures grown on c-plane sapphire.

HL 66.8 Wed 18:45 H15

Superradiant luminescence of GaN nanowires on diamond — •Fabian Schuster, Andrea Winnerl, Saskia Weiszer, Jose Garrido, and Martin Stutzmann — Walter Schottky Institut, Technische Universität München, 85748 Garching

GaN nanowires have attracted much interest in recent years due to their high crystalline quality and large surface area, desirable with respect to optoelectronics, (photo-) catalysis or sensing applications. However, these devices suffer from inefficient p-type doping, especially for AlxGa1-xN ternary alloys. In contrast, diamond with its indirect bandgap of 5.48 eV can be efficiently p-type doped, thus representing a perfect complement to the nitride material system as transparent electrode and efficient heat sink. We have recently demonstrated the growth of self-assembled GaN nanowires on (111) single-crystalline diamond substrates.[1]

In order to investigate waveguiding behaviour of the nanowires, the tips of the GaN nanowires were capped by 10 nm of AlGaN with 40% aluminum content. These capped nanowires exhibit strong superradiant photoluminescence for increasing excitation density at room temperature with a low gain threshold of 50 kW/cm2. A small variation of the emission energy with increasing excitation power indicates efficient heat dissipation by the diamond substrate.

[1] F. Schuster et al., Nano Letters 12, 2199 (2012)

HL 66.9 Wed 19:00 H15

Germanium doping of self assembled GaN nanowires grown by plasma assisted molecular beam epitaxy — •Pascal Hille[1], Paula Neuderth[1], Jörg Schörmann[1], Markus Schäfer[1], Jan Müssener[1], Pascal Becker[1], Matthias Kleine-Boyman[2], Marcus Rohnke[2], Maria de la Mata[3], Jordi Arbiol[3], Detlev M. Hofmann[1], Thomas Sander[1], Peter J. Klar[1], Jörg Teubert[1], and Martin Eickhoff[1] — [1]I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Germany — [2]Physikalisch-Chemisches Institut, Justus-Liebig-Universität Gießen, Germany — [3]ICREA and Institut de Ciencia de Materials de Barcelona,CSIC, Campus de la UAB, 08193 Bellaterra, CAT, Spain

For realization of nanowire (NW) based nano-optical or nano-electronic devices, doping is a crucial issue. Up to now the use of Si-donors prevented a systematic study of the NW electronic properties as a function of the doping-concentration due to changes in the NW morphology during growth and difficulties in quantifying the Si-doping concentration [Si]. Here, we investigate Ge as an alternative dopant. Self assembled GaN:Ge NWs were grown by PAMBE on Si(111) substrates. Time of flight secondary ion mass spectrometry revealed a homogenous Ge distribution along the NW growth direction and a linear dependence of [Ge] on the Ge-flux with a maximum [Ge] of $3 \cdot 10^{20}$ cm^{-3}. The influence of the Ge incorporation on the morphology was analyzed by SEM and TEM. Low temperature PL shows strong and sharp emission even at the highest [Ge]. A linear increase of conductivity with increasing [Ge] was obtained by single wire electrical measurements.

HL 66.10 Wed 19:15 H15

Electrical characterization of doped single GaN nanowires: A comparison of Si- and Ge-doping — •Markus Schäfer, Christian Länger, Marius Günther, Pascal Hille, Jörg Schörmann, Jörg Teubert, and Martin Eickhoff — I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Germany

We present a comparison of the impact of Si- and Ge-doping on the electrical properties of GaN nanowires (NWs). While Si is well established as a shallow donor in GaN thin films, a systematic study of its effect on the electrical properties of NWs has not been reported and no report on Ge-doping of GaN NWs exists. Here, GaN NWs doped with different concentrations of Si and Ge were grown by plasma assisted molecular beam epitaxy on Si(111) substrates. Single NW conductiv-

ity measurements were carried out in four point geometry realized by electron beam lithography processing. A linear increase of the conductivity with increasing Ge-flux was observed. The results are correlated to time-of-flight secondary ion mass spectrometry, revealing a constant doping profile and an estimate for the Ge-concentration. These results are compared to Si-doped NWs. Contact resistances and the effect of Si-doping of n.i.d. GaN NWs due to diffusion from the Si substrate are also discussed.

HL 67: Focus Session (Posters): Crystalline n-type semiconducting oxides - SnO_2, Ga_2O_3, and In_2O_3 for novel devices

Time: Wednesday 16:00–20:00 Location: Poster A

HL 67.1 Wed 16:00 Poster A

Properties of tin oxides prepared by Ion-Beam-Sputtering — •Martin Becker, Robert Hamann, Angelika Polity, Davar Feili, and Bruno K. Meyer — I. Physikalisches Institut, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

The success of n-type oxide semiconductors and its application in oxide-based electronic devices has motivated the interest in p-type oxide based semiconductors. Therefore synthesis of tin monoxide (SnO) recently has received increasing attention. Another phase of this binary system, SnO_2, is of great technological interest in manifold applications, such as transparent electrodes, heat-reflecting filters and gas sensing.

The preparation of tin oxide thin films has been performed by many different procedures such as sol/gel, epitaxial procedures or methods working under vacuum conditions like sputtering techniques. Radio-Frequency-Ion-Thrusters, as designed for propulsion applications, are also qualified for thin film deposition and surface etching if utilized as ion source.

Tin oxide thin films were grown by ion-beam sputtering using a 3 inch metallic tin target. Different aspects of growth and properties of the tin oxide phases were investigated in relation to growth parameters such as substrate temperature or flux of oxygen. Structural, optical and electrical properties of the films will be discussed.

HL 67.2 Wed 16:00 Poster A

Ab-initio investigation of various tin oxides — •Bianca Eifert and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

Tin forms a stable dioxide and monoxide which are of great interest for applications ranging from optoelectronics to electrochemistry. Tin dioxide (SnO_2) is a wide-bandgap n-type semiconductor, and it is the only oxide of tin that has been investigated in some depth experimentally and theoretically so far. Tin monoxide (SnO) is usually regarded as a semimetal or a small-bandgap p-type semiconductor. It is less well examined than the dioxide, and disproportionates to Sn and SnO_2 at elevated temperatures. During this disproportionation reaction, oxides of intermediate stoichiometries such as Sn_2O_3 or Sn_3O_4 are often reported, and some experimental values for possible lattice parameters are available. The preferred stoichiometry and the exact crystal structure, however, remain unknown, and the electronic structure of these oxides is also not known yet. In the present work, we gain new theoretical insight into some of these open questions using density functional theory (DFT). We present calculations for the electronic structure of SnO as well as possible crystal structures of the intermediate oxides. The stabilities of the candidate structures will be compared to those of SnO and SnO_2 in order to suggest whether one of these metastable structures might be grown experimentally.

HL 67.3 Wed 16:00 Poster A

Structural properties and defect-induced conduction mechanism in spinel-type ferrites — •Kerstin Brachwitz, Michael Lorenz, and Marius Grundmann — Linnéstraße 5, 04103 Leipzig, Germany

Zinc ferrite (ZFO), cobalt ferrite (CoFO), and nickel ferrite (NiFO) are promising candidates for application in magnetic tunnel junctions (MTJs) for both, as conducting electrode and as insulating barrier. In this respect we have investigated such spinel-type ferrite thin films grown by pulsed-laser deposition (PLD). We have varied the growth temperature (T_S) by controlling the heater power in a range from 400° to 690°C. The thin films were grown on (100)-oriented strontium titanate (STO) substrates at $p(O_2) = 5 \times 10^{-5}$ mbar. The out-of-plane orientation of the thin films was found to be (100) and the in-plane epitaxial relation to the substrate was confirmed by ϕ-scans. 2Θ-ω XRD scans reveal an increasing out-of-plane lattice constant with decreasing substrate temperature for all investigated ferrites. The film thickness of about 200-400 nm and the large lattice mismatch between ferrite film and STO substrate (6-8%) lead to relaxed film growth. The electrical conductivity of the thin films can be tuned btw. 10^{-4} and 10^2 S/m by different substrate temperatures during growth. It increases with decreasing substrate temperature. The conduction mechanism is not only affected by electron hopping between Fe^{2+} and Fe^{3+}, but also defects like oxygen vacancies and structural disorder have great influence. The conductivity is thermally activated and a model with two activation energies fits the temperature dependent conductivity.

HL 67.4 Wed 16:00 Poster A

Low Rate Deep Level Transient Spectroscopy: A new method for detecting deep levels in wide gap semiconductors — •Rainer Pickenhain[1], Florian Schmidt[1], Otwin Breitenstein[2], Holger von Wenckstern[1], and Marius Grundmann[1] — [1]Universität Leipzig, Institut für Experimentelle Physik II, Abteilung Halbleiterphysik, Linnéstraße 5, 04103 Leipzig — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D - 06120 Halle

Deep level transient spectroscopy (DLTS) has been widely applied to study defect states within the entire bandgap of various semiconductors. The method typically uses time windows in the kHz regime which is not sufficient to study defect states in the entire bandgap of wide bandgap materials such as ZnO. In these materials the emission rates of deep defects are too low to be detected by standard DLTS. Optical DLTS (ODLTS) fails because the photon flux of conventional light sources is too small in order to shift the optical emission rates towards the kHz regime. In this contribution we propose a method (LR-ODLTS) allowing the measurement of capacitance transients in the mHz range maintaining high sensitivity. The method is applied to ZnO and first results will be presented demonstrating that LR-DLTS allows to construct experimental Arrhenius-plots of defects exceeding the emission rate span of conventional ones more than three orders of magnitude. On this basis we easily separated signals from the close-lying defects E3 and E3' in ZnO. Furthermore several defects states within the vicinity of the valance band and close to mid gap in ZnO were detected by LR-ODLTS and will be discussed.

HL 67.5 Wed 16:00 Poster A

$ZnFe_2O_4$ dielectric function — •Tammo Böntgen, Kerstin Brachwitz, Rüdiger Schmidt-Grund, Michael Lorenz, and Marius Grundmann — Universtät Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, Germany

We present a detailed investigation of the dielectric function (DF) of spinel $ZnFe_2O_4$ (ZFO) thin films on a-plane sapphire. The films were grown by pulsed laser deposition at various temperatures and oxygen partial pressures. The optical measurements were carried out using spectroscopic ellipsometry in the spectral range from 0.5 eV to 9.5 eV. For the ZFO DF model dielectric functions (Gauss and critical-point-functions) were used to allow the derivation of transition energies and unravel the effect of the different growth conditions (i.e. temperature, substrate, oxygen pressure). The observed transitions are related to transitions allowed by ligand field theory. The dominant transitions were observed at ≈3.5 eV and ≈6 eV and identified as Fe3d and Fe4s transitions. ZFO has a special position within the spinel ferrites because Zn and its ions have a filled 3d shell. Thus no on site d-d transitions and no transitions from the O2p to the Zn3d band are possible. This results in a high transparency (compared to other ferrites) and reduces the number of observed transitions. While the oxygen partial pressure has a neglectable effect on the optical properties, the growth temperature induces a distinct shift in the transition energies was found. Also a notable shift of the absorption edge is observed. This change can be correlated to a change in the lattice constant as

observed using wide-angle X-ray diffraction.

HL 67.6 Wed 16:00 Poster A

CVD of Epitaxial SnO2 Films grown on c-cut and r-cut Sapphire by SnI2/O2 Precursor — •Yinmei Lu, Gunther Haas, Melanie Pinnisch, Philipp Hering, Martin Becker, Johannes Bieber, and Bruno Meyer — I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen

Thin films of SnO2 have been successfully deposited by CVD using SnI2 powder and O2 as precursor combination. Depositions were carried out at different temperatures (400 - 700 °C) on (001) c-cut and (10-12) r-cut sapphire. Analysis using X-Ray diffraction (XRD) revealed that SnO2 (200) was dominantly grown on c-cut sapphire, but on r-sapphire SnO2 films were strongly (101) oriented. Surface morphology and the dependence of electronic properties on oxygen partial pressures were investigated with scanning electronic microscope/atomic force microscope (SEM/AFM) and Hall measurements, respectively. The absolute average transmittance of the films in the visible and infrared range exceeds 90%. The band gap of the obtained SnO2 films is about 4.2 eV. Optical properties were investigated using low temperature photoluminescence (PL) measurements.

HL 67.7 Wed 16:00 Poster A

Investigation of the Rutile Structure on the Semiconductor Oxides SnO2 Doped with Fe by the Perturbed Gamma-Gamma Angular Correlation Spectroscopy — •Juliana Marques Ramos[1], Thiago Martucci[2], Artur Wilson Carbonari[2], and Reiner Vianden[1] — [1]Helmholtz-Institut für Strahlen- und Kernphysik — [2]Instituto de Pesquisas Energéticas e Nucleares

In the present work the perturbed gamma-gamma angular correlation (PAC) spectroscopy was used to measure hyperfine interactions in the rutile structure of semiconducting SnO2 [1] thin films doped with Fe. The motivation for this study is that both oxides are candidates for diluted magnetic semiconductor in the emerging area of spintronics [2]. The thin films were deposited by sputtering on Si (100) substrate with an applied magnetic field of 500 G. The thicknesses were 100 nm. The implantation of 111In(111Cd) was made into the films at the Bonn Isotope Separator (BONIS) at the University of Bonn. The thermal treatment for the samples was done for 10 minutes at 873 K in vacuum for TiO2 and in air for the SnO2. PAC results are compared with ab-initio first principles calculations [3] and show a week magnetic interaction for the rutile site, what confirms the results of our previous [4] work for thin films as well. REFERENCES [1] J. M. Ramos et al, Hyp. Int., 197 (2010) 239. [2] J. M. D. Coey, New J. of Phys. 12 (2010) 053025. [3] L. A. Errico, G. Fabricius, and M. Rentería, Phys. Stat. Sol. (b) 241 (2004) 2394. [4] J. M. Ramos et al, Phys. Proc., 28 (2012) 90.

HL 67.8 Wed 16:00 Poster A

Electronic properties of Si-doped $(Ga,In)_2O_3$ PLD thin films — •Marcus Purfürst, Stefan Müller, Zhipeng Zhang, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Semiconductor Physics Group, Institut für Experimentelle Physik II, Leipzig, Germany

The wide bandgap oxide semiconductor β-Ga_2O_3 ($E_g = 4.9$ eV at RT) is a promising material for the realization of solar-blind photodetector applications like flame detection or missile warning systems. In order to tune the onset of the photo response as desired we investigated in a first step the incorporation of In into the Ga_2O_3 matrix and the change of the bandgap in dependence on the incorporated In content. The Si-doped $(Ga,In)_2O_3$ thin films were grown by pulsed laser deposition on c-plane sapphire substrates. Thin films grown at 730 °C from a Ga_2O_3 target containing, for example, 1wt.% SiO_2 and 2wt.% In_2O_3 are single crystalline with (-2 0 1)-orientation for oxygen growth pressures (p_{O_2}) up to 2×10^{-3} mbar. For higher p_{O_2} polycrystalline thin films are obtained. According to the Hall measurements the conductivity shows a maximum of 63 S/m at a growth pressure of 2×10^{-3} mbar. The absorption edge decreases with increasing p_{O_2} from 4.8 eV to 4.65 eV in the investigated pressure range. Compared to binary β-Ga_2O_3 thin films, In_2O_3 leads to an increased conductivity and a reduction of the optical band gap.

HL 67.9 Wed 16:00 Poster A

Fabrication and characterization of thin $\beta-Ga_2O_3$ samples — •Srujana Dusari[1], Christine Bülow[1], Saskia F. Fischer[1], Zbigniew Galazka[2], and Martin Albrecht[2] — [1]Novel Materials, Humboldt Universität zu Berlin, D-12489 Berlin — [2]Leibniz Institute for Crystal Growth, D-12489 Berlin

The understanding of transport phenomena in transparent semiconducting oxides is the current subject of great excitement. Among the transparent semi conducting oxides $\beta-Ga_2O_3$ is very much interesting because of its transparency from deep ultraviolet region to infrared region. It has widest energy gap of 4.9 eV [1]. Here we report preparation and characterization of the thin $\beta-Ga_2O_3$ samples. $\beta-Ga_2O_3$ single crystals are grown by Czochralski technique [2]. Thin films are prepared via exfoliation technique. The samples are characterized using confocal microscopy, atomic force microscopy and scanning electron microscopy. Transport measurements will be discussed.

[1] M. Mohamed et.al. Appl. Phys. Lett. 97, 211903 (2010).

[2] Z. Galazka et. al. Cryst. Res. Technol. 45, No. 12, 1229 -1236 (2010).

HL 67.10 Wed 16:00 Poster A

The Seebeck coefficient of In_2O_3 - Inferences on causes of unintentional conductivity and electron effective mass — Natalie Preissler[1], •Oliver Bierwagen[1,2], Ashok T. Ramu[2], and James S. Speck[2] — [1]Paul-Drude-Institut, Berlin, Germany — [2]University of California, Santa Barbara, USA

If synthesized with high quality and purity, In_2O_3 along with SnO_2 and Ga_2O_3 can become true wide band gap semiconductors in their own right, allowing new applications such as transparent electronics or power electronics. A long standing issue with these oxides is the source of the unintentional n-type conductivity, and the more recent suspicion that the In_2O_3 surface dominate the thin film conductivity. Furthermore, literature values on the electron effective mass show a large spread. In this contribution we measured and modeled the room temperature Seebeck coefficient of high-quality, plasma-assisted molecular-beam-epitaxy-grown In_2O_3 for a wide range of electron concentrations, including the previously unexplored non-degenerate regime. We then use Hall and Seebeck measurements to (1.) confirm the bulk nature (and not the surface) of the unintentionally doped electron system in In_2O_3, and (2.) estimate the electron effective mass.

HL 68: Poster Session: GaN: devices & preparation & characterization; III-V semiconductors; Photonic crystals; Semiconductor lasers

Presenters are kindly asked to be near their posters at least 17:00–18:00 or to leave a note at the poster indicating a time period of availability for discussions. — Beverages will be served starting at 18:00.

Time: Wednesday 16:00–20:00 Location: Poster A

HL 68.1 Wed 16:00 Poster A

Characteristics of AlGaN Schottky photodiodes for UV-C detection — •Simon Kapanke[1], Jessica Schlegel[1], Andrea Knigge[2], Xuemei Wang[3], Jens Rass[1], Hassan Gargouri[3], Frank Brunner[2], Markus Weyers[2], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Gustav-Kirchhoff-Str. 4, 12489 Berlin — [3]SENTECH Instruments GmbH, Schwarzschildstr. 2, 12489 Berlin

We have investigated the influence of absorption layer doping on the photoresponse characteristics of solarblind AlGaN Schottky photodiodes by photocurrent spectroscopy, I-V measurements and device simulations. The responsivity maximum of photodiodes with moderate Si-doping of the $Al_{0.45}GaN$ absorption layer shifts to shorter wavelengths compared to devices with non-intentionally doped absorption layer due to a decreased widths of the space charge region. Additionally, the responsivity can be enhanced by increasing the UV-C

transmission of the semi-transparent Schottky contact. Photodetectors with SiO_2 or Al_2O_3 anti-reflection coating showed UV-C responsivities of up to 90 mA/W. The SiO_2 coatings were deposited using a Sentech inductively coupled plasma enhanced chemical vapor deposition (ICPECVD) system SI 500 D and for Al_2O_3 a Sentech atomic layer deposition (ALD) system SI ALD LL was applied. The influence on the spectral and electrical device characteristics of coatings deposited by these techniques in comparison to sputtered SiO_2 will be discussed.

HL 68.2 Wed 16:00 Poster A

Whispering gallery modes in GaN micro- and nanorods by metal-organic vapor phase epitaxy — •Christian Tessarek[1,2], George Sarau[1], and Silke Christiansen[1,3] — [1]Max-Planck-Institut für die Physik des Lichts, Erlangen — [2]Institut für Optik, Information und Photonik, Universität Erlangen-Nürnberg — [3]Institut für photonische Technologien, Jena

Self-assembled catalyst- and mask-free GaN micro- and nanorods on sapphire substrates have been grown by metal-organic vapor phase epitaxy. To obtain these structures a simple three step method was applied consisting of nitridation of the sapphire substrate, deposition of a GaN nucleation layer and growth of GaN rods.

Optical investigations were performed utilizing cathodoluminescence (CL) and photoluminescence (PL). Typical GaN spectra were obtained showing GaN near band edge emission as well as yellow defect band luminescence. In regular hexagonal shaped GaN nano- and microrods whispering gallery modes (WGMs) were observed in the GaN spectra. Q-factors of up to 500 and up to 4000 were measured in CL and PL, respectively.

Further CL investigations will show that the spectral position of the WGMs can be tuned in slighlty tapered GaN nanorods by changing the position of the exposing electron beam. Finally, WGMs were also observed in GaN microrods covered with InGaN quantum wells.

HL 68.3 Wed 16:00 Poster A

DBR for 3D-GaN-LEDs — •Jana Hartmann[1], Lorenzo Caccamo[1], Stephan Merzsch[1], Xue Wang[1], Martin Thunert[2], Helena Franke[2], Rüdiger Schmidt-Grund[2], Hergo-Heinrich Wehmann[1], Marius Grundmann[2], and Andreas Waag[1] — [1]Technische Universität Braunschweig, Institut für Halbleitertechnik, Hans-Sommer-Str. 66, 38106 Braunschweig — [2]Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig

Until now a lot of efforts have been made to achieve low-cost and efficient white LEDs. A relatively new approach is based on micro or nano three dimensional (3D) pillars. We propose to use 1D-Bragg reflectors (DBR) as backside mirror for enhancement of the forward emission of these 3D-LEDs based on GaN/InGaN MQW.

Nanorods with diameter smaller than 200 nm are used as a core to provide a sufficient large evanescent part of the light wave allowing a high interaction between LEDs and the surrounding. To produce such small structures nanoimprint lithography and colloidal lithography are tested.

The DBR layer pairs are composed of yttria stabilized zirconia and Al_2O_3 deposited on sapphire substrates by using pulsed laser deposition. In order to grow nanorods on the sapphire, holes have to be etched into the bottom DBR structure by inductively coupled plasma etching.

First results of lithography, etching process and subsequent metal-organic vapour-phase epitaxial growth of n-doped GaN cores will be presented.

HL 68.4 Wed 16:00 Poster A

Effect of high thermal stress on the internal quantum efficiency of GaInN LED structures — •Fedor Alexej Ketzer, Heiko Bremers, Uwe Rossow, and Andreas Hangleiter — Institut für Angewandte Physik, TU Braunschweig

We investigate high indium content GaInN based light emitting diodes grown via low pressure MOVPE. The efficiency of such structures is rather small due to the high indium content. In order to improve the efficiency we study the growth of the p-doped GaN layer and rapid thermal annealing (RTA), needed to activate the p-dopants (Mg). Due to the high thermal load these processes influence the quantum well (QW) and therefore the internal quantum efficiency (IQE). Both changes in the geometry of the QW due to diffusion and generation of defects are possible. Therefore the effects can be attributed to changes in radiative or nonradiative recombination as well as a combination of both.

To distinguish the effects on the different recombination processes, the IQE and photoluminescence spectra before and after RTA are compared. Furthermore conditions during RTA and growth of the structures were modified to endorse the results. The IQE was determined by temperature and excitation power dependent photoluminescence. These results help optimize growth and processing of LED structures to achieve high internal and external quantum efficiencies.

HL 68.5 Wed 16:00 Poster A

Effect of barrier height and indium composition on the internal quantum efficiency of (In)AlGaN multiple quantum well structures — •Nikolay Ledentsov Jr.[1], Christoph Reich[1], Frank Mehnke[1], Christian Kuhn[1], Tim Wernicke[1], Tim Kolbe[1], Neysha Lobo Ploch[1], Jens Rass[1], Viola Kueller[2], and Michael Kneissl[1,2] — [1]Institute of Solid State Physics, Technische Universität Berlin, Hardenberg-str. 36, 10623 Berlin, Germany — [2]Ferdinand-Braun-Institut, Gustav-Kirchhoff-str. 4, 12489 Berlin, Germany

We studied (In)AlGaN multiple quantum wells (MQWs) emitting in the UV-B spectral region with photoluminescence and electroluminescence spectroscopy. The internal quantum efficiency (IQE) was determined by temperature dependent measurements (5 K - 300 K). The quantum confined Stark effect (QCSE) was investigated by studying the shift of the emission energy with increasing excitation power density. In the first series, $Al_{0.27}Ga_{0.73}N$ MQWs with different $Al_xGa_{1-x}N$ barriers ($0.32 < x < 0.67$) were investigated. Increasing the Al content increased the IQE due to improved carrier confinement. A maximum of the IQE of 24 % at $x = 0.4$ was obtained. Further increase of the Al content in the barriers decreased the IQE due to a stronger QCSE. In the second series, quaternary InAlGaN QWs were investigated. Due to In incorporation, room temperature emission energy shifted from 4.3 eV to 3.9 eV. At low temperatures two peaks were observed. The lower energetic peak was attributed to In-rich clusters. Influence of the In segregation will be discussed.

HL 68.6 Wed 16:00 Poster A

Light trapping in Gallium Nitride nanostructures formed by maskless dry etching — •Anna Haab, Jiehong Jin, Toma Stoica, Beata Kardynal, Andreas Winden, Hilde Hardtdegen, Martin Mikulics, and Detlev Grützmacher — Peter Grünberg Institut (PGI-9), Jülich-Aachen Research Alliance (JARA), Forschungszentrum Jülich, 52425 Jülich, Germany

III-N alloys have attracted much attention as a candidate material system for solar cells, as their band gap can be tuned to cover the solar spectrum. For this application light management is of crucial importance and so patterning is used to reduce surface reflection and therefore to increase efficiency of the photonic devices. In this presentation we show that the simple, maskless reactive ion etching process, using a Cl2/Ar plasma of MOVPE grown GaN layers, can be employed to form arrays of nanowires suitable for light extraction/trapping. Both density and morphology of nanowires (from straight to conical) can be tuned, by varying the inductively coupled plasma power. We performed optimization of procedure to maximize light extraction/trapping in the GaN. The wavelength dependence of absorption was obtained from total transmission and reflection measurements for all samples. Photoluminescence analysis was used to assess potential damage from the etching process. We find that the strongest reduction of reflection is achieved in a dense array of straight nanowires. In such a structure the absorption just above the band gap increased to almost 100%, while the defects did not play a significant role. In future such structures can be used either as an antireflective coating or as substrates for overgrowth.

HL 68.7 Wed 16:00 Poster A

Influence of chemical treatments and the attachment of functional molecules on the surface properties of GaN — •Georg Eichapfel[1], Marcel Himmerlich[1], Stefan Krischok[1], Stefan U. Schwarz[2,3], Volker Cimalla[2], and Oliver Ambacher[2,3] — [1]Institut für Physik and Institut für Mikro- und Nanotechnologien, TU Ilmenau, PF 100565, 98684 Ilmenau — [2]Institut für Mikrosystemtechnik, Albert-Ludwigs-Universität Freiburg, Georges-Köhler-Allee 106, 79110 Freiburg — [3]Fraunhofer-Institut für Angewandte Festkörperphysik, Tullastraße 72, 79108 Freiburg

The functionalization of GaN surfaces is a promising pathway for the realization of semiconductor-based biosensors. Several approaches for the attachment of biosensitive functionalizations to GaN have already been reported in the literature. A detailed knowledge about the mechanisms of molecule attachment and surface reactions are of great im-

portance to understand the electrical behavior of processed sensors. Within this framework, the surface pretreatment and the resulting functional groups play a crucial role. We present photoelectron spectroscopy investigations on the chemical modification of GaN(0001) surfaces and their interaction with ethene. Changes in the surface composition and the formed chemical bonds are characterized and their influence on the electronic properties is discussed. The results are compared with the surface properties of GaN sensor structures that have been thermally or photochemically functionalized with 1-alkenes.

HL 68.8 Wed 16:00 Poster A

Quantification of internal electric fields in InGaN/GaN quantum wells by differential phase contrast microscopy — •Matthias Lohr[1], Ralph Schregle[1], Ines Pietzonka[2], Martin Strassburg[2], Robert Leute[3], Ferdinand Scholz[3], Knut Müller[4], Andreas Rosenauer[4], and Josef Zweck[1] — [1]Fakultät für Physik, Universität Regensburg — [2]Osram Opto Semiconductors, Regensburg — [3]Institut für Optoelektronik, Universität Ulm — [4]Institut für Festkörperphysik, Universität Bremen

LEDs and laser diodes play an important role in our daily lives. A very promising and intensively studied material system is GaN with InGaN quantum wells. It is capable to cover the whole visible spectral range by changing the In content. When trying to tune the output wavelength from blue to green light however, big problems in efficiency emerged. In the literature this became known as the "green gap". An important property of the non-centrosymmetric GaN crystal and possible cause of the efficiency droop is the internal piezoelectric field.

In this work direct and quantitative measurements of InGaN/GaN heterostructures combining STEM and differential phase contrast (DPC) method will be shown. The detected signal is related to the product of the piezoelectric field strength and the sample thickness. The calibration of the inelastic mean free path (IMFP) of electrons in GaN was determined by HAADF STEM and EELS. Using this data, the thickness became accessible. Based on the IMFP thickness maps in combination with calibrated DPC measurements, fields in the range from 10-100 MV/m have been measured in different samples.

HL 68.9 Wed 16:00 Poster A

Investigations of electrolyte/ group-III-nitride interfaces with electrical methods — •Martin Gottschalk, Hartmut Witte, Armin Dadgar, and Alois Krost — Otto-von-Guericke-Universität Magdeburg, Institute of Experimental Physics, MB 4120,39016 Magdeburg

Group-III-nitride materials are well established for detecting chemicals, gases, biological and radiation releases as well as for local stimulation of chemical or biological reactions. Hereby, the electronic properties of the surfaces control the interaction with the different atmospheres and liquids. Therefore, for any application of group-III-nitrides as sensors or actuators these interfaces must be investigated in detail to enable a control of their properties. We focused our investigations on the interface between different group-III-nitride materials such as p-type and n-type GaN, AlGaN, InGaN and InAlN with electrolytes containing chlorine ions. The measurements include cyclic voltammetry and electrochemical impedance- and CV-spectroscopy. To characterize the semiconductor surfaces before contacting with electrolytes we used Hall-effect measurements and CV-characteristics and surface scanning potential spectroscopy. In a systematic study for all investigated materials the redox potentials and the potentials for the hydrogen production were given as well as results of the surface carrier concentrations.

HL 68.10 Wed 16:00 Poster A

Dislocation related luminescence properties in multiple InGaN quantum well structures — •Manuel Frey[1], Ingo Tischer[1], Matthias Hocker[1], Dario Schiavon[2], Matthias Peter[2], and Klaus Thonke[1] — [1]Institut für Quantenmaterie, Gruppe Halbleiterphysik, Universität Ulm, 89081 Ulm — [2]OSRAM Opto Semiconductors GmbH, Leibnizstraße 4, 93055 Regensburg, Germany

The development of InGaN/GaN quantum well structures during the last years resulted in green LEDs with high quantum efficiency.
The indium content and the strain in the InGaN layers increases with the growing number of QWs. Among others, the density of threading dislocations and stacking faults increases leading to V-pit formation when a critical thickness of the QWs is exceeded.
Spatially and spectrally resolved low voltage cathodoluminescence measurements on multiple InGaN/GaN based QWs allow to determine the effect of dislocations and strain on the luminescence properties of multiple QW samples.

HL 68.11 Wed 16:00 Poster A

Design of a high temperature Hall measurement setup — •Dominik Beck, Matthias Hocker, and Klaus Thonke — Institute of Quantum Matter / Semiconductor Physics Group, Ulm University, D-89081 Ulm, Germany

A Hall measurement setup is developed for the temperature dependent characterization of iron doped gallium nitride and other highly resistive materials. For this purpose the whole setup has to meet some special technical requirements.

The Hall chamber has to be vacuum tight to prevent samples from oxidation and other modifications due to reactions with environmental gases. For the thermal activation of deep impurities, the setup is designed to reach temperatures up to 800 °C. Thermal isolation is realized with cascaded stainless steel shields, and water cooling of the outer walls keeps them at low temperature.

Another important point is the measurement of very small electrical currents due to the high resistivity of the samples. The whole setup is optimized for these low currents and high voltages up to 100 V for Hall and Van der Pauw measurements.

Furthermore, the whole setup is designed for minimal size to fit the given geometry of the magnetic pole pieces.

HL 68.12 Wed 16:00 Poster A

Growth of AlN by pulsed and conventional MOVPE — •Hanno Kröncke, Timo Aschenbrenner, Stefan Figge, and Detlev Hommel — Universität Bremen, Institut für Festkörperphysik

Due to low accessibility of pure aluminium nitride substrates, AlN-templates are appropriate for the growth of optoelectronic device emitting in the UV spectral region and high power / frequency electronic devices.

We have grown metal polar AlN layers up to 2 μm thickness on *c*-plane sapphire either by conventional metal organic vapor phase epitaxy (MOVPE) at 1270 °C or in pulsed growth mode at 1050 °C. For both methods we investigated different concepts of nucleation and the influence of V/III ratio and atmospheric conditions. The layers are atomically flat, showing pits in a density lower than $1 \cdot 10^7\,\mathrm{cm}^{-2}$ and edge type dislocations in the density of $3 \cdot 10^{10}\,\mathrm{cm}^{-2}$ (pulsed) and $5 \cdot 10^9\,\mathrm{cm}^{-2}$ (conventionally).

In contrast to other publications on pulsed growth, our growth rate (1μm/h) is much higher than 1 ML/cycle, requiring a different growth mode, which was investigated by *in situ* reflectivity measurements.

For conventionally grown samples we investigated the influence of the growth atmosphere on the growth rate and applied a simple model based on diffusion, viscosity and gas flow velocity. In general the best quality is obtained by low V/III ratio of 100, pure hydrogen atmosphere at 50 Torr at 1250 °C.

HL 68.13 Wed 16:00 Poster A

Epitaxial growth of smooth GaAs layers on non-miscut GaAs (111)A and GaAs (111)B substrates — •Julian Ritzmann[1], Rüdiger Schott[1], Dirk Reuter[2], Arne Ludwig[1], and Andreas D. Wieck[1] — [1]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum — [2]Arbeitsgruppe für optoelektronische Materialien und Bauelemente, Universität Paderborn

(111)A and (111)B oriented GaAs is known for their large piezoelectric effect and light emitting efficiency. Also, these surfaces allow for highly anisotropic etching. The growth by molecular beam epitaxy on these surfaces is however rather challenging and only a limited range of growth parameters leads to smooth layers.

In this work we investigate conditions for the MBE growth of GaAs layers on GaAs (111)A and (111)B substrates without miscut. The samples were grown under different III/V-ratios, different substrate temperatures and growth rates. Atomic force and scanning electron microscopy were used for imaging the surface morphology and photoluminescence measurements were performed to study the optical properties of our samples.

HL 68.14 Wed 16:00 Poster A

Effects of substrate temperature and annealing on structural properties of GaP/Si(100) grown by gas-source molecular-beam epitaxy — •Emad Hameed Hussein, Shabnam Dadgostar, Fariba Hatami, and W. Ted Masselink — Department of Physics, Humboldt Universtät zu Berlin, Newtonstrasse 15, D-12489 Berlin,

Germany

Gallium phosphide (GaP) was grown epitaxially on silicon (100) substrates using gas-source molecular-beam epitaxy. In this study, two growth methods are compared: one-step and two-step growth. In the case of one-step growth, the GaP was grown directly onto the desorbed Si surface at a single substrate temperature between 250°C to 550°C, followed by thermal annealing. In two-step growth, the GaP includes two layers grown at different temperatures. The differences between these methods as well as the effects of growth and annealing temperatures on crystal structure were studied using X-ray diffraction measurements and scanning electron microscopy. Samples grown in two steps method show a better surface quality compared with that grown by one-step. A structurally coherent crystalline GaP layer, on the other hand, was successfully grown by two-step method, as confirmed by asymmetric x-ray curves.

HL 68.15 Wed 16:00 Poster A

In situ characterization of MOVPE grown GaPN/GaP/Si(100) for photoelectrolysis — •Oliver Supplie[1,2], Helena Stange[1,2], Matthias M. May[1,2], Christian Höhn[1], Christian Koppka[3], Katja Tonisch[3], Henning Döscher[1,3,4], and Thomas Hannappel[1,3,5] — [1]Helmholtz-Zentrum Berlin, Institut für Solare Brennstoffe — [2]Humboldt-Universität zu Berlin, Institut für Physik — [3]TU Ilmenau, Institut für Physik, Fachgebiet Photovoltaik — [4]NREL, Golden, CO, USA — [5]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, Erfurt

A photoelectrochemical diode consisting of a Si bottom and a lattice-matched GaPN top cell promises both high photovoltaic energy conversion efficiency and supply of the minimum voltage necessary for photoelectrolysis [1]. Existing devices based on GaPN-on-Si heterostructures, however, suffer from low efficiency due to material quality issues [2]. To achieve in situ control, we monitor the whole MOVPE-preparation with reflection anisotropy spectrom and mass spectrometry in order to compare the established GaP/Si(100) preparation [3] to the dilute nitride system with regard to surface preparation and principal MOVPE growth parameters. We benchmark the in situ signals (i) after contamination-free MOVPE-to-UHV transfer with surface science techniques such as low energy electron diffraction and photoelectron spectroscopy as well as (ii) ex situ by high-resolution X-ray diffraction, photoluminescence and atomic force microscopy.
[1] Döscher et al., *ChemPhysChem* **13**:2899. [2] Geisz et al., *EU-PVSEC* **19**(2004). [3] Döscher et al., *JAP* **107**:123523.

HL 68.16 Wed 16:00 Poster A

Impact of growth temperature on the interface quality of AlP/GaP superlattices grown using gas-source molecular-beam epitaxy — •Shabnam Dadgostar, Fariba Hatami, and William.Ted Masselink — Department of physics, Humboldt-Universität zu Berlin, Newtonstrasse 15, D-12489 Berlin, Germany

High-Q optical cavities in GaP can be realized by incorporating epitaxially grown AlP/GaP Bragg reflectors. Such Bragg reflectors can be prepared as single crystals using gas-source molecular-beam epitaxy, growing the distributed Bragg reflectors adjacent to an active region for optical emission. Electrical transport through such structures depends critically on the interface roughness between the AlP and GaP layers. We have studied the effect of growth temperature on the interface roughness and found the optimum temperature for growth of AlP/GaP superlattice on GaP (100) substrate. For our applications we used structures with AlP and GaP layer thicknesses of 48 and 40 nm. Both scanning electron microscopy and high-resolution x-ray diffraction measurements indicate that interface roughness is minimized for a growth temperature of 450°C.

HL 68.17 Wed 16:00 Poster A

Bandgap engineering of GaAs by ion-implantation and flash lamp annealing — •Kun Gao, Slawomor Prucnal, Wolfgang Skorupa, Manfred Helm, and Shengqiang Zhou — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), P. O. Box 510119, Dresden 01314, Germany

Gallium arsenide based materials have outstanding performances in light-emitting devices in virtue of their remarkable efficiency and thermal stability.

In this contribution we present the successful doping of N, P, Bi, and In into GaAs lattice. First the dopant atoms are implanted into the GaAs wafers. After implantation, the GaAs wafer becomes amorphous within the as-implanted range. Post thermal annealing restores the initial properties of the matrix and leads to formation of the GaAs:X (X:dopants) layers. The optical properties were investigated by μ-Raman spectroscopy, temperature dependence photoluminescence. By N-doping we have successfully narrowed the bandgap. From Bi and In doped GaAs we obtain a strong luminescence peaking at 1.3 μm. On the other hand, Zn-doping has suppressed such luminescence. It is also noticeable that the 1.3 μm light emission only have a slight redshift (about 20 nm) and 60% intensity decline as the temperature rises from 20 K to room temperature. Our investigation suggests that after flash lamp annealing GaAs based materials exhibit a promising prospect on applications of light emitters and detectors, especially for optical communication devices.

HL 68.18 Wed 16:00 Poster A

Treatment of light emitting equipment on the base of III-V semiconductive compound for information visual reflection systems — •Ia Trapaidze[1], Maia Jgenti[1], Lia Trapaidze[2], and Gela Goderdzishvili[1] — [1]Dep. of Physics, Georgian Technical University, 77 Kostava Ave. IV block, 0175, Tbilisi, Georgia — [2]Dep. of Physics, Tbilisi State University, 3 Chavchavadze Ave., 0179 Tbilisi, Georgia

This work includes new methods of treatment and optimization technological processes of light emitting equipment on the base of III-V semiconductive compound. By using local rust thermal method we created high effective light emitting integral scheme. Also was fulfilled new type of integral scheme in the different area of visible spectrum. For made equipment we investigated spectraphotometrical and electro physical parameters. In future we plan to create structures working little consumption current with light radiation elements and will make different configuration semiconductive indicators on the base of these structures.

HL 68.19 Wed 16:00 Poster A

Optical gain and lasing in GaNAsP/BGa(As)P heterostructures grown on (001) silicon substrate — •Markus Finkeldey[1], Nektarios Koukourakis[1], Nils C. Gerhardt[1], Martin R. Hofmann[1], Martin Zimprich[2], Kerstin Volz[2], Wolfgang Stolz[2], and Bernardette Kunert[3] — [1]Photonics and Terahertztechnology, Ruhr-Universität Bochum, Germany — [2]Material Science Center and Faculty of Physics, Philipps-University Marburg, Germany — [3]NAsP III/V GmbH, Marburg, Germany

The realization of electrically pumped lasers on silicon is a huge challenge on the way to optoelectronic integrated circuits. One approach is the heteroepitaxial growth of direct band gap III/V semiconductors on indirect Si. However, the large lattice mismatch between III/V materials and Si leads to a formation of high misfit and threading dislocation densities, reducing the efficiency and lifetime of the lasers dramatically. The dilute nitride material GaNAsP is a very promising candidate to overcome these obstacles. Due to its direct band gap and its capability for lattice matched growth on (001) silicon substrate, GaNAsP is perfectly qualified as an active material for lasers on silicon. Here we investigate gain and temperature dependent lasing in optically pumped GaNAsP/BGa(As)P heterostructures grown on silicon substrate. We obtained high modal gain values at room temperature comparable to the values in common III-V laser materials. However the observed strong dependence of the laser threshold on excitation wavelength indicates significant carrier leakage, which has to be suppressed in order to increase the efficiency in electrically pumped devices.

HL 68.20 Wed 16:00 Poster A

Non-exponential photoluminescence transients in GaNAsP lattice matched to (001) silicon substrate — •Nils C. Gerhardt[1], Nektarios Koukourakis[1], Markus Finkeldey[1], Martin R. Hofmann[1], Martin Zimprich[2], Kerstin Volz[2], Wolfgang Stolz[2], Kakhaber Jandieri[2], Florian Gebhard[2], Sergei Baranovskii[2], and Bernardette Kunert[3] — [1]Photonics and Terahertztechnology, Ruhr-Universität Bochum, Germany — [2]Material Science Center and Faculty of Physics, Philipps-University Marburg, Germany — [3]NAsP III/V GmbH, Marburg, Germany

The novel dilute nitride material GaNAsP which can be grown lattice-matched on silicon substrate is a very promising material for future integrated, electrically pumped lasers on silicon. Here we present an experimental and theoretical study of the time-resolved photoluminescence (PL) of GaNAsP/BGa(As)P heterostructures grown on (001) silicon substrate. The results show a s-shape behaviour for the temperature dependent PL peak energy and a strong non-exponential behaviour for the PL transients, indicating a significant impact of

disorder-induced localization effects. A detailed comparison with theoretical calculations based on Monte-Carlo simulations reveals that the non-exponential PL transient is due to a combination between the fast capture of carriers in non-radiative centers and the slow radiative recombination via localized states. The impact of the localization effects depends strongly on the material composition and growth conditions. Remarkably, the experimental results indicate an unexpected decrease of localization and disorder effects with increasing N content.

HL 68.21 Wed 16:00 Poster A

Time-resolved luminescence studies of rare earth doped III-nitrides grown at high temperature and high pressure — •Oliver Beck[1], Tristan Koppe[1], Takashi Taniguchi[2], Hans Hofsäss[1], and Ulrich Vetter[1] — [1]2. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]National Institute for Materials Science, Namiki 1 - 1, Tsukuba, Ibaraki 305-0044, Japan

We report on luminescence studies of rare earth doped III-nitrides that are synthesized under high temperature and high pressure conditions. The samples are excited with a femtosecond laser system at various wavelengths between 193nm and 1000 nm and the luminescence is collected with a Streak Camera at different time scales in the wavelength range 200-800 nm at room temperature. A special focus is drawn on rare earth doped 2H-AlN as a high power laser material, with a comparison to rare earth doped boron nitride.

HL 68.22 Wed 16:00 Poster A

Investigation of the effective mass in diluted nitride semiconductors — •Faina Lomakina[1,2], Oleksiy Drachenko[1], Harald Schneider[1], Amalia Patanè[3], 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 NG7 2RD, United Kingdom

Dilute nitride semiconductors (DNS), such as GaAsN, with a nitrogen content y of a few percent or even less, have attracted considerable current interest due to the giant bowing effect. That, in turn, offers the possibility to tailor the band structure of new devices, like LEDs, lasers, solar cells, and infrared photodetectors by varying the nitrogen content [1]. Determining proper values of the effective mass (EM) of DNS is a topic of interest because of the inconsistency of previous results (e.g. [2,3]). To clarify the conflict we study a series of GaAsN and InAsN samples (y=0%-1.9%) by cyclotron resonance (CR) spectroscopy, Fourier spectroscopy and photoluminescence spectroscopy in magnetic fields in order to deduce the EM via the CR frequency, plasma frequency and the dielectric shift, respectively. First results of CR measurements indicate that the EM is not significantly affected by the nitrogen doping in contrast to previous publications.

[1] A. Erol, Dilute III-V Nitride Semiconductors and Material Systems, Springer-Verlag Berlin Heidelberg (2008) [2] F. Masia et al. Appl. Phys. Lett. 82, 4474 (2003) [3] Y. J. Wang et al. Appl. Phys. Lett. 82, 4453 (2003)

HL 68.23 Wed 16:00 Poster A

A numerical framework to analyze the nature of guided light in waveguide quantum electrodynamics — •Christoph Martens[1] and Kurt Busch[1,2] — [1]Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, Max Born Str. 2A, 12489 Berlin, Germany — [2]Humboldt-Universität zu Berlin, Institut für Physik, AG Theoretische Optik & Photonik, Newtonstr. 15, 12489 Berlin, Germany

Low-dimensional waveguiding structures combined with embedded single emitters are the basic building blocks of quantum-photonic circuits. The photon transport through such systems is primarily determined by strong quantum interference of single- or few-photon states caused by the restriction of the radiation to the waveguiding elements before and after the scattering. This leads to interesting transport properties, e.g. *interaction–induced radiation trapping* [1] or a variety of the *Hong-Ou-Mandel effect* [2].

In this contribution we present our numerical framework that is used to investigate the dynamics of photon transport in waveguiding systems in the presence of quantum impurities. The framework encloses multi-level atoms of different configurations as impurities, waveguides with nonlinear dispersion relations for photons, and time-dependent driving fields. With the help of this, we can monitor the evolution of certain initial few-photon states in time domain and real space to reveal and understand physical phenomena in these systems.

[1] P. Longo *et al.*, Phys. Rev. Lett. **104,** 023602 (2010)
[2] P. Longo *et al.*, Optics Express **20,** 12326 (2012)

HL 68.24 Wed 16:00 Poster A

Design and Optimization and Fabrication of Photonic Crystal Structures for Single Photon Applications — •Carlo Barth[1], Michael Adler[1], Jürgen Probst[2], Max Schoengen[2], Bernd Löchel[2], Janik Wolters[1], and Oliver Benson[1] — [1]Nano-Optics, Institute of Physics, Humboldt-Universität zu Berlin, Newtonstraße 15, D-12489 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Albert-Einstein-Straße 15, D-12489 Berlin

Photonic crystals are a promising platform for integrated optical hybrid networks on the single photon level. In the last years the controlled coupling of single emitters to photonic crystal cavities has been strikingly demonstrated in several experiments [1]. For future integrated single photon devices efficient wave guiding and coupling structures will be needed. The latter ones are particularly important, as they form the interface between photonic chips and the macroscopic measurement equipment. Our latest results on the design and fabrication of high efficient couplers with large directivity, as well as their integration into photonic networks are presented.

[1] J. Wolters, A.W. Schell, G. Kewes, N. Nüsse, M. Schoengen, H. Döscher, T. Hannappel, B. Löchel, M. Barth, O. Benson. 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(14):141108, 2010.

HL 68.25 Wed 16:00 Poster A

Photon correlations in one-dimensional coupled resonator optical waveguides — •Matthias Moeferdt[1], Peter Schmitteckert[2], and Kurt Busch[1,3] — [1]Humboldt-Universität zu Berlin, Institut für Physik, AG Theoretische Optik und Photonik, Newtonstr. 15, 12489 Berlin, Germany — [2]Institut für Nanotechnologie, Karlsruher Institut für Technologie (KIT), 76344 Eggenstein-Leopoldshafen, Germany — [3]Max-Born-Institut, Max-Born-Str. 2A, 12489 Berlin, Germany

We numerically simulate the propagation of wave packets containing two photons in a one-dimensional coupled resonator optical waveguide, equipped with a side-coupled two-level system.

The two-level system causes an effective photon-photon interaction, resulting in radiation trapping in the immediate neighborhood of the two-level system, as well as strong correlations between the reemitted photons.

To study these correlations, we compute the correlation functions and employ a two-dimensional representation of the two-photon wavefunction in order to visualize the photon transport. We show that its nature depends strongly on the position of the initial pulse in the band.

HL 68.26 Wed 16:00 Poster A

Systematic analysis of intracavity dispersion and absorption effects of a modelocked semiconductor laser — •Benjamin Döpke[1], Jan C. Balzer[1], Andreas Klehr[2], Götz Erbert[2], Günther Tränkle[2], and Martin R. Hofmann[1] — [1]Chair for Photonics and Terahertz Technology, Ruhr-Universität Bochum, D-44801 Bochum, Germany — [2]Ferdinand Braun Institute, D-12489 Berlin, Germany

Modelocked multi-section semiconductor laser diodes are a promising source for ultrafast pulses. They offer a potentially compact and cost-effective alternative to pulsed Ti:sapphire lasers. In addition they have a higher flexibility of the design wavelength compared to fiber lasers. However, in spite of a gain bandwidth greater than 50 nm, intracavity dynamics governed by dispersion limit the obtainable modelocked bandwidth, resulting in typical compressed pulse-widths of more than 200 fs.

We present a systematic study of intracavity dispersion and absorption effects of a multi-segment triple quantum well ridge waveguide semiconductor laser with a central wavelength of 850 nm in an external cavity. The external cavity consists of a folded 4f grating compressor. A spatial light modulator in the Fourier plane of the compressor enables us to modify spectral phase and amplitude. This allows fine-grained control of resonator dispersion and losses in various operating conditions of the laser.

HL 69: Poster Session: II-VI semiconductors; Organic semiconductors; Heterostructures

Presenters are kindly asked to be near their posters at least 17:00–18:00 or to leave a note at the poster indicating a time period of availability for discussions. — Beverages will be served starting at 18:00.

Time: Wednesday 16:00–20:00 Location: Poster A

HL 69.1 Wed 16:00 Poster A

Fabrication and characteristics of ZnO/ZnS core-shell nanotubes based on template-fabrication techniques — •Samar Tarish[1,2], Ahmed Al-Haddad[1,2], Chengliang Wang[1], Huaping Zhao[1], Yan Mi[1], and Yong Lei[1] — [1]Fachgebiet 3D-Nanostrukturierung, Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, Prof. Schmidt Str. 26, 98693 Ilmenau, Germany. — [2]Department of Physics, College of Science, University of Al-Mustansiryah, Baghdad, Iraq.

Here we will introduce a new technique that has been employed by fabricating ZnO/ZnS one-dimensional core-shell nanotubes, where synthesized by a two-step growth process with the assistance of AAO templates. Phase and structural analyses reveal that the ZnO core has a single crystalline phase, whereas the ZnS shell has a polycrystalline phase covering the surface of the core. First ZnO nanotube arrays are synthesized within AAO templates by atomic layer deposition (ALD) at 2500C. Then, by using an electrodepostion route, Na2S and ZnN were employed to supply S and Zn atoms at different temperatures to form ZnS-coated ZnO nanotubes structures. Then ZnO/ZnS core-shell coaxial nanotubes are created .The morphology and structure of ZnO/ZnS coaxial nanotubes are characterized by X-ray diffraction (XRD), field-emission scanning electron microscopy (FESEM), X-ray energy-dispersive spectroscopy (EDX), transmission electron microscopy (TEM).

HL 69.2 Wed 16:00 Poster A

Doping of ZnO micro and nano crystals prepared by sol-gel technique — •Christoph Brodehl, Jahanzeb Azam, Tim Baumgarten, and Sigmund Greulich-Weber — University of Paderborn, 33098 Paderborn, Warburger Str. 100, Germany

Zinc oxide (ZnO) is a wide-bandgap semiconductor with promising applications in the optoelectronic domain. Our main focus is on micro and nano crystalline ZnO as a transparent conductor in solar cells and photonic crystals, and as diluted magnetic semiconductor (DMS) for development of left-handed materials. We prepared ZnO nano and micro crystals via sol-gel routes and doped them with donors, acceptors and regarding to DMS with manganese. Annealing series of doped and as-grown crystals were characterized with electron paramagnetic resonance (EPR), photoluminescence, electron microscopy, X-ray diffraction and conductivity measurements. The annealing studies investigated by EPR together with photoluminescence measurements allow an identification of the commonly observed positively charged oxygen vacancy and the positively charged interstitial zinc as intrinsic defects in as-grown nominally undoped sol-gel ZnO. Beside shallow intrinsic defects and dopants a surface-related defect was always present and determines the crystal conductivity at least at room temperature. Doping with lithium allows a partly compensation of shallow intrinsic defects. Depending on the annealing temperature, we observed changes in EPR spectra of manganese doped ZnO. The samples show paramagnetic behavior for low annealing temperatures and ferromagnetic behavior for temperatures higher than 800°C.

HL 69.3 Wed 16:00 Poster A

Magneto-Stark effect on excitons in ZnO investigated by nonlinear optical spectrosopy — •David Brunne[1], Marco Lafrentz[1], Victor V. Pavlov[2], Roman V. Pisarev[2], Anna Rodina[2], Dmitri R. Yakovlev[1,2], Dietmar Fröhlich[1], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universitaet Dortmund, D-44221 Dortmund, Germany — [2]Ioffe Physical-Technical Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia

The magneto-Stark effect on moving excitons is proved as a driving mechanism enabling resonant second harmonic generation (SHG) in hexagonal ZnO. Strong SHG signals induced by external magnetic fields are observed in the spectral range of 2s and 2p excitons. Theoretical microscopic analysis shows, regardless the fact that the magnetic field is an even parity perturbation, for excitons with a finite k-vector wave functions of opposite parities are mixed by an effective odd parity electric field. Magnetic field, spectral and polarization dependencies of SHG intensity confirm the proposed mechanism.

HL 69.4 Wed 16:00 Poster A

Struktierte Ag-Diffusionsprofile in CdTe durch Cu-Filme — •Johannes Lehnert, Herbert Wolf, Manfred Deicher und Thomas Wichert — Experimentalphysik, Universität des Saarlandes, 66123 Saarbrücken

Das Diffusionsverhalten von Ag in CdTe lässt sich durch das Aufdampfen von Metallfilmen vor der Diffusion stark verändern. Dieser Effekt wurde für Cu, Au, Ni und Al gezeigt. Für die verschiedenen Metalle ergeben sich große quantitative Unterschiede, der stärkste Effekt wird von einem Cu-Film verursacht. Radiotracer-Messungen haben gezeigt, dass sich auf diese Weise das Ag-Diffusionsprofil bei einer Diffusionstemperatur von 500 K und einer Diffusionszeit von 30 min um mehrere 100 μm in das Kristallinnere verlagern lässt [1]. Wird ein CdTe-Kristall lateral homogen mit radioaktivem ^{111}Ag implantiert und anschließend die implantierte Seite mit einem strukturierten Cu-Film bedampft, so lässt sich auf diese Weise ein lateral strukturiertes Tiefenprofil von Ag in CdTe erzeugen. Die laterale Verteilung wurde mit Autoradiographie bestimmt. In Kombination mit der tiefenauflösenden Radiotracer-Technik lässt sich die dreidimensionale Verteilung der radioaktiven ^{111}Ag-Atome rekonstruieren. In diesem Beitrag werden Beispiele für lateral strukturierte Ag-Profile in CdTe vorgestellt. Mit dieser Vorgehensweise konnte z.B. eine Ag-Verteilung im CdTe-Kristall erzeugt werden, die der Form eines Zylinderhutes entspricht.
Gefördert durch das BMBF, Projekt 05K10TS2.
[1] H. Wolf *et al.*, Appl. Phys. Lett. **100** (2012) 171915

HL 69.5 Wed 16:00 Poster A

Bandgap engineering in $Cd_xZn_{1-x}Te$ ternary alloy nanowires — •Nazli Kheirabi[1], Keivan Davami[1], Mehrdad Shaygan[1], Judith Pohl[2], Giovanni Cuniberti[1,2], Jeong-Soo Lee[1], and Meyya Meyyappan[1,3] — [1]Division of IT Convergence Engineering, Pohang University of Science and Technology, Pohang, 790-894, Korea — [2]Institute for Materials Science, Dresden University of Technology, D-01062, Dresden, Germany — [3]NASA Ames Research Center, Moffett Field, CA, USA

Herein, we report Au catalyzed vapor-liquid-solid growth and band gap engineering of single-crystalline alloy $Cd_xZn_{1-x}Te$ nanowires where a continuous tuning of x value ($0<x<1$) and desired nanowire composition were achieved by a precise substrate temperature control. A full investigation of the characteristics of our nanowires such as their morphology, crystal structure, lattice constant and composition was conducted by analyzing SEM and EDS results, TEM images, XRD patterns, Raman and photoluminescence (PL) spectra, and a monotonic increase in the Cd proportion in the alloy composition was confirmed. Near band gap peaks in PL spectra of alloy nanowires revealed a continuous decrease in energy bands from 2.24 eV to 1.52 eV when moving from ZnTe towards CdTe composition. The outcome of this work opens up new frontiers in the field of tunable band gap emission nano photonic devices operating in the range of visible to new infrared regions.

HL 69.6 Wed 16:00 Poster A

Photoresponse properties of ZnTe nanowire photodetectors — •Mehrdad Shaygan[1], Nazli Kheirabi[1], Keivan Davami[1], Jong-Soo Lee[1], Gianaurelio Cuniberti[1,2], and Meyya Meyyappan[1,3] — [1]Division of IT Convergence Engineering, Pohang University of Science and Technology, Pohang, South Korea — [2]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, Dresden, Germany — [3]NASA Ames Research Center, Moffett Field, CA 94035, USA

Photoconductivity in semiconductors is the electrical conductivity enhancement due to the electron hole pair generation induced by radiation exposure. This phenomenon is the main mechanism of photodetection in sensors. There has been increasing interest for nanosensors of all kinds which can be light weight and less expensive and can be easily incorporated into MEMS/NEMS devices. Nanowires as one dimensional high aspect ratio nanostructures have several advantages over their bulk and thin film counterparts when applied as photodetectors. Zinc telluride, an important II-IV semiconductor with a direct

band gap of ~ 2.26 eV, has been considered as a prospective material for photosensing application. In this work, ZnTe nanowires have been synthesized by Vapor-Liquid-Solid method with optimized growth parameters. They have been incorporated in the well known single nanowire field effect transistor (SNFET) device structure to be electrically characterized in dark and under illumination. The wavelength dependent response of our ZnTe NW based photodetector has been investigated under near IR to near UV illumination.

HL 69.7 Wed 16:00 Poster A

Analysis of the energy transfer process in ZnS:Mn and ZnS:Tb by a modified Förster model — •Sebastian Gies[1], Uwe Kaiser[1], Wolfram Heimbrodt[1], Sebastian Geburt[2], and Carsten Ronning[2] — [1]Dept. of Physics, Philipps-University Marburg, Germany — [2]Institute of Solid State Physics, Friedrich-Schiller University Jena, Germany

Zinc Sulphide nanowires doped with different luminescence centers, i.e. Manganese and Terbium, are characterized by means of time-resolved photoluminescence spectroscopy, in order to analyze the energy transfer process quantitatively. To achieve this, a modified Förster model is utilized, describing the energy transfer with respect to migration, quenching processes and dimensionality of the energy transfer.

To test the resilience and validity of the modified Förster model nanowires with doping concentrations from $4 \cdot 10^{-3}$% to 4% were manufactured. The luminescence of the internal $4f^8$- (Tb^{3+}) and $3d^5$-transitions (Mn^{2+}) was measured over four orders of magnitude. Furthermore, the measurements were performed at varying excitation densities and temperatures, leading to a deeper understanding of the energy transfer process and its description via the modified Förster model. We were able to determine the hitherto unknown Förster radius of Tb^{3+} ions. Moreover, using μ-photoluminescence we have performed measurements on single nanowires and compared the results with measurements on macroscopic numbers of wires. We found, that the decay characteristics of single wires resemble the ensemble measurements. The statistical reason will be discussed in detail.

HL 69.8 Wed 16:00 Poster A

Excitons in ZnCdSe/ZnSe quantum dots with parabolic confinement potential — •Tamar Tchelidze[1] and Irakli Noselidze[2] — [1]Iv. Javakhishvili Tbilisi State University , Faculty of Exact and Natural Sciences, 3 Chavchavadze Ave. 0179 Tbilsi, Georgia — [2]Rustaveli National Science Foundation , 1 Aleksidze st . Tbilsi, Georgia

Material distribution profile is found to have significant influence on emission properties of quantum structures. It was reported that core/shell ZnCdSe/ZnSe semiconductor nanocrystals individually exhibit continuous, non-blinking photoluminescence, which was explained by softening the abrupt confinement potential of a typical core/shell nanocrystal, suggesting that the structure is a radially graded alloy of CdZnSe into ZnSe(Xiaoyong Wang et al, Nature 459, 686-689, 2009). We present exact calculation of electronic states for spherical core*shell quantum dots with realistic boundary condition: inside the dot potential is taken equal to -ar2, outside the dot - zero. Calculations are carried out for ZnCdSe/ZnSe structure. We use single band effective mass approximation for finding single particle states of electrons and holes. Exciton states with corresponding energies are calculated by direct diagonalization of Hamilton matrix for 8 lowest excitonic states and their radiative decay probability in dependence of quantum dot radius are calculated. We found that for quantum dots with radius less than 8 nm there is no electron levels inside the dot. For this radius exciton binding energy is 56 meV.

HL 69.9 Wed 16:00 Poster A

Single crystals by vapor and solution growth of organic semiconductors — •Jan-Peter Bäcker, Natalija van Well, and Cornelius Krellner — Physikalisches Institut, Goethe-Universität Frankfurt, Deutschland

The growth and investigations of single crystals of small molecule organic semiconductors is of crucial importance for the deeper understanding of these materials. We apply both a horizontal vapor-growth technique as well as growth from solutions to fabricate mm-sized single crystals of Phenanthrene, Pentacene, and Dibenzopentacene. In this contribution, we present the optimized crystal growth parameters together with investigations of the structural properties.

Recently, it was found that in some of these materials superconductivity can emerge after intercalation with alkali-earth metals [1]. Therefore, these materials are promising with respect to their semiconducting as well as superconducting properties. Here, we show the results of our preliminary intercalation experiments on single crystals to investigate the crossover from semi- to superconducting behaviour.

[1] M. Xue et al., Scientific Reports 2, 389 (2012).

HL 69.10 Wed 16:00 Poster A

Surface functionalization and optical characterization of self-organized surface structures on sublimation grown polyaromatic single crystals — •Teresa Schmeiler[1], Stefan Thoms[1], and Jens Pflaum[1,2] — [1]Inst. Exp. Phys. VI, Julius-Maximilians-University of Würzburg, 97074 Würzburg — [2]ZAE Bayern e.V., 97074 Würzburg

Previously we presented different approaches, such as epitaxial growth or surface etching, to generate micrometer-sized 3D pyramidal surface structures on polyaromatic single crystals of rubrene and diphenylanthracene. By means of FDTD-simulations as well as photoluminescence measurements an enhanced luminescence emission at the lateral edges has been observed. Upon further optimization this could lead to cavity structures with defined optical properties. In this context, one of the major drawbacks are refection losses at the interfaces of these organic structures resulting in a significantly reduced quality factor Q. In this contribution we will discuss a possible solution to this problem by means of an additional metallic, e.g. gold, cover layer. Optical investigation revealed an enhanced emission at the pyramidal cone ends when covered by a 50 nm gold layer. Consequently, the influence of surface functionalization on the cavity quality factor as well as on the population density of optical states was investigated as a function of material and cover layer thickness. Complementary, the coated surface structures were analysed by AFM as well as SEM which showed a homogenous metallic surface coverage. Financial support by the DFG research unit FOR1809 is gratefully acknowledged.

HL 69.11 Wed 16:00 Poster A

Influence of the presence of residual gases during sample fabrication on the performance and lifetime of OLEDs — •Florian Wölzl[1], Ines Rabelo de Moraes[2], Björn Lüssem[1], Karl Leo[1], and Malte C. Gather[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Str. 1, 01062 Dresden, Germany — [2]Institut für Photonische Technologien Jena Albert-Einstein-Straße 9 07745 Jena

Due to their application potential in lighting and display technology, organic light emitting diodes (OLEDs) have been attracting considerable attention. However, the lifetime of these devices is still a bottleneck for a broad application of the technology. Revealing the degradation processes, especially the chemical degradation is of great interest. In particular the processing conditions, such as the amount of residual gases during the deposition of the materials might have considerable influence. To manipulate their partial pressures during evaporation, a needle valve was added to the processing chamber which can be connected to a nitrogen or oxygen gas bottle as well as to a water-filled gas-washing bottle. This allows us to intentionally contaminate the chamber with these gases. The devices are prepared under a base pressure of $5 \cdot 10^{-6}$ to 10^{-8} mbar. In this work we will focus separately on the influence of nitrogen oxygen and water during the OLED preparation on the performance and lifetime of a p-i-n OLED based on the stable red triplet emitter tris(1-phenylisoquinoline) iridium(III) ($Ir(piq)_3$). By LDI-TOF-MS technique, the chemical degradation processes of an electrically driven OLED are investigated.

HL 69.12 Wed 16:00 Poster A

Simulations of electronic states at grain boundaries in polycrystalline naphthalene — •Marko Mladenović, Nenad Vukmirović, and Igor Stanković — Scientific Computing Laboratory, Institute of Physics Belgrade, University of Belgrade, Serbia

One of the limiting factors for charge carrier transport in polycrystalline organic semiconductors based on small molecules are grain boundaries. We investigated the electronic structure of grain boundaries in polycrystailline organic semiconductor naphthalene. Energy of the system was modeled using TraPEE potential for the interaction between atoms. Atomic structure was obtained by a Monte Carlo method. Electronic structure was obtained using the Charge patching method (CPM) [1], which is based on Density Functional Theory (DFT).

Results for small systems (1000 molecules) indicate that grain boundaries produce trap energy states within the band gap of the material. These states are localized on molecule pairs (called trapping pairs) at the grain boundaries with the distance between molecules sig-

nificantly smaller than the distance between two adjacent molecules in a naphthalene crystal. Strong correlation between trapping pair mutual distance and trap state energy relative to the top of the valence band energy was found. As a consequence, on the basis of the densities of trapping pairs, densities of trap states for bigger systems (100 000 molecules) were calculated.

[1] N. Vukmirovic, L. Wang, J. Chem. Phys. 128, 121102 (2008)

HL 69.13 Wed 16:00 Poster A

Polarization-resolved absorption of perfluoropentacene — •Jan Kuhnert, Kolja Kolata, Tobias Breuer, Gregor Witte, and Sangam Chatterjee — Philipps-Universität Marburg

Organic semiconductors are promising materials for future electronic applications. A well investigated and prototypical organic semiconductor is the p-type pentacene (PEN). Crystalline PEN films exhibit a pronounced Davydov-splitting of the excitonic excitations owing to the herringbone arrangement of both molecules within the unit cell (adopting an angle of about 52°). Perfluorination yields an n-type semiconductor (perfluoropentacene, PFP) which also exhibits a herringbone packing in the crystalline phase but with almost orthogonal arrangement (91,2°) between both molecules. Using polarization-resolved absorption measurements we demonstrate the presence of a Davydov-splitting in crystalline PFP films that were epitaxially grown on NaF(100) substrates. Moreover, by employing micro-spot illumination single crystalline domains and their azimuthal dependent excitation were analyzed. Measurements were performed at room temperature and at 10K, and yield an energetic splitting of both Davydov components of 27meV. Azimuthal resolved measurements reveal that the transition dipole moment of the high energy component is maximal for polarization parallel to the b-axis; accordingly, the transition dipole of the low energy component is oriented along the c-axis. The experiments demonstrate a Davydov-splitting like behavior despite an almost orthogonal molecular packing in the unit cell where a degeneration of excitonic components is anticipated.

HL 69.14 Wed 16:00 Poster A

Optical Spectroscopy on planar ZnO/Pentacene Hybrids — •Ingo G. Meyenburg, Manuel Demper, Jonatan Helzel, Mira El Helou, Tobias Breuer, Gregor Witte, and Wolfram Heimbrodt — Philipps Universität Marburg department of physics and material sciences centre Germany, Renthof 5, D-35032 Marburg

In recent years organic semiconductors have attracted considerable attention because of their unique optical, electronic and mechanical properties. It has been shown, for example that inorganic organic hybrids like p-type Pentacene on ZnO are feasible to prepare p-n-junction. To study the excitonic properties of the organic layer we prepared pentacene films with thicknesses in the range between 10 nm and 100 nm on different ZnO surfaces by molecular beam deposition under ultra-high vacuum. By varying the growth temperature we obtain pentacene films in an amorphous, in the thin film and the Campbell phase which were characterized by AFM and X-ray diffraction measurements. Due to a formation of crystalline islands in the range of several micrometres in the non-amorphous phases we were able to study the absorption behavior of these single crystals by varying the temperature and the light polarization. In comparison to the pentacene molecules in solution the absorption spectra of the crystalline pentacene exhibit additional pronounced Davydov-splitted excitonic features with characteristic polarization dependence. A detailed discussion will be given of the exciton properties at the organic-inorganic interface in dependence on the crystallographic structure and the orientation of the ZnO surfaces.

HL 69.15 Wed 16:00 Poster A

Temperature dependent exciton diffusion length in organic solar cells — •Bernhard Siegmund, Johannes Widmer, Christian Körner, Debdutta Ray, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, Dresden, Germany

The photo-current of organic solar cells is the result of a multi-step process from the generation and diffusion of excitons to their separation into free charge carriers being then transported to the electrodes and extracted. In this work, the exciton diffusion length as function of temperature as well as a combined probability for charge carrier recombination and extraction are investigated in devices with a flat heterojunction between ZnPc and C60. To accomplish this, jV-characteristics of organic solar cells and the optical properties of the constituting single layers are studied at different temperatures in the range of 100 to 350K. Furthermore, the thickness of ZnPc is systematically varied from 7 to 70nm as well as the illumination intensity over two orders of magnitude to verify the obtained values. The results may lead to a better understanding of the temperature behaviour of organic solar cells.

HL 69.16 Wed 16:00 Poster A

Excitation of surface plasmon polaritons via prism coupling and metallic nanostructures for applications in organic solar cells — •Michael Mayr, Björn Gallheber, Mark Gruber, and Wolfgang Brütting — University of Augsburg, Germany

Organic photovoltaic cells based on diindenoperylene (DIP) exhibit high crystallinity in thin films resulting in long-range exciton transport and high charge carrier mobilities[1,2]. Due to nearly perpendicular orientation of the transition dipole moment with respect to the substrate, however, DIP exhibits only weak absorption for direct illumination, but tends to couple strongly to the near-field of surface plasmon polaritons (SPPs). Moreover, DIP provides a low lying HOMO and LUMO, which results in high open circuit voltages when using it as acceptor in combination with commonly used donor materials like oligo- or polythiophenes[3]. This makes DIP a promising candidate for using SPPs to increase the efficiency of organic solar cells. Due to the need for conservation of momentum and energy, light induced far-field excitation of SPPs at metal/dielectric medium interfaces is impossible. We use glass prisms and metallic nanostructures made by nanosphere lithography to overcome this problem, as they can manipulate the in-plane wave vector of incident photons to fulfill this condition. Particularly metallic nanostructures permit tuning of the excited SPPs by adjusting the size of the used nanospheres.

[1] J. Wagner et al. *Adv. Func. Mater.* **20**, 4295 (2010).
[2] D. Kurrle et al. *Appl. Phys. Lett.* **92**, 133306 (2008).
[3] U. Hörmann et al. *phys. stat. sol. RRL* **5**, 241 (2011).

HL 69.17 Wed 16:00 Poster A

Loss mechanisms in organic bulk heterojunction solar cells investigated by differential photocurrent density measurements — •Philipp Pelchmann[1], Simon Hein[1], Andreas Zusan[1], Vladimir Dyakonov[1,2], and Carsten Deibel[1] — [1]Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [2]Bavarian Centre for Applied Energy Research (ZAE Bayern e.V.), D-97074 Würzburg

Organic solar cells are interesting for contributing to the solution of the growing demand for renewable energy sources. One of the main problems is their lower efficiency compared to their inorganic counterparts. For its optimization, a fundamental understanding of the loss mechanisms, i.e. geminate and non-geminate recombination, is crucial. The non-geminate recombination, a function of light intensity under short-circuit conditions, can be investigated by differential photocurrent (DPC) measurements [1]. Therefor, the electrical response of a solar cell to a superposition of a continuous background light and a modulated low intensity light is determined. We measured the DPC signal for bulk heterojunction solar cells made from poly(3-hexylthiophene) (P3HT) blend with [6,6]-phenyl C61-butyric acid methyl ester (PCBM) with various active layer thicknesses. The results are discussed with regard to non-geminate recombination of free and trapped charge carriers.

[1] L. J. A. Koster et al., Adv. Mater., 23, 1670 (2011)

HL 69.18 Wed 16:00 Poster A

Hybrid Organic Photodetectors for Radiography — •Patric Büchele[1,2], Oliver Schmidt[2], Sandro Tedde[2], David Hartmann[2], Moses Richter[3], and Uli Lemmer[1] — [1]Light Technology Institute, Karlsruhe Institute of Technology. Karlsruhe, Germany — [2]Siemens AG. Corporate Technologies. Erlangen, Germany — [3]Institute for Materials for Electronics and Energy Technology, Friedrich-Alexander University. Erlangen, Germany

Most of todays x-ray detectors are using an indirect conversion mechanism. The x-ray radiation is converted into visible light within a thick scintillator layer. The visible light is then absorbed by standard thin-film photodetectors. The isotropic propagation of light in the scintillator reduces the resolution of the x-ray imager. This work avoids the stacked structure by integration of inorganic PbS quantum dots directly into the bulk hetero junction (BHJ) of an organic photodetector. X-ray photons are immediately converted into charge carriers and travel in direction of the electrical field towards the electrodes. However, this concept demands much thicker organic layers than known from conventional OLED and OPV processing. We demonstrate that thick diodes can be achieved with a spray coating process and the

influence of spraying parameters on device performance is discussed.

HL 69.19 Wed 16:00 Poster A

Investigation of carrier dynamics in Ga(As1-xBix)/GaAs heterostructures by time-resolved photoluminescence — •Dimitri Kalincev[1], Mohammad Khaled Shakfa[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

The ternary Ga(AsBi) semiconductor alloys have received considerable attention over the last decade due to their potential application in photonic and spintronic devices, especially in the near- and mid-infrared spectral range. Bi incorporation into GaAs leads to a great reduction in the band gap resulting from the giant band gap bowing effect. In our recent work, time-resolved photoluminescence (TR-PL) is used to investigate carrier dynamics of Ga(As1-xBix)/GaAs single quantum wells (SQWs) with different Bi contents. The TR-PL measurements are performed as function of excitation density and lattice temperature. The disorder effects and the presence of Bi clusters within the alloy structure are found to strongly influence the spectra and the dynamics.

HL 69.20 Wed 16:00 Poster A

The band alignment of the cuprous and cuprite oxide — •Benedikt Kramm, Philipp Hering, Daniel Reppin, Angelika Polity, and Bruno K. Meyer — 1. Physikalisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen

In recent work we showed the band alignment for the heterostructures of cuprous oxide, gallium nitride and zinc oxide. We found a conduction band offset (CBO) value of 0.97 eV for Cu_2O/ZnO and 0.24 eV for Cu_2O/GaN [1]. The low conduction band offset of Cu_2O/GaN making GaN a more suitable candidate for the front contact of Cu_2O based solar cells. Now we investigated heterostructures of CuO/GaN and CuO/Cu_2O. Details about the copper oxide thin films can be found here [2]. We analyzed the photoelectron characteristics of the heterostructures, on the surface and in the depth, and out of this we determined the band alignment of the copper oxide phases among each other and to gallium nitride and zinc oxide.

[1] B. Kramm et al., Appl. Phys. Lett. 100, 094102 (2012), DOI: 10.1063/1.3685719
[2] B.K. Meyer et al., Phys. Status Solidi B, 1-23 (2012), DOI: 10.1002/pssb.201248128

HL 69.21 Wed 16:00 Poster A

Exciton-polariton pseudospin in a planar ZnO based microcavity under external magnetic field — •Steffen Richter, Chris Sturm, Helena Franke, Rüdiger Schmidt-Grund, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig, Germany

Strong light-matter coupling between excitons and photons leads to the formation of exciton-polaritons. These quasi-particles inherit exciton spin orientation as well as light polarization. Both are expressed by the pseudospin of a polariton ensemble. The effect of magnetic fields on the pseudospin was studied experimentally and theoretically. External magnetic fields of 3T were applied in three spatial orientations while the polarization was measured in photoluminescence experiments. The experimental findings cannot be explained by a simple model consisting of pseudospin precession, spin-independent scattering and decay. For the total magnetic field, an effective field arising from linear polarization splitting was considered additionally to the external one.
The planar microcavity under study consists of a $\lambda/2$ layer of ZnO with a slight wedge shape. The complete Stokes vector of the lower polariton branch was determined under non-resonant excitation. For the probed detuning, an energetic splitting of about 20meV between the TE- and TM-polarized eigenmodes is found for an emission angle of 37°. Unexpectedly, the emission from these modes shows even without external magnetic field a fraction of ca. 5% circular polarization with different sign for the TE and TM mode, respectively.

HL 69.22 Wed 16:00 Poster A

Magneto thermopower measurements on rolled-up 2DESs — •Nils Gayer, Matthias Schmidt, Gunnar Schneider, David Sonnenberg, and Wolfgang Hansen — Institut für Angewandte Physik, Universität Hamburg

We present magneto thermopower and magnetotransport measurements on an evenly curved two-dimensional electron gas (2DEG). The 2DEG is confined in a rolled-up GaAs/AlGaAs high electron mobility heterostructure (HEMT) grown by molecular beam epitaxy. In a rolled-up 2DEG the perpendicular magnetic field component is sinusoidally modulated and the density of states changes along the roll. This arises because in a magnetic field the 2D electronic density of states condensates on the Landau levels (LL) and the filling of the LL depends on the strength of the magnetic field component perpendicular to the 2DEG. We rotate the rolled up structure in the magnetic field and show the dependence of the diagonal and the off-diagonal (Nernst-Ettingshausen) magneto thermopower on the rotation angle.

HL 69.23 Wed 16:00 Poster A

Investigation of light emitting indicators — •Lia Trapaidze[2], Ivane Beragchian[1], Ia Trapaidze[1], and Gela Goderdzishvili[1] — [1]Dep. of Physics, Georgian Technical University, 77 Kostava Ave. IV block, 0175, Tbilisi, Georgia — [2]Dep. of Physics, Tbilisi State Univeristy,3 Chavchavadze Ave., 0179 Tbilisi, Georgia

In the system of information represent and transmission, widely used, light emitting monolithic construction indicators with multi-elements. In our work we investigated: radiation diagrams of neighbor elements in multi-element indicators; dependence of emitting angle on the construction element, also we investigated influence of isolating protective thin films on the technology. We improved measurement method and created experimental equipment. By using our method, we can exactly determine expected parameters, optimally choose element construction and as well their technological method during planning process.

HL 70: Poster Session: Devices; Preparation and characterization; C/diamond; Si/Ge

Presenters are kindly asked to be near their posters at least 17:00–18:00 or to leave a note at the poster indicating a time period of availability for discussions. — Beverages will be served starting at 18:00.

Time: Wednesday 16:00–20:00 Location: Poster A

HL 70.1 Wed 16:00 Poster A

Solution processed doped zinc oxide field-effect transistors on flexible substrates — •Florian Mathies[1,2], Sebastian Hietzschold[1,2], Wolfgang Kowalsky[1,2,3], Uli Lemmer[4], and Norman Mechau[2,4] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Germany — [2]InnovationLab, Heidelberg, Germany — [3]Institut für Hochfrequenztechnik, Technische Universität Braunschweig, Germany — [4]Light Technology Institute, Karlsruhe Institute of Technology, Germany

In order to build efficient printed inorganic electronic devices, solution processable semiconductors and adequate fabrication techniques are required. Metal oxides have been considered a promising material because of their excellent electrical performance and stability, in addition to good solubility and printability. In this work, soluble zinc oxide precursor systems doped with aluminium or tin (AZO, ZTO) are used to fabricate field-effect transistors (FETs) in top- and bottom gate configuration. The bottom gate FETs are prepared on top of thermally oxidized doped silicon wafers. For the top gate configuration flexible glass-substrates with a polymer dielectric were used. The characteristics of the devices are found to be strongly affected by material- and process parameters which correlate to differences in the layer morphology and the charge carrier concentration.

HL 70.2 Wed 16:00 Poster A

Optimization of (Mg,Zn)O-based thin-film transistors with high-k WO_3 dielectric gates — •Anna Reinhardt, Michael Lorenz, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Semiconductor Physics Group

Recently, room-temperature deposited tungsten trioxide (WO_3) was demonstrated to be an advantageous high-k gate dielectric for transparent metal-insulator-semiconductor field-effect transistors (MISFETs) with large on/off-current ratios and low gate-voltage sweeps [1].

We present our results on the optimization of WO_3-gated thin-film transistors deposited on (Mg,Zn)O-channel material by pulsed-laser deposition. The gate dielectric thickness was varied in order to minimize the subthreshold slope and leakage currents. Furthermore, results on the reduction of the (Mg,Zn)O-channel thickness and its impact on the turn-on voltage will be presented. In combination with Pt as gate metal normally-off transistors were realized. In addition, we investigated the long-term stability of the transfer characteristics of unpassivated devices in comparison to passivated transistors.

[1] M. Lorenz *et al.*, Adv. Mater. **23**, 5383-5386 (2011)

[2] M. Lorenz, A. Reinhardt *et al.*, Appl. Phys. Lett. **101**, 183502 (2012)

HL 70.3 Wed 16:00 Poster A

Comparison of ZnO-based JFETs, MESFETs and MISFETs — •Fabian J. Klüpfel, Friedrich L. Schein, Michael Lorenz, Heiko Frenzel, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Fakultät für Physik und Geowissenschaften, Linnéstr. 5, 04103 Leipzig

We compare the device characteristics of field-effect transistors (FETs) based on ZnO. From the same ZnO thin film, junction FETs with $ZnCo_2O_4$-based gates, metal-semiconductor FETs with reactively sputtered Pt Schottky contacts and metal-insulator-semiconductor FETs with WO_3 as gate insulator were fabricated. By using a common thin film for the channel, the influence of the different gate architectures on the device performance can be distinguished from other fabrication-induced factors. Similar operation voltages for all FET types support the comparability of the devices. The transistors were characterized electrically by dc measurements at room and elevated temperatures and by frequency-dependent measurements. It was found, that the transfer curves of all devices exhibit a shift towards positive gate voltages with increasing temperature. This is in contrast to other semiconductors, e.g. InGaZnO or a-Si, and is attributed to the ZnO channel material. Several differences in the device characteristics were observed, which make the device types suitable for different fields of application.

HL 70.4 Wed 16:00 Poster A

Transparent, highly rectifying p-CuI/n-ZnO heterojunctions — •Friedrich-Leonhard Schein, Holger von Wenckstern, and Marius Grundmann — Institut für Experimentelle Physik II, Abt. Halbleiterphysik, Universität Leipzig, Germany

We investigated the wide bandgap ($E_g = 3.01$ eV [1]) p-type semiconductor γ-copper(I)-iodide (CuI) [2] as an alternative candidate to p-type transparent semiconducting oxides like SnO [3] or $ZnCo_2O_4$ [4]. Our method to transform dc-sputtered Cu into CuI is easy to handle and uses temperatures below 120 °C. Hall-effect measurements of these CuI films on glass substrates revealed a hole mobility of about $6\,cm^2/Vs$, a hole density of $5 \times 10^{18}\,cm^{-3}$ and a resistivity of $0.2\,\Omega$cm. Atomic force microscopy and optical transmission measurements will be discussed.

Heterostructures consisting of p-CuI and pulsed-laser deposited n-ZnO were fabricated on a-sapphire substrates and characterized electrically. The diodes showed rectification ratios $I_{on}/I_{off} > 10^7$ at ± 2 V. Capacitance-voltage and temperature-dependent current-voltage measurements were analyzed to obtain a clear understanding of the diode characteristics.

[1] B.-L. Zhu and X. Z. Zhao, Phys. Status Solidi A **208**, 91 (2011).

[2] K. Bädeker, Annalen der Physik textbf327, 749 (1907)

[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 70.5 Wed 16:00 Poster A

Synthesis of single crystalline Cu2O nanowires for electrochemically-gated PMOS transistors — Suneeti Purohit[1], •Anna Stösser[1], Robert Kruk[1], Subho Dasgupta[1], and Horst Hahn[1,2] — [1]INT, Karlsruhe Institute of Technology, D-76344 Eggenstein-Leopoldshafen, — [2]Joint Research Laboratory Nanomaterials, TU Darmstadt, Petersenstr. 32, D-64287 Darmstadt

One-dimensional nanomaterials such as nanorods or nanowires (NWs) are very attractive for various nanoelectronic devices. Cuprous oxide (Cu2O), a well-known p-type semiconductor with a band gap of 2 eV, has cubic crystal structure and is a very good candidate for conversion of solar energy into electrical or chemical energy; optoelectronic or light-emitting devices and as well as for catalysis. We present a low-cost, large scale solution-phase synthesis of single crystalline cuprous oxide NWs that shows very high aspect ratio. Synthesis has been done with hydrothermal treatment of Cu(Ac)2 and pyrrole at 250°C for 5hr. The powder X-ray diffraction (XRD) confirms cubic cuprite structure. Scanning electron microscopy (SEM) images show smooth and straight NWs with minimal surface roughness. The length of most Cu2O NWs exceeds 100 *m, while the diameter varies between 100-150 nm. Fourier transformed infrared spectroscopy (FTIR) and High resolution transmission electron microscopy (HRTEM) has also been performed. Subsequently, the NWs are harvested and used to build low voltage operated, single-nanowire transistors that are gated with composite solid polymer electrolytes; detailed transistor characteristics will also be presented.

HL 70.6 Wed 16:00 Poster A

Narrow bandwidth ultraviolet photodetectors based on wide band gap semiconductors — •Zhipeng Zhang, Friedrich-Leonhard Schein, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Fakultät für Physik und Geowissenschaften, Institut für Experimentelle Physik II, Linnéstraße 5, 04103, Leipzig

The integration of an optical filter layer allows fabrication of wavelength-selective, visible-blind ultraviolet photodetectors (PDs) based on (Mg,Zn)O-heterostructure being only sensitive in a defined, narrow spectral range [1]. Up to now, this was accomplished by growing the active layer of a backside detector on top of a buffer layer having a slightly higher band gap. In this contribution we demonstrate the potential of a novel device layout allowing to achieve much narrower bandwidth by the decoupling of the optical filter and the active layer. Within this approach interdiffusion between the layers is avoided and carriers generated in the filter layer will not contribute to the photocurrent. The achieved bandwidth of this kind at 3.4 eV was 12 meV smaller than that of the previous design.

Furthermore, the properties of a p-$ZnCo_2O_4$/n-ZnO heterojunction [2] under illumination were investigated. This bipolar diode can be used as PD similar to the PDs described above. Additionally, such pn-junction can be used as visible-blind solar cells. A first wavelength selective PD with a bandwidth of 60 meV was realized.

[1]: Z. Zhang et al., Appl. Phys. Lett. **99**, 083502 (2011)

[2]: F-L. Schein et al., IEEE Electron Device Lett. **33**, 676 (2012)

HL 70.7 Wed 16:00 Poster A

Two-photon quantum well infrared photodetectors in the THz regime — •Carsten Franke[1], Harald Schneider[1], and Martin Walther[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf — [2]Fraunhofer IAF Freiburg

Two-photon quantum well infrared photodetectors (QWIPs) are interesting nonlinear devices for autocorrelation measurements in the mid-infrared and THz-regime. Here, we present first results on two-photon THz-QWIPs with intersubband transition frequencies below 7 THz, based on the GaAs/AlGaAs material system with an aluminium content of 5% and below. We performed dark current measurements and observed large current discontinuities which can be attributed to impact ionisation. We also present photocurrent spectra which show, in addition to the expected intersubband transitions, evidence of further signatures related to optical-phonons.

HL 70.8 Wed 16:00 Poster A

Construction of a heterodyne nearfield optical microscope — •Jan Siebels, Jens Ehlermann, Lena Simone Fohrmann, and Stefan Mendach — University of Hamburg, Germany

Here we describe the technical realization of a phase-resolved scanning near field optical microscope. In general, the frequency of visible light oscillating between 384 THz and 789 THz is too fast to be detected directly with today*s electronics. In order to obtain information about the phase of light one can utilize heterodyne detection. In combination with a near field scanning optical microscope it is possible to directly

detect the amplitude and phase of near field distribution on sample surfaces [1][2]. . The near-field microscopeis placed in one branch of a Mach-Zehnder like interferometer. The frequency of the laser beams within the two branches, i.e. reference and signal beam, is slightly shifted via acousto-optic modulators. As a result, the interference of the beams results in beating pattern which is demodulated with a Lock-in amplifier to retrieve amplitude and phase of the SNOM signal.

We gratefully acknowledge financial support of the Deutsche Forschungsgemeinschaft via the Graduiertenkolleg 1286.

[1] M.L.M. Balistreri, J. Korterik, K. Kuipers, and N. van Hulst, Phys. Rev. Lett. 85, 294 (2000)

[2] A. Nesci, R. Dändliker, and H.P. Herzig Optics Letters, Vol. 26, Issue 4, pp. 208-210 (2001)

HL 70.9 Wed 16:00 Poster A

Production and characterization of ZnO nanorods from various precursors for single- and multi-rod transistors — •Falk von Seggern[1,2], Subho Dasgupta[1], Robert Kruk[1], and Horst Hahn[1,2] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [2]TU Darmstadt and KIT Joint Research Laboratory Nanomaterials, , Petersenstr. 32, 64287 Darmstadt, Germany

There is still a large research interest for ZnO for many applications due to its relatively wide band gap (3.37 eV), its transparency, its high carrier mobility, the easy production and non-toxicity. We present different routes for bulk synthesis (in the gram range) of ZnO nanorods, which are later used for single, as well as multi-nanorod transistor fabrication. Starting from different precursors we vary the process parameters systematically in order to obtain nanorods in bulk amounts and with an optimum morphology for the field-effect device fabrication. Structural characterizations are performed on as-grown nanorods using XRD, SEM and EDX techniques. Initially, devices have been made by structuring with e-beam lithography (in order to define the passive structures) and tested for transistor characteristics thereafter. Further work is in progress to fabricate completely solution processed single or multi nanorod field-effect devices.

HL 70.10 Wed 16:00 Poster A

strain and temperature evaluation of electro-thermal actuators using raman spectroscopy — •pramodh srinivasa[1], evgeniya sheremet[1], raul rodriguez[1], alexey shaporin[2], ovidiu gordan[1], gianina schondelmaier[3], and dietrich zahn[1] — [1]Semiconductor Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]Microsystems and Precision Engineering, Chemnitz University of Technology, Chemnitz, Germany — [3]Materials and Reliability of Micro-Technical Systems, Chemnitz University of Technology,Chemnitz, Germany

Strain and temperature changes in Micro-Electro-Mechanical Systems devices are key factors to determine the performance and reliability. Movable parts are the main components of MEMS actuators responsible for sensing and actuating. Upon applying a potential to the actuator,resulting current flow heats up the comb structures leading to strain and temperature effects in turn making them move and elongate. Optical techniques are adopted for quantifying strain and temperature in comparison to other techniques, as they are highly accurate, non-destructive, and non-invasive. Micro-Raman Spectroscopy is used in this work to estimate the temperature and localized strain based on the analysis of the shift in the position of the optical phonon. The excitation wavelength used is 632nm(HeNe laser)with a spectral resolution of 0.23cm-1. We report the characterization of electro-thermal actuators in idle and working conditions under different external temperature and potentials.Spatially resolved temperature and stress maps of different components of the device are discussed.

HL 70.11 Wed 16:00 Poster A

Simulated annealing of nanodiamonds in vaccum, oxygen and water vapor — •Moloud Kaviani, Peter Deák, Bálint Aradi, and Thomas Frauenheim — BCCMS University of Bremen TAB Building, Entrance 1 A, Level 3 The case of Tower 1 28359 Bremen

Biocompatible luminescent nanodiamonds (ND) have received considerable attention as markers in biophysics and nanomedicine. For these applications NDs should be produced as small as possible. Transmission electron microscopy studies have shown that NDs are polyhedra with a diamond core, partly covered by a shell of graphitic or amorphous carbon. Our goal is to estimate how small can NDs be to preserve the diamond core at elevated temperatures under various ambient conditions: in vacuum, in oxygen, and water vapor. We investigate the stability of diamond nanoparticles upon annealing as a function of the size and shape, with the help of molecular dynamics (MD) simulations, using the self-consistent density functional based tight-binding method (SCC-DFTB). Simulated isochronal annealing was carried out at 500K, 1000K, 1500K for 30ps with a linear ramp between the stages (for 10ps).The diamond core of cuboid and cuboctahedral clusters with as like as ~250 atoms survives such short anneals. As accelerated MD at 5000K, as well as tests at 1500K for 250 ps indicate that they are likely to survive also longer annealing times. The primary effect of oxygen seems to be saturated threefold-coordinated surface carbon atoms and the etching of coordinated ones.The application process becomes somewhat quicker and stronger but about a ~250 atom cluster still retains its diamond core in the longer run.

HL 70.12 Wed 16:00 Poster A

Determination of the Depth of Shallow Implanted NV Centers in Diamond by Confocal Microscopy and Statistics — •Andreas Häussler, Pascal Heller, 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 magnetic sensing in solid state. However, to measure a magnetic field outside of the diamond, the NV probe has to be positioned close to the point of interest, i.e. near the surface of the diamond. For the sake of good sensitivity and precision, knowing the exact depth of a NV center below the surface is crucial.

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. A 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 70.13 Wed 16:00 Poster A

Influence of surface treatment on NV centers in diamond — •Lina Elbers[1], Aniela Scheffzyk[1], Daniel Laumann[1], Christian Klump[1], Sani Noor[1], Sébastien Pezzagna[2], Jan Meijer[2], and Ulrich Köhler[1] — [1]Experimentalphysik IV, AG Oberflächen, Ruhr-Universität Bochum — [2]RUBION, Ruhr-Universität Bochum

Color centers in diamond especially NV centers are practical single photon emitters due to RT operations and candidates for applications in quantum computing. The implantation of NV centers near the surface for a possible electrical addressing is still a problem. Therefore, we survey the influence of different surface and bulk treatments on the diamond and the 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 intensity of their luminescence could be reduced down to $\frac{1}{8}$. In one set of the experiments we deposited silicon on the diamond to test the influence on the luminescence spectra and the charge states. The spectra show that the Si only influences the overall intensities. The H-termination in contrast seems to be practical for the manipulation of the charge state. Hence the diamond surface was treated by an H_2 plasma under varying parameters until the diamond becomes conductive. HREELS and AFM measurements were made to test the surface after the plasma treatment. The influence of an Al_2O_3 passivation layer that was deposited by sputtering on the conductivity was investigated. Additionally, a UHV chamber is modified to implant directly under UHV conditions and to allow in situ spectroscopic access to the diamond samples.

HL 70.14 Wed 16:00 Poster A

Microwave Driven Nanoscopic Resolution of Two Neighbour Single NV Centres in Diamond: Micro-(wave)-scopy (MWS) — •Andreas Häussler[1], Luca Marseglia[1], Florian Striebel[1], Manfred Bürzele[1], Ressa Said[2], Pascal Heller[1], Philip Hemmer[3], and Fedor Jelezko[1] — [1]Institut für Quantenoptik, Universität Ulm, Germany — [2]Institut für Quanteninformationsverarbeitung, Universität Ulm, Germany — [3]Electrical and Computer Engineering, Texas A&M University, College Station, TX 77843, USA

The negatively charged Nitrogen Vacancy color center (NV) is a spin active defect in diamond with a long spin lifetime at room temperature. We aim to resolve two different NV centres separated by a distance in nanoscopic regime by exploiting Rabi oscillations of the spin of the NV centre which show a spatial dependence due to applied microwave fields. Therefore we fabricate a microwave circuit on the diamond, which will allow us to apply different high intensity microwave fields

and gradients. Finally the relation between the Rabi oscillations and the microwave field of two NV centres close to each other can be used in order to compute the distance between them, with a resolution below 50 nm.

HL 70.15 Wed 16:00 Poster A

Entanglement of a pair of two nitrogen-vacancy centers — •Christian Osterkamp[1], Christoph Müller[1], Liam McGuinness[1], Takashi Yamamoto[2], Boris Naydenov[1], and Fedor Jelezko[1] — [1]Institut für Quantenoptik, Universität Ulm, Germany — [2]Japan Atomic Energy Agency, 1233 Watanuki-machi, Takasaki, Gunma, 370-1292, Japan

Entanglement is the most counter-intuitive state in the quantum mechanics and it is the main part of the most quantum information protocols. Entangled states can be also used to enhance magnetic field sensitivity. Here we report on experiments towards the creation of entanglement between two single electron spins associated to nitrogen-vacancy defect centers in diamond (NV). The NV is a very promising system as a solid state qubit as well as a nano-scale magnetic field sensor. The fluorescence of single NVs can be detected and its electron spin can be polarized, read-out and manipulated at ambient conditions. We produced a pair of coupled single NV centers by using nitrogen ion implantation in 12C enriched ultra pure single crystalline diamond. Both NVs show long electron spin coherence time T2 ~ 1 ms and a magnetic dipolar coupling of 55 kHz, corresponding to 13 nm distance between the spins. Using this system we will be able to create a variety of entangled states with reasonable fidelity.

HL 70.16 Wed 16:00 Poster A

Temperature and gate dependent electrical characterization of carbon nanotube networks — •Fabian Fritz[1,2], Michael Schnee[1,2], Marlou Slot[1,2], Robert Frielinghaus[1,2], Claus M. Schneider[1,2], and Carola Meyer[1,2] — [1]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA – Fundamentals of Future Information Technologies

Carbon nanotubes (CNTs) show outstanding electronic properties and therefore they are a promising material for future nanoelectronic applications. Their electrical transport behavior depends on the environment. Here, we investigate the influence of gate dielectrics and chemical functionalization on the transport properties of carbon nanotube networks.

Networks of single-walled CNTs of different densities are grown by means of chemical vapor deposition. The structure of the networks is characterized by atomic force microscopy and scanning electron microscopy. Electrical measurements have been conducted at room temperature and down to 4 K in a helium flow cryostat.

At low temperature, the networks show clear non-ohmic current-voltage characteristics, which is interpreted within the framework of two-dimensional variable range hopping. The influence of oxidation on the transport through the networks is investigated, since this is the first step for a chemical functionalization based on ligand exchange reaction. First results of magneto-transport measurements on chemically functionalized CNTs as well as gate dependent transport measurements are presented.

HL 70.17 Wed 16:00 Poster A

Carbon Nanotube spectroscopy in optical microcavities — •Thomas Hümmer[1,2], Hanno Kaupp[1,2], Matthias S. Hofmann[1], Jonathan Noe[1], Alexander Högele[1], Theodor W. Hänsch[1,2], and David Hunger[1,2] — [1]Ludwig-Maximilians-Universität München, Deutschland — [2]Max-Planck Institut für Quantenoptik, Garching, Deutschland

We use fiber-based Fabry-Perot optical microcavities [1] with mode volumes down to a few tens of wavelengths cubed and high quality factors up to 10^7 to study single-walled carbon nanotubes (SWCNTs). Very recent progress in the growth of freestanding narrow-diameter SWCNTs has demonstrated that this system can show exceptional fluorescence properties, including a strong optical dipole transition, single photon emission characteristics, and close to Fourier limited linewidth [2]. Placing nanotubes inside an optical microcavity promises ultimative sensitivity for absorption spectroscopy and strong Purcell enhancement of fluorescence emission. Harnessing the full tunability and open access of fiber-based microcavities allows us to address a variety of CNTs at different locations and wavelengths with a single cavity. We show first experimental results on cavity enhanced spectroscopy of individual SWCNTs and discuss the potential for cavity QED with this system.

[1] Hunger, Reichel *et al.*, NJP **12**, 065038 (2010)
[2] Hofmann, Högele *et al.*, arXiv: 1209.3429 (2012)

HL 70.18 Wed 16:00 Poster A

Ab-initio study of metal-decorated carbon nanotubes for interconnect and sensor applications — •Florian Fuchs[1], Christian Wagner[1], and Jörg Schuster[2] — [1]Center for Microtechnologies, Chemnitz University of Technology, Chemnitz, Germany — [2]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany

Carbon nanotubes (CNTs) are promising candidates for novel applications in various technical fields. They are discussed as metallization layers in interconnect systems, thanks to their extraordinary electronical properties. Furthermore, the electromechanical sensitivity of CNTs can be used to construct new sensors. For all these various application fields, CNTs with suitable properties are required. Still, producing them in high purity is a challange and multiple approaches are being considered. One of the possibilities is to functionalize the CNTs in order to adjust their electronical properties.

We present the results of an ab-initio study of metal-decorated single walled CNTs (SWCNTs) based on density functional theory. The influence of different metals adsorbed on a semiconducting SWCNT are investigated and compared. We demonstrate that the decoration significantly changes the properties and that the choice of the metal is essential. Furthermore, the decorated SWCNTs are strained to judge their applicability for sensors. It is shown, that the electromechanical properties of SWCNTs are conserved and that the metal decoration can therefore be used to control the properties of SWCNTs for future sensors as well as for interconnect applications.

HL 70.19 Wed 16:00 Poster A

Untersuchungen zur Absorption von Thz-Strahlung durch einwandige Kohlenstoffnanoröhren — •Frieder Ostermaier[1], Hans-Georg von Ribbeck[2], Michael Mertig[1] und Lukas Eng[2] — [1]TU Dresden, Professur für Physikalische Chemie, Mess- und Sensortechnik, 01062 Dresden, Germany — [2]TU Dresden, Institut für Angewandte Photophysik, 01062 Dresden, Germany

Einwandige Kohlenstoffnanoröhren (SWCNT) kann man sich als Hohlzylinder vorstellen, die durch das Aufrollen von Graphen entstanden sind. Je nach Richtung des Aufrollens kommt es zu Änderungen in der Bandstruktur im Vergleich zum halbmetallischen Graphen. Die Bandlücken sind z.T. sehr klein und weisen daher Absorptionsbanden im THz-Wellenlängenbereich auf, was sich ideal für sensorische Anwendungen im tiefen Infrarot anbietet. Bisherige Studien haben stets Netzwerke von SWCNT zur Messung der Absorption verwendet. Dabei findet eine Mittelung über viele SWCNT statt.

Um die Absorption im THz-Wellenlängenbereich an einzelnen SWCNT zu messen, wurden mit Hilfe der Dielektrophorese SWCNT zwischen Elektroden abgelegt, so dass Stränge aus einzelnen SWCNT entstanden. Zur Vermessung der Absorption wurde ein streuendes optisches Nahfeldmikroskop verwendet, welches den durchstimmbaren Freie-Elektronen Laser am Helmholtz-Forschungszentrum Dresden-Rossendorf als THz-Strahlungsquelle einsetzt.

Die Messungen legen eine selektive Absorption nahe. Kleine Bündel von SWCNT zeigen zudem eine höhere Absorption. Die Messungen fanden dabei an der Grenze des Signal-Rauschabstandes statt.

HL 70.20 Wed 16:00 Poster A

Thermoelectric measurements of strained silicon using electrical and optical methods — •Jiehong Jin, Markus Hagedorn, Beata Kardynal, Stephan Wirths, Dan Mihai Buca, Detlev Grützmacher, and Toma Stoica — Peter Grünberg Institut (PGI-9), Jülich-Aachen Research Alliance (JARA), Forschungszentrum Jülich, 52425 Jülich, Germany

Semiconductor nanowires (NWs) have been shown to greatly suppress phonon heat conduction without a significant decrease in the Seebeck coefficient or electrical conductivity. Variety of methods can be used for structure fabrication. Irrespective of the fabrication process the specific geometry of NWs renders the heat transport measurements difficult. In this work, NWs of strained silicon on insulator (SSOI) were defined using e-beam lithography with metallic lines for local heaters and thermoelectric contacts. Two different methods of measuring temperature along the NWs are compared. We measured the temperature as resistance change of the thin metal lines in contact with the NWs. We also used the temperature dependence of the Si-Si Raman vibration mode to measure the NWs temperature. Both techniques can be used as accurate thermometers. However, optical readout using micro-

Raman scattering proved to be more flexible. Using this technique, the temperature change along the NWs can be monitored with a resolution of the order of laser wavelength. Importantly, since the Raman peaks of the strained Si NWs and the substrate are clearly separated, the parasitic heat transport into the substrate can be evaluated.

HL 70.21 Wed 16:00 Poster A

BCS-type condensate in the electron-hole plasma of silicon — •Dietrich Schneider, Dirk Semkat, and Heinrich Stolz — University of Rostock

Quantum condensation phenomena in highly excited semiconductors comprise, besides the Bose-Einstein condensate of excitons, also a BCS-type condensate of weakly correlated electron-hole pairs at very low temperatures and high densities, where excitons can no longer exist. The key quantity of the BCS condensate is the so-called gap function. We present theoretical results for this quantity based on a recent approach. The gap function modifies the single-particle spectrum of the carriers. These modifications are transformed in the usual way into alterations of the high-energy tail of the electron-hole pair luminescence spectrum. Therefore, the occurrence of BCS condensed electron-hole pairs, i.e., a nonzero gap function, should manifest itself in the luminescence spectrum. We present first experiments where the electron-hole plasma in silicon is captured in a stress-induced potential trap at temperatures below 100 mK. Results for the measured spectra are shown and compared to the theoretical predictions.

HL 70.22 Wed 16:00 Poster A

Analysis of the fabrication process of x-ray waveguides — •Sarah Hoffmann, Henrike Neubauer, Mike Kanbach, and Tim Salditt — Institut für Röntgenphysik, Universität Göttingen

Small sized x-ray sources as provided by x-ray waveguide channels are required for a multitude of applications such as high resolution spectroscopy, diffraction, microscopy and holography [1,2]. We report on a processing scheme which among other techniques involves e-beam lithography, reactive ion etching and Silicon wafer bonding [3], allowing for the fabrication of sub-100 nm sized waveguide channels [4]. Both waveguide geometry and material can be adapted to meet the requirements of a specific experiment, such as the x-ray energy (7.9-17.5 keV) or the desired source size, or the application of a reference beam in a holography setup. As the tunability of the optical properties provided by the waveguide, as the coherence of the beam, its divergence or the waveguide transmission, depends sensitively on the precise control over the several processing steps, an iterative process of diagnostics and optimization is essential. Thereby, the surface roughness of the channel walls could be identified as a key parameter in fabrication of high transmission x-ray waveguides. To study this attribute in detail, complementary methods like AFM, SEM and ellipsometry are employed in addition to x-ray analysis both at synchrotron and lab sources.

[1] A. Jarre et al., Phys. Rev. Lett. 94, 074801 (2005)
[2] C. Krywka et al., J. Appl. Cryst. 45, 85*92 (2012)
[3] A. Kohlstedt et al., Appl. Phys. A 91, 6*12 (2008)
[4] H. Neubauer et al., in preparation

HL 71: Exciton polaritons and their condensates (HL, jointly with TT)

Time: Thursday 9:30–12:15 Location: H2

HL 71.1 Thu 9:30 H2

Polariton lasing in III-nitride based microcavities: How far are we from the Mott-transition? — •Georg Rossbach, Jacques Levrat, Etienne Giraud, Eric Feltin, Jean-Francois Carlin, Raphael Butte, and Nicolas Grandjean — ICMP, Ecole Polytechnique Fdérale de Lausanne, 1015 Lausanne, Switzerland

Non-equilibrium polariton condensates producing a coherent light source referred to as polariton laser have attracted a lot of interest as they should allow the realization of ultralow threshold coherent light-emitting devices due to the release of the population inversion condition. Polariton lasing under ambient conditions was demonstrated for the first time in a III-nitrid based microcavity, where the increased exciton stability and oscillator strength facilitate the strong coupling regime even for high carrier injection. Nevertheless, the generally observed emission energy blueshift toward the polariton lasing threshold indicates a significant altering of the light-matter coupling with increasing carrier density. Such non-linearities arise from the interacting excitonic fraction of cavity-polaritons.

Based on the investigation of the Mott-transition occurring in GaN/AlGaN single quantum wells and the microcavity bare active medium by means of non-resonant photoluminescence, the impact of the exciton renormalization on the polariton branch dispersion is discussed. Contrary to the usually assumed picture the exciton energy shift is shown to play a negligible role, while saturation effects emerging from phase space filling and exchange interaction govern the polariton renormalization already far below threshold.

HL 71.2 Thu 9:45 H2

Weak periodic modulation of exciton-polariton condensates — •Edgar Cerda-Mendez[1], Dipankar Sarkar[2], Klaus Biermann[1], Dmitry Krizhanovski[2], Maurice Skolnick[2], and Paulo Santos[1] — [1]Paul Drude Institut for Solid State Physics, Berlin, Germany — [2]Department of Physics and Astronomy, University of Sheffield, Sheffield, United Kingdom

Macroscopic quantum behavior manifest when bosonic particles undergo a phase transition to a condensate state described by a single quantum wavefunction. Such behavior also occurs in microcavities containing quantum wells (QWs), where quasiparticles called polaritons arise from the strong coupling of photons and the QW excitons. In this work, we study the properties of polariton condensates in a shallow square lattice created via acoustic modulation. We demonstrate the formation of an extended state with negative effective mass at the corners (i.e. M-points) of the square lattice mini-Brillouin Zone. Also, optical threshold intensities for condensation are reduced, which is attributed to the lower density of states at the M-points and to the negative effective mass which compensates polariton drift induced by repulsive interactions. Both effects may allow to reach the critical density for condensation more efficiently than at the center of the MBZ (i.e. the Γ point). Finally, the momentum spread of the M-point states is independent from the area covered by the MCP, showing that the wavefunction of the MCP has a self-induced intrinsic coherence length. This work opens the way for investigation of polariton quantum phases such as a Bose Glass, Mott insulator or bright gap solitons.

HL 71.3 Thu 10:00 H2

Coherent Propagation of blue Polaritons in Cu_2O — •Johannes Schmutzler, Dietmar Fröhlich, and Manfred Bayer — Experimentelle Physik 2, Technische Universität Dortmund, D-44221 Dortmund, Germany

The lowest excitons in Cu_2O are intensively studied as they are considered as candidates for Bose-Einstein Condensation. The excitons of the so-called yellow and green series are of even parity and thus only quadrupole allowed. There are, however, two other series of excitons (blue and violet series) which are dipole allowed and should thus exhibit a pronounced polariton structure.

Despite the fact that Cu_2O has inversion symmetry we report sum-frequency generation of blue exciton polaritons. This is possible since in our case the SFG is of quadrupole-dipole type. Typically the observation of non-linear effects requires power levels in the kW to MW range, necessitating pulsed laser sources. Here, we achieve strong sum-frequency (SF) signals far above the bandgap by spectrally narrow excitation of two exciton-polariton resonances in Cu_2O with two continuous wave lasers in the mW to W power range.

In the case of an antiparallel laser beam configuration pronounced oscillations of the SF-signal can be observed. We attribute these oscillations to a phase matching effect. This observation is rather surprising since the absorption length in one-photon absorption is in the range of 150 nm [1]. The occurrence of oscillations clearly indicates the creation of coherent exciton-polaritons, the damping of which is suppressed.

[1] S. Brahms et al., Physics Letters. 21, 31 (1966)

HL 71.4 Thu 10:15 H2

Polariton condensates in GaAs-based microcavities: influence of the spot size — •Matthias Salewski[1], Marc Assmann[1], Jean-Sebastian Tempel[1], Franziska Veit[1], Sven Höfling[2], Martin Kamp[2], Alfred Forchel[2], and Manfred Bayer[1] —

[1]Experimentelle Physik 2, Technische Universität Dortmund, 44221 Dortmund — [2]Technische Physik, Physikalisches Institut, Universität Würzburg, 97074 Würzburg

Microcavity-polaritons consist of excitons strongly coupled to the photon field of the cavity. Photons leaking out of the cavity show the same energy-momentum dispersion as the polariton, which allows for easy experimental accessibility of the polariton states. It has been shown, that microcavity polaritons are able to undergo Bose-Einstein condensation.

Here, we investigated the influence of the excitation-spot size on the threshold carrier density necessary to create polariton condensates in a GaAs-based quantum-well microcavity. Different cavity-exciton detunings were examined.

By measuring the far-field emission of the cavity, we mapped the polariton dispersion relation as a function of the excitation power. Carriers were created by two excitation spots of different sizes. First, the intensity of the larger spot was varied. Second, while keeping the intensity of the larger spot fixed, the intensity of the second, much smaller spot was increased in the sub-milliwatt range. This way, we could measure the excitation efficiency of different spot sizes. Different results are observed for various detunings.

HL 71.5 Thu 10:30 H2

Optically and structurally trapped exciton-polariton systems — •Tom Michalsky, Helena Franke, Chris Sturm, Rüdiger Schmidt-Grund, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstraße 5, 04103 Leipzig

The formation and properties of exciton-polaritons in microcavities (MCs) have been intensively investigated in the last years, since they can undergo a Bose-Einstein condensation (BEC). In this work we present the investigation of the momentum and spatial distribution of polaritons in the uncondensed as well as in the condensed phase for planar ZnO-based MCs with a wedge-shaped cavity layer and also in mesa structures. In the mesa structures we found an enhancement of the trapping as a result of the reduced potential energy therein. For MCs without mesa structures we demonstrate the manipulation of propagation of condensed polaritons. It turns out that for small negative detuning values the condensate is trapped by the excitation laser spot whereas for larger negative detunings an acceleration of the polaritons out of the pumping region accompanied by ballistic propagation [1] is observed.

[1] M. Wouters, I. Carusotto and C. Ciuti, Phys. Rev. B **77**, 115340 (2008)

Coffee break

HL 71.6 Thu 11:00 H2

Influence of disorder on the propagation of polariton BEC — •Martin Thunert[1], Helena Franke[1], Chris Sturm[1], Rüdiger Schmidt-Grund[1], Alexander Janot[2], Bernd Rosenow[2], and Marius Grundmann[1] — [1]Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig — [2]Universität Leipzig, Institut für Theoretische Physik, Brüderstr. 16, 04103 Leipzig

We report on the influence of disorder effects on the propagation of exciton-polariton Bose-Einstein condensates (BEC) in a ZnO-based bulk planar microcavity (MC). Due to their composite nature, the spatial distribution is affected by electronic (inhomogeneous carrier distribution) as well as photonic (thickness fluctuations, rough interfaces) disorder. The energy(E)-k-space emission patterns of the condensate show in dependence on temperature (T) and detuning (Δ) two different regimes: 1) ballistic polariton propagation for low (T,Δ) values and 2) disorder effects for increasing (T,Δ) values, which are reflected by a fragmentation of the (E,k) emission patterns. This can be explained by interference of localized condensates or by propagating condensates with different discrete velocities determined by scattering events at the disorder potential. For each (T,Δ) parameter set increasing pump power causes an increase of the fragmentation parameter which is deduced quantitatively from the (E,k) emission patterns. A theoretical investigation shows that a non-equilibrium exciton-polariton condensate remains stiff at finite length scales only. This indeed suggests a scenario of fragmentation caused by the interplay of disorder and gain-loss of the condensate.

HL 71.7 Thu 11:15 H2

Exciton-polariton pseudospin polarization in a planar 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. An interesting feature is their pseudospin. It expresses at the same time the average exciton spin orientation and the photonic light polarization of a polariton ensemble.

A planar ZnO-based microcavity of thickness $\lambda/2$ was investigated by angle-resolved photoluminescence experiments. A slight wedge shape of the cavity allows probing of different detunings. The Stokes vector of the emission from the lower polariton branch was determined under non-resonant excitation. The energetic splitting between the TE- and TM-polarized eigenmodes is found to increase with in-plane wavevector $k_{||}$ until the polariton becomes mostly exciton-like. It reaches about 20meV at most. Contrary to expectations, a circular polarization degree of up to 5% is found in the emission from these supposedly linear modes. The extent of this circular polarization reveals the same $k_{||}$-dependence as the TE-TM splitting.

The pseudospin model and the impact of related effective magnetic fields are discussed in order to explain the observed polarization behavior. Influences by different detunings, crystal quality and local anisotropic effects are considered.

HL 71.8 Thu 11:30 H2

Magnetic field interaction of exciton-polariton-condensates in a GaAs-quantum-well microcavity — •Julian Fischer[1], Ingo Lederer[1], Alexander Chernenko[2], Sebastian Brodbeck[1], Arash Rahimi-Iman[1], Matthias Amthor[1], Alfred Forchel[1], Christian Schneider[1], Martin Kamp[1], and Sven Höfling[1] — [1]Technische Physik, Physikalisches Institut, Universität Würzburg and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, 142432 Russia

In this work we investigate the interaction of exciton-polaritons with an external magnetic field in a GaAs-quantum-well-microcavity. The magnetic field up to B=5T is applied in Faraday configuration. We focus on measurements of the Zeeman-splitting for the three regimes of our quantum-well microcavity: uncondensed exciton-polariton at low excitation power, exciton-polariton-condensate and a photon dominated regime above the mott density of excitons. For the uncondensed polaritons we measure the expected linear dependence of the Zeeman-splitting on the magnetic field, while we observed a quenching of the Zeeman-splitting for the condensate case, referred to as "Spin-Meissner-effect". Above the mott-density the Zeeman-splitting is not measurable anymore due to the negligible excitonic content. Hence, the Zeeman-splitting is a reliable tool to distinguish a polaritonic system from a photonic one.

HL 71.9 Thu 11:45 H2

Electroluminescence from spatially confined exciton polaritons in a textured microcavity — •Karol Winkler[1], Christian Schneider[1], Julian Fischer[1], Arash Rahimi-Iman[1], Matthias Amthor[1], Alfred Forchel[1], Stephan Reitzenstein[1,2], Sven Höfling[1], and Martin Kamp[1] — [1]Wilhelm Conrad Röntgen Center for Complex Material Systems, Technische Physik, Universität Würzburg — [2]Institut für Festkörperphysik, Technische Universität Berlin

Strong coupling between microcavity photons and quantum well excitons results in the formation of exciton polaritons. Spatial trapping of these quasi-particles in three dimensions allows for the observation of long-range coherence phenomena and could be exploited for new kind of coherent or non-classical light sources.

While electrical injection of quasi-2D-polaritons has been already archived, we report on electrically pumped formation of spatially confined polaritons. The trapping scheme is based on an elongated textured cavity which results in a three-dimensional confinement potential for the photonic part of the polaritons. An external bias can be used for fast manipulation of the exciton energy through the quantum confined stark effect with a simultaneous read out via resonant photocurrent measurements.

HL 71.10 Thu 12:00 H2

Zeeman split nonlinear emission from electrically injected exciton-polaritons — •Matthias Amthor[1], Christian Schneider[1], Arash Rahimi-Iman[1], Na Young Kim[2,3], Ju-

lian Fischer[1], Matthias Lermer[1], Martin Kamp[1], Stephan Reitzenstein[1,4], Alfred Forchel[1], Yoshihisa Yamamoto[2,5], and Sven Höfling[1] — [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]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany. — [5]National Institute of Informatics, Hitotsubashi, Chiyoda-ku, Tokyo 101-8430, Japan.

We report on magneto-optical measurements of an electrically driven GaAs based exciton-polariton light-emitting diode. The system under investigation is a p-i-n GaAs microcavity with a stack of four InGaAs quantum wells in the center of a one-lambda cavity, etched into circular pillars with diameters of 20 μm. 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. Additionally, we prove the conservation of the strong coupling regime above the first threshold by investigating the Zeeman splitting of the cavity resonance in the non-linear regime.

HL 72: Focus Session: Extended defects in semi- and nonpolar GaN I

Semipolar GaN was sucessfully used for the realization of the green laser diode and is also a promising material for LEDs, due to the changed symmetry and binding configuration on the surface. However, growth on large area low cost substrates like sapphire typically leads to the formation of a high density of extendend defects, especially stacking faults and threading dislocations. These defects can be also formed by strain relaxation of heterostructures grown on GaN substrates with low defect density. This focus session aims to explain the mechanism for formation, methods of identification and growth methods for reduction of such defects as well as optoelectronic devices grown defect reduced GaN. (Organizers: Ulrich Schwarz, Fraunhofer IAF Freiburg, Tim Wernicke, TU Berlin)
Morning session: Origin and identification and reduction of defects in semipolar GaN / Semipolar heterostructures and devices

Time: Thursday 9:30–13:15 Location: H13

Topical Talk HL 72.1 Thu 9:30 H13
Defect reduction methods for GaN heteroepitaxial films grown along semipolar orientations — •Philippe Vennéguès — Centre de Recherche sur l'Heteroepitaxis et ses Applications, rue Bernard Gregory 06560 VALBONNE FRANCE

Heteroepitaxially-grown semipolar GaN films contain a high density of extended structural defects, mainly basal stacking faults, which prohibit their use for the fabrication of efficient optoelectronic devices. After a short description of the microstructure and of the origin of the crystalline defects, this presentation will focus on a few methods which have been developed to improve the crystalline quality. Thanks to transmission electron microscopy, the behavior of the defects and the mechanisms resulting in the reduction of their density are investigated. Two main efficient defect reduction techniques will be presented: epitaxial lateral overgrowth and growth on inclined facets. Problems encountered in the implementation of such growth techniques and the perspective towards the developments of high quality heteroepitaxial GaN templates will be presented.

Topical Talk HL 72.2 Thu 10:00 H13
Identification of defects in semipolar GaN and (Al,Ga,In)N by cathodoluminescence spectroscopy — •Klaus Thonke[1], Ingo Tischer[1], Matthias Hocker[1], Manuel Frey[1], and Ferdinand Scholz[2] — [1]Institute of Quantum Matter / Semiconductor Physics Group, Ulm University, 89081 Ulm, Germany — [2]Institute of Optoelectronics, Ulm University, 89081 Ulm, Germany

The growth of nitride semiconductor layers on semipolar planes typically introduces specific crystalline defects in relatively high concentrations. These defects create local strain, deteriorate the electrical properties, and act as nonradiative recombination centers. Mainly basal plane stacking faults of I_1 and I_2 type are introduced, terminated eventually by prismatic stacking defects or dislocations. To correlate specific types of defects with the commonly observed multiple mostly broad sub-bandgap luminescence emission bands, optical methods with very high spatial resolution in the range of few 10 nm are required. Here, either transmission electron microscope (TEM) or low-energy scanning electron microscope (SEM) based cathodoluminescence (CL) setups yield valuable information. By spatial correlation of CL maps with high-resolution TEM micrographs recorded on exactly the same sample cross section, direct correlation can be obtained. These defects also affect the incorporation of dopant atoms like Mg, or of In and Al atoms when quantum well structures are grown. We discuss the most prominent cases, and look also into the characteristic shift of the emission bands with changes in the (Al,Ga,In) composition.

Topical Talk HL 72.3 Thu 10:30 H13
Stacking fault elimination in heteroepitaxial semi-polar GaN — •Armin Dadgar — Institut für Experimentelle Physik, Otto-von Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg

Heteroepitaxially grown semi- and non-polar GaN layers typically suffer from high densities of stacking faults or require elaborate growth techniques as epitaxial lateral overgrowth. Recently a simple method to eliminate stacking faults of the dominant I1 type by the insertion of AlN interlayers in GaN has been demonstrated for GaN layers inclined towards the m-plane. For semipolar GaN layers with different inclination angles X-ray diffraction and TEM studies of GaN / AlN layer stacks show in detail the annihilation of stacking faults, but also the generation of short segments of I2 type stacking faults.

HL 72.4 Thu 11:00 H13
Enhanced stacking fault induced indium diffusion on semipolar gallium nitride based ridges — •Matthias Hocker[1], Ingo Tischer[1], Klaus Thonke[1], Junjun Wang[2], Robert A.R. Leute[2], Ferdinand Scholz[2], Johannes Biskupek[3], Willem van Mierlo[3], and Ute Kaiser[3] — [1]Institute of Quantum Matter / Semiconductor Physics Group, Ulm University, D-89081 Ulm, Germany — [2]Institute of Optoelectronics, Ulm University, D-89081 Ulm, Germany — [3]Central Facility of Electron Microscopy, Ulm University, D-89081 Ulm, Germany

Semipolar indium gallium nitride (InGaN) quantum wells are promising candidates for long wavelength output light emitting devices with increased efficiency. For this purpose, gallium nitride (GaN) based non-*c* plane structures are overgrown with several InGaN quantum wells. With increasing number of quantum wells on top of these structures, a higher density of stacking faults and dislocations leads to an enhanced incorporation and diffusion of indium towards the ridge of these structures.

Samples with different structures were investigated by spatially and spectrally resolved cathodoluminescence (CL), transmission electron microscopy (TEM), and energy dispersive X-ray spectroscopy (EDX). The CL measurements allow to identify indicators of these defects to avoid tedious TEM measurements.

Coffee break

Topical Talk HL 72.5 Thu 11:30 H13
Strain and Relaxation in Nonpolar and Semipolar GaN-based LEDs and Laser Diodes — •Kathryn Kelchner, Shuji Nakamura, Steven DenBaars, and James Speck — Materials Depart-

ment, University of California, Santa Barbara, USA

Due the noncentrosymmetric nature of the hexagonal wurtzite crystal structure, heterostructures employing InN and AlN alloys on the (0001) basal plane of GaN experience large internal electric fields due to discontinuities in spontaneous and piezoelectric polarizations. Alternative crystal orientations that are nonpolar or semipolar in nature may offer improved device performance, however are also subject to anisotropic in-plane strain of lattice mismatched layers which may impact device design due to limits in critical thickness. In this talk, we will overview some of the basic mechanisms of strain relaxation of InGaN and AlGaN layers on nonpolar and semipolar GaN, including dislocation glide along the basal plane, prismatic slip, and crack formation. Measurement techniques for determining onset and degree of strain relaxation in addition to other materials and growth issues for LED and laser diodes on intentionally strain-relaxed buffers will also be covered.

Topical Talk HL 72.6 Thu 12:00 H13

Semipolar GaN substrate grown on patterned sapphire substrate by hydride vapor phase epitaxy — •Kazuyuki Tadatomo, Keisuke Yamane, Narihito Okada, Hiroshi Furuya, and Yasuhiro Hashimoto — 2-16-1 Tokiwadai, Ube, Yamaguchi, Japan

This paper presents the growth of thick semipolar {10-11}, {11-22}, and {20-21} GaN layers on n, r, and {22-43} patterned sapphire substrates (PSSs), respectively, by hydride vapor phase epitaxy. The reduction rate of the dislocation density varied with growth planes. For {10-11} GaN layers, the dislocation density drastically decreased at over 100 *m, which was as fast the reduction rate as in the case of the c-plane. It was revealed that the reduction rate of the dislocation density could be controlled by the proper selection of the growth plane. We obtained a freestanding GaN of 2 inch diameter. Thick GaN growth led to the self-separation of the GaN layer from the PSS during cooling process. The separation plane formed at the interface between GaN and PSS, which is different from the case of a conventional c-plane GaN/sapphire. The separationability of the GaN layer from the PSS depended on the selective growth area of the sapphire sidewall. A freestanding semipolar GaN substrates were then obtained.

HL 72.7 Thu 12:30 H13

Optical properties of MBE grown cubic AlGaN/GaN double quantum well structures — •Tobias Wecker, Christian Mietze, Dirk Reuter, and Donat J. As — Department of Physics, University of Paderborn, Warburger Str. 100, 33098 Paderborn, Germany

The spatial separation of electrons and holes in $Al_xGa_{1-x}N/GaN$ quantum well structures due to polarization effects can be avoided by growing cubic quantum well samples in the (001) direction. Therefore the optical recombination efficiency in quantum well structures can be increased compared to the hexagonal phase with their strong spontaneous polarization along the hexagonal c-axis [1].

Cubic $Al_xGa_{1-x}N/GaN$ double heterostructures were grown on 3C-SiC(001) substrates by radio-frequency plasma-assisted molecular beam epitaxy. The coupling of the two quantum wells with varying barrier thicknesses was investigated by photoluminescence spectroscopy at room temperature as well as low temperature. The good crystal quality of the samples is demonstrated by high resolution X-ray diffraction.

The strain effects for different Al contents due to the pseudomorphically strained AlGaN barriers were investigated employing photoluminescence spectroscopy and X-Ray diffraction reciprocal space maps around the (113) reflection.

[1] D.J. As, K. Lischka, "Nonpolar cubic III-nitrides", In: Henini M, "Molecular Beam Epitaxy: From research to mass production", Elsevier Inc., 2013, p.203-215, ISBN: 9780123878397

HL 72.8 Thu 12:45 H13

InGaN/GaN based semipolar light emitting diodes — •Junjun Wang[1], Matthias Hocker[2], Robert Leute[1], and Ferdinand Scholz[1] — [1]Institute of Optoelectronics, Ulm University, Germany — [2]Institute of Quantum Matter, Ulm University, Germany

Non- and semipolar III-nitrides are promising to fabricate highly efficient light-emitting devices due to a reduced piezoelectric field leading to an increased overlap of electron and hole wavefunctions. In our research, three-dimensional stripes are realized by selective area growth on patterned masks providing semipolar surfaces. We focused on improving the electrical and optical performance of the stripe light emitting diodes with the semipolar InGaN/GaN quantum wells (QWs). Defects are generated at the tip via strain relaxation during the semipolar InGaN/GaN QWs resulting in a large leakage current. It is reduced from ~5mA to ~0.3mA at a reverse bias of 5V by including a 50nm p-GaN layer before the p-AlGaN electron blocking layer (EBL). Mg doping induces lateral growth in the ~50nm p-GaN layer leading to a plateau at the tip. Under a suitable epitaxial condition, AlGaN EBL grows more vertically recovering the sharp tip with an AlGaN triangle to block the leakage current there. The growth of the undoped GaN between the QWs and p-(Al)GaN was controlled to avoid any plateau or current crowding at the tip.

HL 72.9 Thu 13:00 H13

Epitaxy of $Al_{1-x}In_xN$ on different GaN-surface orientations — •Ernst Ronald Buss, Uwe Rossow, Heiko Bremers, and Andreas Hangleiter — Institute of Applied Physics, TU Braunschweig

$Al_{(1-x)}In_xN$ with thicknesses exceeding 250 nm deposited on c-plane oriented GaN exhibits a distinct splitting of the composition and a very strong roughening of the surface. An increase in indium incorporation efficiency of $Al_{(1-x)}In_xN$ on the $(11\bar{2}l)$ side facets (l=1,2,3) of the V-pits, compared to c-plane orientation, has been frequently mentioned in the literature to be the origin of the composition splitting and strong roughening. To clarify possible dependencies $Al_{(1-x)}In_xN$ layers grown on differently oriented GaN substrates and templates, with various thicknesses have been investigated regarding surface morphology, composition splitting and orientation of the V-pits. It became apparent that the growth rates, as well as the incorporation efficiency of $Al_{(1-x)}In_xN$ are comparable for the polar (0001), and the non polar $(1\bar{1}00)$ surfaces. On semi-polar $(11\bar{2}2)$ surface $Al_{(1-x)}In_xN$ incorporates indium more efficiently as compared with (0001) and $(1\bar{1}00)$ surfaces. $Al_{(1-x)}In_xN$ grown on pitted GaN with typical $(1\bar{1}01)$ side facets does not reveal an additional composition on this semi-polar surface orientation. The formation of differently oriented V-pits in the $Al_{(1-x)}In_xN$, compared with the V-pits in other group III-nitrides, is the key to understand the seemingly intrinsic behavior of composition splitting of $Al_{(1-x)}In_xN$. These results are in perfect agreement with investigations of higher indium content inside the pits formed during growth of $Al_{(1-x)}In_xN$ with $(11\bar{2}l)$ side facets in the literature.

HL 73: Devices

Time: Thursday 9:30–11:15 Location: H15

HL 73.1 Thu 9:30 H15

Does Scaling help making HEMTs faster? — Sabbir Ahmed[1], Kyle David Holland[1], Navid Paydavosi[1], Christopher Martin Sinclair Rogers[1], Ahsan Ul Alam[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]Theoretische Physik I, Universität Bayreuth

The scaling-down of channels has been the basis to design faster transistors. Particularly III-V high-electron-mobility transistors (HEMTs) have been favored for terahertz applications thanks to their low-effective mass. However, experimentally it is known that the unity-current gain and power-gain cut-off frequencies (f_T and f_{max}) of HEMTs exhibit the tendency to saturate with shorter channel lengths and thus become insensitive to scaling. In this talk we employ a self-consistent, quantum-mechanical NEGF solver to quasi-statically extract the f_T of intrinsic III-V devices, focusing on InGaAs and GaN HEMTs with channel lengths of 50 nm down to 10 nm. We show that the non-scaling behavior of HEMTs is a result of short-channel effects (DIBL) leading to a weaker quantum confinement, so that the subbands are positioned lower in energy resulting in a larger-than-expected charge modulation and gate capacitance, respectively. It is also shown that the InGaAs HEMTs have faster f_T at long gate lengths, but as a

consequence of their lower effective mass, they experience a more rapid f_T saturation than the GaN HEMTs, such that the two devices have a comparable f_T at very short gate lengths down to 10 nm.

HL 73.2 Thu 9:45 H15

Structural and magnetic properties of iron on modulation-doped (001) GaAs and on modulation-doped InAs heterostructures — •Boris Landgraf, Taras Slobodskyy, Christian Heyn, and Wolfgang Hansen — Institut für Angewandte Physik, Universität Hamburg, 20355 Hamburg, Germany

We study hybrid structures comprising a ferromagnetic metal layer on III/V compound heterostructures in view of spintronic applications [1]. While iron on modulation-doped (001) GaAs is a well established system [2], corresponding experiments of iron on InAs-HEMTs are not appeared so far. InAs is of high interest because of the low Schottky barrier and strong spin-orbit coupling.
In this talk, I will give an account of the growth and strain relaxation of iron on modulation-doped (001) GaAs and on inverted modulation-doped InAs heterostructures investigated with in-situ reflection high-energy electron diffraction (RHEED). Furthermore, we employed high-resolution X-ray diffraction and magneto-optical Kerr measurements to investigate structural as well as magnetic properties of these structures.

[1] S. Datta, B. Das, „Electronic analog of the electro-optic modulator“, Apllied Physics Letters 56, 665-667 (1990)

[2] X. Lou, C. Adelmann, S. A. Crooker, E. S. Garlid, J. Zhang, K. S. M. Reddy, S. D. Flexner, C. J. Palmstrøm, and P. A. Crowell, „Electrical detection of spin transport in lateral ferromagnet-semiconductor devices“, Nature Physics 3, 197-202 (2007)

HL 73.3 Thu 10:00 H15

Interrelation between the Charge Transport and the Electronic Structure of Transparent Printed Metal Oxide Semiconductors — •M. Häming[1,2], A. Issanin[1,3], P. Pacak[1,2], W. Jägermann[3], and K. Bonrad[1,2] — [1]Merck-TU-Darmstadt Laboratories, Darmstadt, Germany — [2]Merck KGaA, Darmstadt, Germany — [3]Materials Science Department, TU Darmstadt, Germany

Printed Indium-Zinc-Oxide (IZO) and Indium-Gallium-Zinc-Oxide (IGZO) semiconductor thin films have rapidly become of high interest due to recent observations of a surprisingly high field effect mobility ($\mu > 10$ cm^2/Vs) in printed IZO and IGZO thin film transistors (TFTs) which opens up the opportunity for high-performance transparent printed electronics. The charge transport and the electronic structure of a systematic series of solution processed IZO thin films with high field effect mobility has been studied with particular focus at the aspects of doping and the energy position of the charge transport states. A consistent picture of the interrelation between the charge transport properties and the electronic structure can be developed by correlating the data from TFT and four-point probe measurements with UV/VIS transmission spectroscopy and photoelectron spectroscopy data.

HL 73.4 Thu 10:15 H15

A novel bottom-up approach for single photon emitters based on self-aligned quantum dots — •Jan-Hindrik Schulze, Waldemar Unrau, David Quandt, Tobias Heindel, Tim Germann, Ole Hitzemann, André Strittmatter, Stephan Reitzenstein, Udo Pohl, and Dieter Bimberg — Institut für Festkörperphysik, Technische Universität Berlin

Low-cost single or entangled photon sources are basic components of future semiconductor based quantum communication systems. We present a method for fabricating electrically driven single photon sources based on site-controlled quantum dots (QD). The QD positioning is induced by a buried stressor consisting of an oxide aperture which simultaneously self-aligns the current path in the pin-diode structure to the QD site. Due to the long range impact of the buried stressor this approach allows to embed QDs in defect-free matrix material leading to excellent optical properties comparable to Stranski-Krastanow QDs grown on planar surfaces. Moreover, the entire process relies only on conventional photolithographic processes compatible to mass production. Devices exhibit electroluminescence spectra of single QDs featuring linewidths of excitonic recombinations down to 25 μeV (resolution limited). The fine-structure splitting of the excitonic ground state could be measured to be (84 $\pm$ 2) μeV. Also electrically driven anti-bunching measurements confirm single photon emission with $g^2(0) = 0.05$.

HL 73.5 Thu 10:30 H15

Cathodoluminescence spectroscopy and electron-beam induced current mapping of quantum devices — •Manuel Gschrey, Tuan Minh Do, Sven Rodt, Waldemar Unrau, David Quandt, Jan-Hindrik Schulze, Tim Germann, André Strittmatter, Dieter Bimberg, and Stephan Reitzenstein — Insititut für Festkörperphysik, Technische Universität Berlin

Electrically-driven single-photon sources (SPSs) are key components for future quantum communication systems. For the further development of cavity-enhanced quantum-dot (QD) based SPSs, the spatial and spectral control of the QDs, as well as the design of the current path through the device, are of utmost importance. We report on high-resolution cathodoluminescence (CL) spectroscopy and electron-beam induced current (EBIC) mapping of novel electrically driven SPSs. The SPSs are fabricated by an self-alignment process where an oxide aperture defines not only the current path through the device, but also initiates the site-controlled growth of single QDs aligned to the aperture, which provide true single photon emission with $g^{(2)}(0) = 0.05$. The combination of CL spectroscopy and EBIC mapping under variation of the applied bias voltage allows us to prove the small size and high quality of the oxide aperture, as well as the spatial position of the emission lines of single QDs within the active layer of the device.

HL 73.6 Thu 10:45 H15

d-DotFET: Using locally strained silicon for mobility enhancement in MOSFET devices — •Jürgen Moers[1,2], Julian Gerharz[1,2], and Detlev Grützmacher[1,2] — [1]Peter Grünberg Institut 9 (PGI-9), Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]JARA -Fundamentals of Future Information Technology (JARA-FIT)

In MOSFET devices strained silicon is regarded as material to improve device performance due to enhanced mobility. In the d-DotFET approach we use ordered Ge dots to facilitate locally strained silicon layers. The growth sites of the Ge dots, which serve as local pseudosubstrate for the subsequently grown Si, are defined by template assisted self assembly: the Ge dots grow on prepatterned sites only. By integrating the MOSFET on top of this locally strained layer the strain can be utilized to improve device performance. The applied strain in the Si layer can be larger as in the planar case, because the Ge content in the dots is larger than possible in normal blanket epitaxy of SiGe-layers. Transistors with gate length between 60 nm and 1 μm were processed with different gate width ranging from 60 nm to 180 nm. In comparison to transistors fabricated on the same chip, but without strained layer, the drain current enhancement is up to 35%. In devices where the Ge-dot is not removed the drain current increase is 22.5%, showing that removing the Ge dot further increases performance. In conclusion exploiting locally strained silicon in the d-DotFET concept offers an alternative route to get higher strain and hence improved device performance in MOSFET applications.

HL 73.7 Thu 11:00 H15

Electrostatic Doping in III-V Nanowire Tunnel FETs — •Thomas Grap and Joachim Knoch — Institute of Semiconductor Electronics RWTH University, D-52074 Aachen

Tunnel FETs (TFETs) have attracted a great deal of attention due to their potential superior off-state performance which would enable a substantial reduction in power consumption of highly integrated circuits. In order to improve the TFET performance, a nanowire (NW) device layout with ultrathin diameter and wrap-gate architecture with high-k gate dielectrics is proposed. Of special interest are III-V semiconductors, since they offer a low effective mass and a small band gap. As a result, in such a device structure electronic transport is one-dimensional (1D). Due to the particular band profile (p-i-n) excellent screening of the gate action on the source is mandatory in order to obtain a steep source-channel p-n junction. However a large doping concentration increases the Fermi-Level in source - due to a 1D transport and a low density of states of the III-V NW - limiting the inverse subthresholdslope of the TFET to 60mV/dec. As an alternative to the conventional doping, we successfully designed various device layouts using a triple-gate structure to electrostatically dope the NW. This allows us to adjust the screening and the Fermi-Level independently. We will show simulations performed for different TFET device geometries discussing the advantages of electrostatic doping over conventional doping with respect to the TFET performance. First experimental results on the proposed device layouts will be presented as well.

HL 74: Quantum dots: Optical properties

Time: Thursday 9:30–12:15 Location: H16

HL 74.1 Thu 9:30 H16

Strongly size dependent polar exciton-LO-phonon interaction in GaN/AlN quantum dots — •Johannes Settke, Andrei Schliwa, Gordon Callsen, Juri Brunnmeier, Axel Hoffmann, and Christian Thomsen — Institut für Festkörperphysik, Technische Universität Berlin, Germany

Recently, strongly size dependent exciton-LO-phonon interaction for epitaxial GaN/AlN quantum dots (QD) was observed experimentally by analyzing the LO-phonon sidebands of single-QD excitonic peaks. Depending on the exciton energy, ranging from 3.2 eV to 4.3 eV, values of the Huang-Rhys parameter S between 0.5 and 0.01 were deduced. Since the polar coupling strength (described by S) for an exciton is proportional to the squared absolute value of the Fourier transformed difference of the probability densities of the electron and hole, S provides a measure for the electron-hole separation.

GaN/AlN QDs are well known for their strong intrinsic piezo- and pyroelectrical fields along the c-axis, giving rise to excitonic charge separation analogous the quantum confined Stark effect. As this charge separation is known to be dependent on the QD height, it is mirrored by a variation of the parameter S.

Here, we calculate the Huang-Rhys parameter for the ground-state exciton as function of size and composition using a strain dependent 3D implementation of the eight-band k*p model taking into account piezo- and pyroelectric effects. We discuss the interrelation of QD size, built-in fields, exciton energy, dipole-moment and Huang-Rhys parameter S.

HL 74.2 Thu 9:45 H16

Spin-flip Raman scattering on Γ-X mixed excitons in indirect band-gap (In,Al)As/AlAs quantum dots — •Dennis Kudlacik[1], J. Debus[1], D. Dunker[1], V. F. Sapega[2], T. S. Shamirzaev[1], E. L. Ivchenko[2], D. R. Yakovlev[1,2], and M. Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44227 Dortmund, Germany — [2]Ioffe Physical-Technical Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia

We studied the fine structure of the indirect exciton in self-assembled (In,Al)As/AlAs quantum dots (QDs) by means of spin-flip Raman scattering (SFRS). The QDs are characterized by a type-I band alignment, wherein, dependent on the dot size, a crossover between the energetically lowest conduction-band states of the Γ- and X-valley occurs. This Γ-X mixing of the electron levels is used to optically study the indirect in momentum-space exciton. It has a long recombination lifetime and longitudinal spin relaxation time of up to several milliseconds. Using the resonant SFRS the g-factor tensors of the indirect exciton, Γ-valley heavy-hole, and X-valley electron are determined. The spin-flip scattering mechanisms are based on acoustic phonon interaction in tilted magnetic field geometries. The efficiencies of the electron and heavy-hole spin scattering strongly depend on the excitation energy across the inhomogeneously broadened QD ensemble. The Γ-valley electron cannot be observed because of its short lifetime and the broad dispersion of its g-factor corresponding to the strong variation in the QD sizes, which is evidenced in experiment and theory.

HL 74.3 Thu 10:00 H16

GaAs Quantum Dot Molecules of ultra-low density — •Achim Küster, David Sonnenberg, Andreas Graf, Christian Heyn, and Wolfgang Hansen — Institut für Angewandte Physik, Universität Hamburg, 20355 Hamburg, Germany

We present the fabrication and optical properties of GaAs quantum dot molecules (QDM). The QDM are fabricated by filling nanoholes in an AlGaAs surface with a GaAs/AlGaAs/GaAs layer sequence. The nanoholes are formed using local droplet etching with Al droplets on AlGaAs substrates. By optimizing the arsenic flux during droplet deposition an ultra-low density of some $\cdot 10^6$ cm^{-2} can be achieved [1], allowing the study of single QDM. With our fabrication method we have good and independent control on the dot size and the tunnel barrier in the QDM. The AlGaAs layer between the GaAs layers forms the tunnel barrier with thickness that is tuned from 1 nm to 20 nm in our experiments. Also, the dot size can be tuned separately in these structures. In samples with tunnel barrier thickness below 5 nm we observe non-resonant tunnelling [2] in these QDMs as a clear sign of coupling, while at a barrier thickness of 15 nm the optical spectra show no signature of tunnelling any more. Furthermore, we have integrated the QDMs into Schottky-diode structures and observed strong Stark-shifts up to 25 meV at typical fields of $2 \cdot 10^7$ V/m. [1] D. Sonnenberg et al., APL **101**, 143106 (2012); [2] M. Reischle et al., PRB **76**, 085338 (2007)

HL 74.4 Thu 10:15 H16

MOVPE grown InAs quantum dots with strain reducing layer — •Matthias Paul, Jan Kettler, Michael Jetter, and Peter Michler — IHFG, Universität Stuttgart, Deutschland

In recent years, InAs semiconductor quantum dots (QDs) have been studied extensively due to their potential application in quantum information networks. Based on their good optical properties and small area densities InAs QDs are excellent candidates for sources of entangled or indistinguishable photons. An implementation in fiber-coupled networks, however, requires emission wavelengths of 1310 nm or 1550 nm to minimize absorption losses.

Therefore, typical emission energies of InAs QDs need to be redshifted, e.g. by a strain reducing InGaAs layer on top of the QDs. This leads to both a reduction of the effective band gap and to an increase of the size of the QDs which results in lower emission energies.

The fabrication of InAs QDs for the aforementioned spectral range by metal-organic vapor-phase epitaxy usually leads to high area densities. In this case, a structuring a posteriori is necessary to investigate single QDs. By choosing the presented sample structure and growth parameters our samples show area densities of around 10^6 cm^{-2}. This renders an additional patterning unnecessary. The emission wavelengths of the QDs are around 1050 nm. Distributed Bragg reflectors (DBR), optimized for this spectral range, are used to increase the collection efficiency for micro-photoluminescence measurements. Correlation experiments and time-resolved measurements show the good optical properties of our InAs QDs.

HL 74.5 Thu 10:30 H16

Spectroscopy on single buried InAs quantum dots by scattering scanning near-field infrared microscopy — •Markus Fehrenbacher[1], Rainer Jacob[1], Stephan Winnerl[1], Jayeeta Bhattacharyya[1], Harald Schneider[1], Marc Tobias Wenzel[2], Hans-Georg von Ribbeck[2], Lukas M. Eng[2], Paola Akinson[3], Oliver G. Schmidt[3], and Manfred Helm[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]TU Dresden, Dresden, Germany — [3]Leibniz Institute for Solid State and Materials Research, Dresden, Germany

Quantum dots are a highly interesting material system for many application purposes such as single photon emitters in the near-infrared, but also for mid- and far-infrared applications. Studying the linewidth of involved optical transitions offers valuable clues to the dephasing mechanisms of the trapped electrons. However, due to size fluctuations of the quantum dots, inhomogeneous broadening of the signals usually hides this information when investigating ensembles of dots. Therefore, single-dot spectroscopy has to be performed for this purpose. In contrast to studies of interband transitions this is not well established at all for intersublevel transitions. In this work, scattering type scanning near-field optical microscopy (s-SNOM) in combination with a free-electron laser is used to investigate intersublevel transitions in single self-assembled buried InAs quantum dots. Thereby, spectrally resonant optical contrast to the surrounding GaAs substrate is observed at photon energies of 83 meV and 123 meV, which can clearly be assigned to the s-d and p-d transitions of single conduction band electrons.

Coffee break

HL 74.6 Thu 11:00 H16

Tailoring the optical properties of single semiconductor quantum dots with metallic planar- and nano-structures — •Hongyi Zhang[1,3], Klas Lindfors[1,3], Yongheng Huo[2], Armando Rastelli[2], Oliver G. Schmidt[2], Harald Giessen[1,3], and Markus Lippitz[1,3] — [1]Max Planck Institute for Solid State Research — [2]Institute for Integrative Nanosciences, IFW- Dresden — [3]4th Physics Institute, University of Stuttgart

Coupling plasmonic nanostructures with single quantum emitters is of

high interest for both fundamental research and a wide range of applications such as ultra-bright non-classical photon sources. The luminescence properties of the emitter can be significantly modified because of the localized electromagnetic field close to the metal nanostructures.

We have studied the optical properties of single GaAs/AlGaAs QDs at different distances to a gold mirror. Both the luminescence intensity and the recombination rate of the QDs were enhanced because of coupling to surface plasmons. We have also investigated the influence of optical antenna on the luminescence of the QDs. With the help of a state of the art positioning technique, we positioned gold nanorods above single QDs and observed significant modification of the emission properties, which manifests the coupling between the QD and localized plasmons. We have also taken first steps to fabricate plasmonic nanocavities for the self-assembled GaAs QDs.

HL 74.7 Thu 11:15 H16

Fabrication of a thin membrane of InP/AlGaInP quantum dots — •Hendrik Niederbracht, Elisabeth Koroknay, Fabian Hargart, Christian Alexander Kessler, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen und SCoPE Forschungszentrum, Universität Stuttgart, Deutschland

For applications based on the single photon emission from quantum dots (QDs) like quantum key distribution or quantum communication high collection efficiency is important. An easy way to achieve this is to guide the emission of semiconductor QDs into the direction of the detection by growing distributed Bragg reflectors below the QDs and using optics with a high numerical aperture. But often the setup can limit the use of such objectives. An alternative is offered by very thin samples in combination with solid immersion lenses.

The QD samples are fabricated via metal-organic vapor-phase epitaxy on a (100) GaAs substrate with a 6 degree miscut. The challenge is the fabrication of the thin membrane of InP/AlGaInP QDs. Therefor the sample is glued topside down on Si and afterwards thinned using mechanical and wet chemical methods. Optical measurements on an 80 nm thick sample are carried out in order to proof the single photon emission and the results are compared with an unprocessed reference.

HL 74.8 Thu 11:30 H16

Optical excitation channels of a single site-controlled quantum dot — •Ole Hitzemann[1], Erik Stock[1], André Strittmatter[1], Andrei Schliwa[1], Jan-Hindrik Schulze[1], Tim D. Germann[1], David Quandt[1], Waldemar Unrau[1], Udo W. Pohl[1], Axel Hoffmann[1], Dieter Bimberg[1], and Vladimir Haisler[2] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Germany — [2]Institute of Semiconductor Physics, Russian Academy of Sciences, Novosibirsk, Russian Federation

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

Above a sub-micrometer aperture we observe sharp luminescences lines, originating from a single QD as demonstrated by autocorrelation measurements. Micro photoluminescence excitation spectroscopy shows efficient excitation channels through hybridization with the wetting layer, excited states, and coupling with phonon modes as well as distinctively different photoluminescence spectra for different excitation energies. Excitation power dependent measurements reveal the saturation behavior of excitonic and high excitation luminescence lines.

HL 74.9 Thu 11:45 H16

Cascaded emission of linearly polarized single photons from positioned InP/GaInP quantum dots — •Tristan Braun[1], Vasilij Baumann[1], Sebastian Unsleber[1], Manuel Gschrey[2], Sven Rodt[2], Stephan Reitzenstein[1,2], Sven Höfling[1], 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]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany

We report on the in-depth optical characterization of red-emitting site-controlled InP/GaInP Quantum Dots. In order to prove the long-range ordering of the buried emitters scanning cathodoluminescence with a high spatial resolution was performed, revealing a yield of $\approx 90\%$ of optically active QDs on the pre-determined positions and the absence of emitters on interstitial positions. Polarization dependent investigations on the emission of single QDs show a pronounced degree of linear polarization along the (1-10) crystal axis with an average degree of polarization as large as 80%. Photon correlation measurements of the biexcitonic and excitonic emission of a single dot are employed to reveal the single-photon character of each emission line as well as the cascaded nature of the photon pair emission.

HL 74.10 Thu 12:00 H16

Comparison of the energy transfer in colloidal core-shell Q-dots in solution and in a Q-dot layer — •Uwe Kaiser[1], Robert Malinowski[1], Wolfram Heimbrodt[1], Faheem Amin[2], Dorleta Jimnez de Aberasturi Arranz[2], and Wolfgang Parak[2] — [1]Experimental semiconductors group of Philipps-University Marburg — [2]Biophotonics group of Philipps-University Marburg

There is a great interest in functionalized colloidal Q-dots (CQDs) with diameters of a few nanometers for physical as well as biological applications. A fundamental understanding of the energy transfer processes in these materials for different experimental environments is necessary.

We studied the temporal spectral behavior of CdSe quantum dots functionalized with chromophores with time resolved photoluminescence spectroscopy. With a laser pulse of a few nanoseconds we are able to observe the luminescence decay in the range of nanoseconds up to microseconds for the luminescence of the dot as well as for the chromophore.

Measurements have been done for nanoparticles in solution as well as on particles transferred to a substrate. The fluorescence resonant energy transfer (FRET) between the dot and the chromophores has been studied in a temperature range between 10K and room temperature. A detailed comparison of the FRET process will be presented for the Q-dots in different environments.

HL 75: Transport: Spintronics and magnetotransport 1 (TT, jointly with HL, MA)

Time: Thursday 9:30–13:00 Location: H18

HL 75.1 Thu 9:30 H18

A relativistic implementation of the non-equilibrium Green's function formalism for layered systems — •S Wimmer[1], M Ogura[2], H Akai[2], and H Ebert[1] — [1]Department Chemie, Ludwig-Maximilians-Univeristät München — [2]Department of Physics, Graduate School of Science, Osaka University

The non-equilibrium Green's function formalism has been implemented within the Korringa-Kohn-Rostoker (KKR) multiple scattering theory following previous work [1,2]. First results for the transport in layered systems are presented and compared to available results of other authors [1–3]. Using a fully relativistic approach within the Dirac-formalism allows us to investigate the influence of spin-orbit coupling. This will be discussed for various transport properties including the spin-transfer torque.

[1] C. Heiliger et al., J. Appl. Phys. **103**, 07A709 (2008)
[2] S. Achilles, Ph.D. thesis, Martin-Luther-Universität Halle-Wittenberg (2012)
[3] P. M. Haney et al., Phys. Rev. B **76**, 024404 (2007)

HL 75.2 Thu 9:45 H18

Persistent Spin Helix Conditions in Two-Dimensional Electron and Hole Gases — •Tobias Dollinger, Andreas Scholz, Paul Wenk, John Schliemann, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg

We discuss magnetotransport in systems with nonnegligable cubic in momentum Dresselhaus Spin Orbit Interaction (SOI). The latter has been found responsible for diminishing and shifting the parameter regime where weak localization signatures, attributed to the so called "Persistent Spin Helix"(PSH) symmetry [1,2], are detected in magneto-

conductance traces [3]. Building on the electronic results, we present an effective model for the heavy hole band of a confined twodimensional hole gas, where typically SOI terms with cubic structure are relevant. We investigate numerically and analytically the magnetotransport propery of this model, in which we can identify an analogue to the PSH.

[1]J. Schliemann et al., PRL **90** 146801 (2003)
[2] Bernevig et al., PRL **97** 236601 (2006)
[3] Kohda et al., PRB **86** 081306 (2012)

HL 75.3 Thu 10:00 H18

Aharonov-Casher effect in quantum rings: geometric phase shift by in-plane magnetic field — Diego Frustaglia[1], •Henri Saarikoski[2], Klaus Richter[2], Fumiya Nagasawa[3], and Junsaku Nitta[3] — [1]Departamento de Física Aplicada II, Universidad de Sevilla, Sevilla, Spain — [2]Department of Theoretical Physics, Regensburg University, Germany — [3]Department of Materials Science, Tohoku University, Sendai, Japan

We study transport through Rashba spin-orbit coupled quantum rings where the spin-orbit field causes the Aharonov-Casher effect [1, 2]. The ring is subject to an in-plane magnetic field which gives rise to a shift in the geometric phase. We show that the in-plane field allows control of the geometric phase independently from the dynamic phase and without competing with Aharonov-Bohm phases. We use perturbation theory to calculate the resulting phase shift in quasi-1D rings for weak in-plane fields. The resulting phase shift is quadratic in the in-plane field. Numerical Recursive Green's function algorithm is used to study the effect in multi-mode quantum rings and in the case of large in-plane fields. We demonstrate the effect in InGaAs/InAlAs based quantum rings where the Rashba spin-orbit field is modulated by an external gate. As the in-plane magnetic field is increased we find a quadratic phase shift in the Aharonov-Casher effect towards lower spin-orbit fields in good agreement with calculations.

[1] F. Nagasawa, J. Takagi, Y. Kunihashi, M. Kohda, and J. Nitta, Phys. Rev. Lett. 108, 086801 (2012)
[2] K. Richter, Physics 5, 22 (2012).

HL 75.4 Thu 10:15 H18

Quantum Feedback in nuclear spin-assisted electronic transport — •Klemens Mosshamer and Tobias Brandes — Institut für theoretische Physik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin

We investigate theoretically the electronic transport through quantum dot systems that interact with the nuclear environment via the hyperfine interaction. We show that the non-linear dynamics arising due to the hyperfine interaction can be controlled via closed-loop feedback operations, such as time-dependent modifications of the tunneling rate.

HL 75.5 Thu 10:30 H18

Projective Boltzmann approach to thermal drag in spin-1/2-ladder systems coupled to phonons — •Christian Bartsch and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig

We quantitatively investigate the spin-phonon drag contributions to the thermal conductivity of a two-leg-spin-1/2-ladder coupled to lattice vibrations in a magnetoelastic way. By applying suitable transformations the system is mapped onto a weakly interacting quantum gas model of bosonic spin excitations (magnons) and phonons. We adequately construct a collision term of a linear(ized) Boltzmann equation from the underlying quantum dynamics by means of a pertinent projection operator technique. From the Boltzmann equation we obtain concrete numerical values for the drag conductivity and relate it to the individual thermal conductivities of magnons and phonons for parameter ranges which are typical for certain material classes.

HL 75.6 Thu 10:45 H18

Rashba spin-orbit-interaction-based quantum pump in graphene — •Dario Bercioux[1], Daniel F. Urban[2,3], Francesco Romeo[4], and Roberta Citro[4] — [1]Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität, 79104 Freiburg, Germany — [2]Physikalisches Institut, Albert-Ludwigs-Universität, 79104 Freiburg, Germany — [3]Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstraße 11, 79108 Freiburg, Germany — [4]Dipartimento di Fisica "E. R. Caianiello" and Spin-CNR, Università degli Studi di Salerno, I-84084 Fisciano (Sa), Italy

We present a proposal for an adiabatic quantum pump based on a graphene monolayer patterned by electrostatic gates and operated in the low-energy Dirac regime [1]. The setup under investigation works in the presence of inhomogeneous spin-orbit interactions of intrinsic- and Rashba-type and allows to generate spin polarized coherent current. A local spin polarized current is induced by the pumping mechanism assisted by the spin-double refraction phenomenon [2].

[1] Citro, Appl. Phys. Lett. **101**, 122445 (2012)
[2] D. Bercioux, A. de Martino, Phys. Rev. B **83**, 012106 (2011)

HL 75.7 Thu 11:00 H18

First-principles calculation of ballistic transport in single-atom contacts — •Fabian Otte[1], Björn Hardrat[1], Frank Freimuth[2], Yuriy Mokrousov[2] und Stefan Heinze[1] — [1]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Peter-Grünberg-Institut, Forschungszentrum Jülich, 520425 Jülich, Germany

Recently, the spin-valve effect of single-atom contacts has been demonstrated using scanning tunneling microscopy [1]. In these measurements a magnetic tip approaches magnetic adatoms on a surface and the distance-dependent conductance and magnetoresistance is obtained. Here, we report first-principles calculations of ballistic transport in model systems of such single-atom contacts using our recently developed approach [2] which allows to include spin-orbit coupling and non-collinear spin structures. We present the conductance between two ferromagnetic Co monowires terminated by single Mn apex atoms while varying the distance between the two Mn atoms. Due to frustration of exchange interactions a non-collinear spin state is favorable in the contact regime. We show that it leaves a fingerprint in the distance-dependent conductance and magnetoresistance [3]. We also study the ballistic anisotropic magnetoresistance from the tunneling to the contact regime for leads whose structure is modeled with Fe monowires.

[1] M. Ziegler et al., New J. Phys. 13, 085011 (2011)
[2] B. Hardrat et al., Phys. Rev. B 85, 245412 (2012)
[3] B. Hardrat et al., Phys. Rev. B 86, 165449 (2012)

15 min. break

HL 75.8 Thu 11:30 H18

A carbon nanotube quantum dot in the intermediate coupling regime: Conductance and tunnel magnetoresistance — •Alois Dirnaichner, Johannes Kern, and Milena Grifoni — Universität Regensburg

We discuss transport through carbon nanotube quantum dots with intermediate coupling to ferromagnetic leads. In a density matrix approach we sum up infinite-order corrections due to charge fluctuations within the dressed second order approximation (DSO) [1], allowing us to go beyond the sequential tunneling regime. From the master equation we deduce conductance and tunnel magnetoresistance (TMR). The results are compared to experimental data with a pronounced gate modulation of the TMR and negative TMR features in particular.

[1] J. Kern and M. Grifoni, arXiv:1209.4995v1

HL 75.9 Thu 11:45 H18

Spin transport in carbon nanotubes in the Fabry-Perot regime — •Miriam del Valle and Milena Grifioni — Institute of Theoretical Physics, University of Regensburg

We investigate the spin-dependent transport through carbon nanotubes connected to two ferromagnetic leads in the ballistic regime. The effect and origin of the phases acquired by electrons upon scattering at the contact interfaces are analyzed. These phases greatly determine the Fabry-Perot patterns obtained in this transport regime. With stress on the nanotube fingerprints, the magneto-resistance is calculated with the inclusion of spin-orbit effects, which are not negligible due to the finite curvature of the nanotubes.

HL 75.10 Thu 12:00 H18

Investigation of spin transfer torques in $Mn_{1-x}Fe_xSi$ — •Christoph Schnarr, Robert Ritz, Andreas Bauer, Christian Franz, and Christian Pfleiderer — Technische Universität München, Physik-Department E21, D-85748 Garching, Germany

Small angle neutron scattering and Hall effect measurements recently revealed sizeable effects of spin transfer torques in the skyrmion lattice phase of MnSi [1,2]. The associated critical current densities of $\sim 10^6$ A/m^2, are exceptionally small and about 5 orders of magnitude

smaller than the spin transfer torque observed in conventional systems. The low critical current density is due to a very efficient gyromagnetic coupling exhibited by a topological Hall contribution that arises in the topologically non-trivial magnetic structure of a skyrmion lattice. We report spin transfer torque experiments, measuring the Hall effect in $Mn_{1-x}Fe_xSi$ for a wide range of x, where the topological Hall effect increases by up to a factor of ten characteristic of a much more efficient coupling of the electric currents to the magnetic structure. The dependence of j_c on the doping concentration is discussed in view of the increased topological Hall effect as well as the increased pinning by disorder.

[1] F. Jonietz *et al.*, Science **330**, 1648-1651 (2010)
[2] T. Schulz *et al.*, Nat Phys **8**, 4, 301-304 (2012)

HL 75.11 Thu 12:15 H18

Magnetotransport along a boundary: From coherent electron focusing to edge channel transport — •Thomas Stegmann, Dietrich E. Wolf, and Axel Lorke — University of Duisburg-Essen, Department of Physics and CENIDE

In a two dimensional electron system with a boundary, electrons are injected at one point on the boundary and focussed by a perpendicular magnetic field B onto another voltage probe on the boundary. Using the nonequilibrium Green's function approach we study theoretically the 4-point Hall resistance R_{xy} as a function of B. For low fields, R_{xy} shows the characteristic equidistant peaks observed in the experiment, which can also be explained by simple classical trajectories: The electrons are guided on cyclotron orbits, are reflected speculary at the boundary, and end finally at the collector when a multiple of the cyclotron diameter equals the distance between injector and collector. In a strong magnetic field, the current is carried by edge channels parallel to the boundary and the typical fingerprint of the quantum Hall effect is observed. Here, we study the transition from the classical cyclotron motion to the edge channel transport and discuss its influence on the focussing spectrum. In intermediate fields, we find that R_{xy} shows sets of oscillations, which are neither periodic in B (such as the magnetic focussing peaks) nor in $1/B$ (quantum Hall effect). These oscillations can be understood as interference between adjacent edge states.

HL 75.12 Thu 12:30 H18

Entanglement detection in Cooper pair splitters based on carbon nanotubes in magnetic fields — •Pablo Burset[1,2], Bernd Braunecker[1], and Alfredo Levy Yeyati[1] — [1]Departamento de Fisica Teorica de la Materia Condensada, Universidad Autonoma de Madrid, E-28049 Madrid, Spain — [2]Institute for Theoretical Physics and Astrophysics, University of Wuerzburg, Am Hubland, 97074 Wuerzburg, Germany

The production of entangled electron pairs in a solid state device from the splitting of a Cooper pair is currently attracting much attention. Recent experiments have shown that Cooper pairs can be split in a controlled fashion in double quantum dot structures. In this talk I will describe how spin-orbit interaction in carbon nanotubes presents unique characteristics for the study of the entanglement of injected pairs of electrons.

I will briefly introduce the double dot Cooper pair splitter device based on carbon nanotubes. In this setup, I will review the form of spin-orbit interaction and demonstrate that it leads to a perfect spin filter with spin orientations tunable by external fields. Tunable spin-orbit induced spin-filtering allows to implement entanglement detectors, such as probing a Bell inequality. These detectors can rely on conductance measurements alone and do not require the precise knowledge of the spin orientations of the spin filter. Yet if in addition the spin orientations are known, the same setup can be used for full quantum state tomography.

HL 75.13 Thu 12:45 H18

Electronic correlations in magnetic heterostructures. — •Liviu Chioncel[1,2] and Junya Otsuki[2,3] — [1]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany — [2]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [3]Department of Physics, Tohoku University, Sendai, Japan

Heterostructures that contain semiconducting and magnetic monolayers offer the possibility to adjust simultaneously band-gap and magnetic properties. Dynamical Mean Field Theory is a necessary theoretical tool to address physical properties of multilayer systems containing correlated electrons. Here we solve a simplified Hubbard model within DMFT using the recently developed CT-QMC solver, for several magnetic monolayers embedded into semiconducting/insulating host. Our approach is relevant for the Cr/Mn-doped semiconducting heterostructures. We discuss possible half-metallic properties in these systems in the presence of dynamic correlations at finite temperatures.

HL 76: Focus Session: Organic materials for spintronics – From spinterface to devices (DS, jointly with HL, MA, O)

Since the first report of an organic spin valve in 2004, novel devices such as spin-OLEDs (organic light emitting diodes) and spin-OFETs (organic field effect transistors) as well as sensors based on magnetic resonance were developed. This rapid development of the field of organic spintronics is driven by the large spin life time in organic molecules, combined with the large diversity and flexibility of molecular synthesis and technological processing. Despite the tremendous progress, there are still many challenges which must be tackled. On one hand, it is desirable to achieve a computer-aided design for novel molecules that can keep their properties at the interfaces with the spin-injecting electrodes. On the other hand, novel technologies for the fabrication of spin devices and the spin transport properties of various molecules are being tested. Last but not least, the spin injection at spinterfaces, i.e. at the interface between the organic molecules and the ferromagnetic electrodes, is a key factor that still needs to be understood and controlled. This topical session aims to give an overview of the latest developments in the dynamic field of organic spintronics. (Organizers: Martin Aeschlimann, Uni Kaiserslautern; Bernd Büchner, IFW Dresden; Dietrich R. T. Zahn, TU Chemnitz)

Time: Thursday 9:30–13:30 Location: H32

Invited Talk HL 76.1 Thu 9:30 H32

Organic Magnetoresistance: The effect of excitons on charge transport in organic semiconductors — •William Gillin — Queen Mary, University of London, UK

It has been known since 2003 that applying a magnetic field to an organic light emitting diode (OLED) will cause changes in both the light output (efficiency) of a device and the current through the device (organic magnetoresistance or OMR). The observation of this phenomenon has spurred a number of models to explain the observations but these can be classified in to two broad classes: excitonic and bipolaron. As the effect of the magnetic field is to apply a small perturbation to existing spin dependent processes that are affecting charge transport and recombination, the study of OMR provides an interesting new tool for understanding these processes. In this talk I will highlight the recent developments in the study of organic magnetoresistance and illustrate that the effect probably has several components which are all acting in parallel and which can have different signs and magnetic field dependencies. By developing an understanding of the different magnetic field characteristics of different processes we may open a door on to a new way of studying the interactions responsible

for the fundamental operation of organic electronic devices.

Topical Talk HL 76.2 Thu 10:00 H32

Metal-phthalocyanines: Materials for molecular spintronics — •Jens Kortus[1], Rico Friedrich[1], Torsten Hahn[1], Claudia Loose[1], and Martin Knupfer[2] — [1]TU Bergakademie Freiberg, Germany — [2]IFW Dresden, Germany

Metal-phthalocyanines (MPc) are very stable and can have different spin states depending on the transition metal ion. In this contribution we will discuss electronic, (magneto)optical and transport properties of MPc in view of possible application in spintronic devices.

In particular a recently investigated layered system of MnPc and F_{16}CoPc shows charge transfer at an interface between two metal phthalocyanines, which is investigated in detail using density functional theory. These results are of importance for the application of such interfaces in organic electronic devices because charge transfer considerably affects the energy level alignment and the transport behaviour of the respective hetero-junction. Since the transfer of charge is also connected to a transfer of spin and the hybrid system has a net spin of $S = 2$, such compounds could also be termed *spin-transfer materials* with future applications in the area of spintronics [1].

[1] S. Lindner, M. Knupfer, R. Friedrich, T. Hahn, J. Kortus Phys. Rev. Lett. 109 (2012) 027601-1/5

Topical Talk HL 76.3 Thu 10:30 H32

Magneto-optical Kerr Effect Spectroscopy of Selected Phthalocyanines and Porphyrines — •Georgeta Salvan[1], Peter Robaschick[1], Frank Lungwitz[1], Michael Fronk[1], Carola Mende[1], Heinrich Lang[1], Rico Friedrich[2], Jens Kortus[2], and Dietrich R.T. Zahn[1] — [1]TU Chemnitz, 09126 Chemnitz, Germany — [2]2TU Bergakademie Freiberg, Freiberg 09596, Germany

Phthalocyanines and porphyrines find nowadays many applications from pigments to organic electronics. Nevertheless, they still have a special charm for fundamental investigations thanks to the large flexibility of their molecular structure. This work focuses on the influence of the molecular spin ground state on the room temperature magneto-optical activity of some phthalocyanines and porphyrins. The films in the typical thickness range between 30 nm and 100 nm were prepared by organic molecular beam deposition in high vacuum. Magneto-optical Kerr effect (MOKE), which is commonly used to study the magnetic properties of inorganic ferromagnetic layers or magnetic nanostructures, is measured here spectroscopically in the region of the Q and B absorption bands of phthalocyanines and porphyrines. From this the magneto-optical Voigt constant is calculated numerically and can be correlated to the electronic properties of the molecules. For instance, the hybridisation of Co3d states with the HOMO π-orbital of CoPc leads to additional features in the magneto-optical spectra compared to e.g. CuPc. The magnitude of the Voigt constant in the Q band is hardly sensitive to the molecular spin, but highly sensitive to the orientation of the molecules with respect to the substrate plane.

Topical Talk HL 76.4 Thu 11:00 H32

Molecular Quantum Spintronics — •Mario Ruben — Institut für Nanotechnologie (INT), Karlsruhe Institut für Technologie (KIT) — Institut de Physique et Chimie (IPCMS); Université de Strasbourg (UdS)

Molecules can be considered as physical Quantum Objects. Magnetic molecules consist of an atomic core of one-to-few open spin ions surrounded by a shell of organic material. At low temperature such molecular spin objects behave as simple, few-level systems.[1,2] Since quantum coherence and stable entanglement of electron spins are extremely difficult to achieve, alternative concepts propose the use of nuclear spins as quantum information carrier. Nuclear spins are extremely well isolated from environment and less prone to decoherence, and the coherent manipulation can be adapted by tailoring the molecular environment. However, although being well isolated from their surroundings, nuclear spins have to be addressed, ideally electronically since complementary with existing technologies. The delicate balance between decoupling of the magnetic molecule for stable coherence and connecting it for read out can be carried out by synthetic engineering of the molecular components. The first example of a completely electronic read out of a nuclear spin of a lanthanide ion (bearing electron and nuclear spins) embedded in a magnetic molecule TbPc2, was recently reported.[3] [1] M. Urdampilleta et.al. Nature Mater. 10, 502 (2011) [2] J. Schwöbel, et. al. Nature Comms. 2, 1953 (2012) [3] R. Vincent, et. al. Nature 488, 357 (2012)

Coffee break (15 min)

Topical Talk HL 76.5 Thu 11:45 H32

Nanomembrane based electrodes for contacting ultra-thin organic layers — •Carlos Cesar Bof Bufon[1], Celine Vervacke[2], Maria Esperança Navarro Fuente[2], Dominic J. Thurmer[2], Christian Müller[5], Michael Fronk[3], Georgeta Salvan[3], Dietrich R. T. Zahn[3], and Oliver G. Schmidt[2,4] — [1]Brazilian Nanotechnology National Laboratory, CNPEM, PO Box 619, 13083-970, Campinas, Brazil — [2]Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstraße 20, 01069, Dresden, Germany — [3]Semiconductor Physics, Chemnitz University of Technology, Reichenhainerstrasse 70, 09107, Chemnitz, Germany — [4]Material Systems for Nanoelectronics, Chemnitz University of Technology, Reichenhainerstrasse 70, 09107 Chemnitz, Germany — [5]Physics Departament, UFPR, Curitiba, Brazil

One of the main challenges for accessing the electronic properties of ultrathin organic layers (UOL), and consequently their application for future devices, consists of connecting such layers to the external word. Two main problems usually arise by trying to vertically connect UOLs: i) the interdiffusion of metallic atoms into the sub-10nm molecular layers, which leads to the damaging and/or the modification of the final device behavior; ii) the presence of pin-holes across the molecular layer, which is responsible for short circuited junctions. Here we discuss the fundamentals, potentialities and limitations of using rolled up nanomembranes as top electrodes for contacting a variety of UOLs, including self-assembled monolayer's and ultra-thin organic semiconducting layers.

Topical Talk HL 76.6 Thu 12:15 H32

Spinterfaces as microscopic spin traps — •Mirko Cinchetti — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Kaiserslautern, Germany

Interfaces between ferromagnetic materials and organic semiconductors - also known as spinterfaces - constitute an incredibly rich playground in the field of spintronics. For example, spinterfaces have the potential to be implemented as tunable spin filters, which will pave the way to a whole new class of advanced, i.e., actively controlled spintronics devices. The progress in the field of spinterface science depends thus critically on elucidating the still unexplored spin-dependent carrier dynamics at such hybrid interfaces.

We use time-resolved two-photon photoemission to optically pump and probe a hybrid electronic state forming at the prototypical spinterface between cobalt and the organometallic complex tris(8-hydroxyquinolinato)aluminium (Alq3). We generate a transient spin polarization in the hybrid interface state, and follow its behavior in four dimensions: energy, time, spin and momentum. We find that electrons are confined at the Co-Alq3 interface for times in the range of 0.5-1 ps, and that the confining potential is strongly spin dependent. Such spin-dependent trapping behavior elucidates the fundamental microscopic origin of the spin-filtering properties at spinterfaces, which is important for the design of next-generation spintronics devices based on tunable organic spin filters.

HL 76.7 Thu 12:45 H32

ESR study of the magnetic properties of the MnPc – F_{16}CoPc dimer — •Azar Aliabadi, Susi Linder, Martin Knupfer, Yulia Krupskaya, Vladislav Kataev, and Bernd Büchner — IFW Dresden, 01069 Dresden

Photoemission spectroscopy has demonstrated a charge transfer at the interface between two transition metal phtalocyanines (MnPc and F_{16}CoPc) indicating the formation of a $MnPc^{\delta+}/F_{16}CoPc^{\delta-}$ heterojunction [1]. In this work, the MnPc-F_{16}CoPc dimer system with charge transfer was investigated using ESR spectroscopy at different temperatures. Comparison between ESR spectra of the parent compounds (MnPc and F_{16}CoPc powders) and of the product of the reaction (MnPc/F_{16}CoPc mixed powder) has revealed characteristic features due to the formation of the MnPc – F_{16}CoPc dimer. We discuss distinct magnetic properties of the MnPc – F_{16}CoPc dimer and their possible relation to the charge transfer in the studied complex.

[1] S. Lindner, M. Knupfer, R. Friedrich, T. Hahn, and J. Kortus, *Phys. Rev. Lett.* **109**, 027601 (2012).

HL 76.8 Thu 13:00 H32

Influence of surface interaction on the properties of single-molecule-magnets — •David Klar[1], Andrea Candini[2], Bernhard Krumme[1], Loic Joly[3], Svetlana Klyatskaya[4], Jean-Paul

Kappler[3], Mario Ruben[3,4], and Heiko Wende[1] — [1]Fakultät für Physik und CENIDE, Universität Duisburg-Essen — [2]Centro S3 Modena, Istituto Nanoscienze - CNR — [3]Institut de Physique et Chimie des Matériaux de Strasbourg, Université de Strasbourg — [4]Institute of Nanotechnology, Karlsruhe Institute of Technology

Due to the consecutive downsizing of devices, single-molecule-magnets as building blocks for spintronic applications are of high interest for actual research. The remanent behavior, caused by the single-ion anisotropy, of $TbPc_2$ molecules in bulk samples at less than 5 K is reported in the literature. Our goal is to investigate and to understand the influence of the surface on the properties of the $TbPc_2$ molecules deposited onto a substrate. Therefore we study submonolayer coverages of $TbPc_2$ molecules on ferromagnetic surfaces like Ni, and on a very inert surface of highly oriented pyrolytic graphite (HOPG) that should maintain the properties of isolated molecules. By XAS and XMCD we analyze the element specific magnetic and electronic properties. The low interaction with the HOPG surface hardly affects the magnetic properties of the molecules and we were able to observe a remanent magnetization, but only at very low temperatures ($T < 4$ K). On the Ni surface an indirect exchange leads to an antiferromagnetic coupling between the molecules and the surface. As a result, we obtained a remanent magnetization at higher temperatures ($T \approx 100$ K).

HL 76.9 Thu 13:15 H32

Paramagnetic organic radicals on rutile TiO2(110) single crystals — •Reza Kakavandi, Sabine-Antonia Savu, Thomas Chassé, and Maria Benedetta Casu — Institute of Physical and Theoretical Chemistry, University of Tübingen, Germany

A novel class of organic compounds, namely the nitronyl nitroxide radicals, has recently gained attention because of its magnetic property. In this work a pyrene-substituted nitronyl nitroxide radical (NitPyn) deposited on well characterized rutile TiO2(110) single crystals has been investigated by using X-ray photoemission spectroscopy (XPS) and near edge X-ray absorption fine structure spectroscopy. The mechanism of molecular adsorption on the well defined surface, the chemical environment at the interface and the electronic structure of thin films are discussed by analyzing the XPS core level signals. The persistence of the paramagnetic character of the molecules is also discussed with respect to the chemisorption on the surface. Our studies clarifies the orientation of the molecule in the thin films as a function of film thickness as well as the influence of the substrate, identifying the fine balance between molecule-molecule and molecule-substrate interactions.

HL 77: Organic electronics and photovoltaics IV (CPP, jointly with DS, HL, O)

Time: Thursday 9:30–13:00 Location: H34

Invited Talk HL 77.1 Thu 9:30 H34

Influence of morphology on organic solar cell performance comparing crystalline diindenoperylene (DIP) and its amorphous derivative tetraphenyldibenzoperiflanthene (DBP) — Stefan Grob, Mark Gruber, Ulrich Hörmann, and •Wolfgang Brütting — Institute of Physics, 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, the four 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. In contrast, the structural disorder in DBP combined with a little smaller optical gap leads to light absorption which is about eight times higher than in DIP, whereby the short-circuit current density almost doubles in corresponding solar cell devices. Moreover, open circuit voltages are high and - due to similar energy level alignments - comparable, by using the materials both as donor with C60 (0.9 V) and as acceptor with 6T (1.2 V). Based on these results, we discuss the influence of different film structure and morphology on electrical transport and device performance.

HL 77.2 Thu 10:00 H34

Influence of fluorine content in manipulating the nanomorphology of PTB7:PC70BM bulk heterojunction systems — •Shuai Guo[1], Jing Ning[1], Volker Körstgens[1], Yuan Yao[1], Chen Lin[1], Stephan Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]HASYLAB at DESY, 22603 Hamburg, Germany

Polymer-based photovoltaics have drawn tremendous attention in both basic research and application fields during the last decade. Here, the up-to-date highest efficient bulk heterojunction system PTB7 with varied fluorine content and the fullerene derivative PC70BM are thoroughly investigated. It is known that the amount of fluorine along the polymer chain strongly influences the film formation and therefore the solar cell performance. Additionally, it is of great interest to explore the effect of solvent additive 1,8-diiodooctane (DIO) on differently fluorinated films. To address the relation between the morphology and efficiency completely, a series of measurements have been done. The film surface structure is investigated by optical microscopy and AFM. The inner film structures, crystal orientation as well as the crystallinity are probed by advanced scattering techniques such as XRR, GISAXS and GIWAXS. By integrating all data, the three-dimensional morphology of the active layer is detected. Consequently, the different morphologies introduced by varying the fluorine content and the addition of DIO are determined and compared with the corresponding performance of these systems.

HL 77.3 Thu 10:15 H34

Influence of nanostructural changes on the charge carrier dynamics in PTB7 based solar cells — •Andreas Zusan[1], Andreas Baumann[2], Jens Lorrmann[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [2]Bavarian Centre for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg

For organic bulk heterojunction solar cells, the blend morphology is one of the most crucial parameters influencing the device performance. Inducing nanostructural changes by means of the use of processing additives is a common practice to increase the power conversion efficiency. Hence, understanding the effect of modified structural properties of organic layers on the charge carrier transport and lifetime is a key issue for further progress in organic photovoltaics. In this context, we applied our novel charge extraction technique OTRACE (Open Circuit Corrected Transient Charge Extraction) to high efficiency solar cells made from the low-bandgap polymer PTB7 in combination with $PC_{70}BM$ using the solvent additive diiodooctane (DIO). The results show two different nongeminate decay regimes identified as a fast direct recombination of free polarons and a trap assisted decay. We find that the DIO induced alteration of the morphology significantly reduces the recombination order of the first regime, whereas it has no influence on the second part arising from the delayed emission of trapped charges. Our explanation based on a multiple-trapping-and-release approach clarifies the large impact of phase separation on charge carrier dynamics.

HL 77.4 Thu 10:30 H34

Diffusion limited charge generation from fullerene excitons in low bandgap polymer solar cells — •Clare Dyer-Smith, Ian Howard, and Frédéric Laquai — Max Planck Institut für Polymerforschung, Mainz, Germany

Organic solar cells with high power conversion efficiencies have been realised in recent years by the use of low bandgap polymers in combination with C70-based electron acceptors to provide good absorption coverage across the entire solar emission spectrum. Diffusion-limited charge generation from fullerene excitons has been observed in such blends, including the high-performance PTB7:PC70BM blend system which is the subject of the present study. We characterise the diffusion-limited charge generation from fullerene excitons in this system using

transient absorption and photoluminescence spectroscopy. Fitting to a simple exciton quenching model allows us to determine the size of fullerene domains in the blend, showing quantitatively how blend morphology limits device performance, and allowing us to identify selection criteria for the optimum blend morphology in devices based upon light-absorbing fullerene acceptors.

HL 77.5 Thu 10:45 H34

Impact of molecular weight on the intrinsic charge carrier mobility of Si-PCPDTBT:[C70]PCBM thin films — •Andreas Fritze[1], Andreas Sperlich[1], Andreas Zusan[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

We investigated the influence of the molecular weight on the performance of solar cells from solution processed Si-PCPDTBT:[C70]PCBM blends. A significant increase in the short circuit current density j_{SC} was found with increasing molecular weight of the polymer. To explain this behavior, we performed transient microwave conductivity (TRMC) experiments and found much higher intrinsic mobilities in thin films based on the higher molecular weight donor. In order to distinguish between the influence of intra- and intermolecular charge transport on the obtained intrinsic TRMC mobility, we used two different solvents to influence the molecular environment in the film. We discuss our findings in view of the impact of the local order, influenced by the molecular weight on the performance of organic solar cells.

HL 77.6 Thu 11:00 H34

Charge generation and recombination in PCPDTBT:PCBM and PSBTBT:PCBM bulk heterojunction photovoltaic blends — •Fabian Etzold, Ian Howard, Michael Meister, and Frédéric Laquai — Max Planck Research Group for Organic Optoelectronics, Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

We present a comparative study of the photophysical processes leading to photocurrent generation and photocurrent loss in photovoltaic blends of the low-bandgap polymer PCPDTBT with PCBM and its silicon-substituted analogue PSBTBT with PCBM studied by Vis-NIR transient absorption pump-probe spectroscopy and variable time-delay double-pump photocurrent extraction experiments. Our experiments demonstrate that the power conversion efficiency of PCPDTBT:PCBM blends is largely limited by sub-nanosecond geminate recombination of interfacial charge-transfer states plus fast non-geminate recombination of free charges competing efficiently with charge extraction. In comparison photovoltaic blends of the silicon-substituted polymer PSBTBT with PCBM exhibit significantly less geminate recombination in conjunction with much slower non-geminate recombination of free charges leading in turn to substantially higher photocurrents and fill factors and thus overall increased photovoltaic performance. We also observed a pronounced excitation wavelength dependence of the photophysical processes occurring after excitation of either the polymer or the fullerene component of the blend at different photon energies. [1] F. Etzold et al., J. Am. Chem. Soc. 2012, 134 (25), 10569-10583.

15 min. break

HL 77.7 Thu 11:30 H34

Charge Generation in PBDTTPD:PCBM and Si-PCPDTBT:PCBM Solar Cells: The Influence of Excess Photon Energy and Electronic Energy Level Offsets — •Steve Albrecht[1], Koen Vandewal[2], Alberto Salleo[2], and Dieter Neher[1] — [1]University of Potsdam, Soft Matter Physics, Potsdam, Germany — [2]Stanford University, Department of Materials Science and Engineering, Stanford, USA

In the last years a dramatic increase in organic solar cell efficiency has been reported with polymers and fullerene derivatives processed from solution. However, the fundamental process involved in the conversion of absorbed photons to free charges is still not fully understood. In this work, we use time delayed collection field (TDCF) **[1]** with variable excitation wavelength to gain inside into the effect of the excess photon energy on the quantum efficiency and field-dependence of free charge carrier generation. With two high efficiency model systems showing either field independent CT-state splitting (PBDTTPD:PCBM) or a weak field-dependence of free charge formation (Si-PCPDTBT:PCBM), we show how the field-dependence changes with direct CT state excitation in the absorption region below the band-gap. Additionally, we show how generation and bimolecular recombination is affected when the fullerene derivative PCBM is exchanged by higher LUMO adducts ICMA, ICBA or ICTA with reduced driving force for CT-state splitting.

[1] Albrecht, S.; Janietz, S.; Schindler, W.; Frisch J.; Neher D., Journal of the American Chemical Society 134 (36), 14932 (2012).

HL 77.8 Thu 11:45 H34

Sub-Bandgap Absorption in Polythiophene–Fullerene Heterojunctions: Experiment and Theory — •Wichard Beenken, Felix Herrmann, Martin Presselt, Harald Hoppe, Sviatoslav Shokhovets, Gerhard Gobsch, and Erich Runge — Technische Universität Ilmenau, Institut für Physik and Institut für Mikro- und Nanotechnologien, 98693 Ilmenau, Germany

Most high-performance organic solar cells base on P3HT/PCBM bulk-heterojunctions. Spectroscopy of the sub-bandgap region, i.e., below the bulk absorption of the individual components, provides unique opportunities to study interface-related properties. In order to characterize some of the unsettled spectral features, we applied quantum-chemical calculations of a oligothiophene–fullerene model complex, which in particular allow us to identify spectral signatures of charge-transfer excitons in the sub-bandgap absorption and external quantum efficiency.

HL 77.9 Thu 12:00 H34

A new multiscale modeling method for simulating the loss processes in polymer solar cell nanodevices — •Anton Pershin, Sergii Donets, and Stephan A. Baeurle — Institute of Physical and Theoretical Chemistry, University of Regensburg, D-93040 Regensburg, Germany

The photoelectric power conversion efficiency of polymer solar cells is till now, compared to conventional inorganic solar cells, relatively low with maximum values ranging from 7% to 8%. This essentially relates to the existence of exciton and charge carrier loss phenomena, significantly reducing the performance of polymer solar cells. Here, we introduce a new computer simulation technique [1], which permits to explore the causes for the occurrence of such phenomena at the nanoscale and to design new photovoltaic materials with optimized opto-electronic properties. Using our approach, we find that the disjunction of continuous percolation paths leads to the creation of dead ends, resulting in charge carrier losses through charge recombination. Moreover, we observe that defects are characterized by a low exciton dissociation efficiency due to a high charge accumulation, counteracting the charge generation process. Finally, by analyzing the photovoltaic behavior of the nanostructures under different circuit conditions, we demonstrate that charge injection at the electrodes determines the impact of the defects on the solar cell performance. [1] A. Pershin, S. Donets, S.A. Baeurle, J. Chem. Phys. 136, 194102 (2012).

HL 77.10 Thu 12:15 H34

Morphology and Charge Transport in Polythiophene/PCBM Blends: Insight from Molecular Simulations — •Olga Guskova[1], Julia Romanova[2], Andreas John[1], Peter Friedel[1], and Jens-Uwe Sommer[1,3] — [1]Leibniz Institute of Polymer Research, Dresden, Germany — [2]University of Namur, Namur, Belgium — [3]TU Dresden, Dresden, Germany

Combined structural-computational approach to study the organic photovoltaic materials, namely mixtures of polythiophenes (donor, D) and [6,6]phenyl-C61-butyric acid methyl ester (acceptor, A) was applied. The quantum mechanical computational level was used (1) to improve the force field for subsequent molecular dynamics (MD) modeling, (2) to calculate the ionization energies, electron affinities, HOMO/LUMO energies and charge transfer characteristics of D/A pair. We have performed a large-scale all-atomistic MD simulation to investigate both the geometry of D/A interface between two crystals and the D/A blend morphology in self-organized systems (the ordering and molecular orientation, the formation of polythiophene paracrystalls and PCBM-rich phases in amorphous regions of polythiophene).

HL 77.11 Thu 12:30 H34

Electroabsorption spectroscopy on organic pin solar cells — •Ellen Siebert-Henze, Vadim G. Lyssenko, Janine Fischer, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, George-Bähr-Str. 1, Dresden, Germany

The built-in voltage has a significant impact on the solar cell performance, but its origins are controversially discussed. In our work

we determine the built-in voltage of small molecule organic solar cells based on the pin concept by electroabsorption spectroscopy (EA).

EA detects the change in absorption caused by an electrical field (Stark effect). A change in DC bias on the device results in a variation of the Stark signal. It is probed adding an AC voltage on top of the DC bias enabling the detection using a lock-in amplifier. Thus, the information about the built-in voltage can be evaluated.

As a model system, flat heterojunction solar cells containing C_{60} as acceptor and MeO-TPD as donor material are investigated. The doping concentration of both the hole and the electron transport layer is modified and it is shown that there is an influence of the consequential change of their work functions on the built-in voltage. Both the short-circuit current as well as the fill factor increase for larger built-in voltages.

HL 77.12 Thu 12:45 H34

First-principles calculations of the TCO-Organic interface in an OLED — •Arno Fey[1], Paul Erhart[2], and Karsten Albe[1] — [1]Fachbereich Material- und Geowissenschaften, Technische Universität Darmstadt, Darmstadt, Germany — [2]Department of Applied Physics, Chalmers University of Technology, Gothenburg, Sweden

The ongoing development in the field of organic light emitting diode (OLED) technology and the continuously improvement towards higher efficiencies has created a need to understand the interaction between the different layers in an OLED. In this contribution we focus on the interface of the transparent conductive oxide (TCO) and the organic molecule. The interaction between the polar and hydrophilic oxide surface on the one side and the organic and non-polar thin film on the other side determines the growing of the organic film and therefore directly influences the conductivity. The calculations based on the density functional theory (DFT) were carried out using the Vienna ab initio simulation Package (VASP) with Generalized Gradient Approximations (GGA).

HL 78: Graphene: Preparation and characterization I (O, jointly with HL, TT)

Time: Thursday 10:30–13:15 Location: H17

HL 78.1 Thu 10:30 H17

Synthesis of graphene on $(6\sqrt{3}\times 6\sqrt{3})$R30° reconstructed SiC surfaces by molecular beam epitaxy — •Timo Schumann[1], Martin Dubslaff[1], Myriano H. Oliveira Jr.[1], Michael Hanke[1], Felix Fromm[2], Thomas Seyller[2,3], J. Marcelo J. Lopes[1], and Henning Riechert[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]Lehrstuhl für Technische Physik, Friedrich-Alexander-Universitt Erlangen-Nürnberg, Erlangen, Germany — [3]Institut für Physik, Technische Universität Chemnitz, Chemnitz, Germany

We report on the synthesis of graphene on a $(6\sqrt{3}\times 6\sqrt{3})$R30° reconstructed SiC(0001) surface (a.k.a. *buffer layer*) by means of molecular beam epitaxy (MBE). Raman spectroscopy reveals that the quality of the MBE-grown graphene films increases with growth time and that the average crystallite size exceeds 20 nm. X-ray photoelectron spectroscopy confirms that the thickness of the films increases as a function of the growth time and proves that the buffer layer is preserved during the growth process. In addition, grazing-incidence X-ray diffraction measurements were performed at the beamline ID10 of the ESRF in Grenoble. In-plane reflections of the buffer layer, the SiC, as well as from the MBE-synthesized graphene, were investigated. Strikingly, despite their nanocrystalline nature, it is observed that the graphene films grown by MBE show an in-plane alignment to the substrate, revealing that a conventional epitaxial growth on the buffer layer takes place. The results will be discussed in the context of MBE growth of graphene considering the most recent data reported in the literature.

HL 78.2 Thu 10:45 H17

Microscopic characterization of CVD grown graphene suspended on TEM grids — •Florian Studener[1], Luca Bignardi[1], Willem van. Dorp[1], Steffano Gottardi[1], Oleksii Ivashenko[1], Pavel Dudin[2], Alexei Barinov[2], Petra Rudolf[1], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG Groningen, Netherlands — [2]Sincrotrone Trieste S.C.p.A, 34149 Basovizza, Trieste, Italy

We investigated CVD grown graphene, which was transferred and suspended on a TEM grid. Both electronic and structural properties were investigated. The former were investigated with angle resolved photoelectron spectroscopy and microscopy, while the latter were analysed with Raman spectroscopy and transmission electron microscopy. We could observe that CVD grown graphene has comparable characteristics with free standing graphene produced with micro cleavage, e. g. the Fermi velocity of 1*10-6 m/s is close to the theoretically expected value. Despite the polycrystalline nature of the Cu foil used as a substrate for the graphene growth, the obtained graphene exhibits large single-crystalline domains up to tens of microns. Thus, the presented transfer method can be successfully exploited for clean TEM substrates for further investigations.

HL 78.3 Thu 11:00 H17

Graphene-enhanced versus Surface-enhanced Raman Scattering — •Fatemeh Yaghobian, Tobias Korn, and Christian Schüller — Institute of Experimental and Applied Physics University of Regensburg D-93040 Regensburg, Germany

Graphene-enhanced Raman scattering (GERS) is emerging as an important method due to the need for highly reproducible, quantifiable and biocompatible active substrates. As a result of its unique two dimensional carbon structure, graphene provides particularly large enhanced Raman signals of molecules at its surface. In this work, it is demonstrated that graphene works as active substrate for enhanced Raman scattering and has a great potential in biosensing because of its ability to quench interfering fluorescence. Obtained GERS signals of different molecules with reproducible enhancement factors are discussed and compared with surface-enhanced Raman scattering (SERS) signals on highly active substrates, covered with spherical silver nanoparticles. We have also observed an upshift in the frequency of the breathing mode of a test molecule, when adsorbed on graphene, in contrast to measurements on silver nanoparticles, where the frequencies remain unchanged.

HL 78.4 Thu 11:15 H17

Dynamics of adsorbate layers on freestanding graphene probed by ultrafast low-energy electron diffraction — •Max Gulde[1], Simon Schweda[1], Manisankar Maiti[1], Hakki Yu[2], Sascha Schäfer[1], and Claus Ropers[1] — [1]Materials Physics Institute and Courant Research Centre, University of Göttingen, Germany — [2]Department of Dynamics at Surfaces, Max Planck Institute for Biophysical Chemistry, University of Göttingen, Germany

Ultrafast structural dynamics in solids and nanostructures can be observed by an increasing number of sophisticated electron and x-ray diffraction techniques. Despite successful implementations of ultrafast reflection high-energy electron diffraction (1,2), the diffractive probing of ultrafast structural processes at surfaces remains an experimental challenge. We have implemented ultrafast low-energy electron diffraction (ULEED) to study structural changes with high temporal resolution and ultimate surface sensitivity, at electron energies from 100 eV to 500 eV. Specifically, we ultilize nanoscopic needle emitters in an electrostatic lens geometry as high-brightness sources of pulsed electrons. With this approach, the ultrafast melting dynamics of ordered adsorbate structures on freestanding graphene is investigated in transmission with a temporal resolution below 5 ps.

(1) A. Hanisch-Blicharski, A. Janzen, B. Krenzer, S. Wall, F. Klasing, A. Kalus, T. Frigge, M. Kammler, and M. Horn-von Hoegen, Ultramicroscopy (accepted) (2012)

(2) S. Schäfer, W. Liang, and A. H. Zewail, J. Chem. Phys. 135, 214201 (2011)

HL 78.5 Thu 11:30 H17

High-Temperature STM of the Ordering of an Amorphous Carbon Layer into Graphene on Ru(0001) — Sebastian Günther[1], Sebastian Dänhardt[2], •Martin Ehrensperger[2], Patrick Zeller[2], Stefan Schmitt[3], and Joost Wintterlin[2] — [1]Chemie Department, Technische Universität München, Germany — [2]Department Chemie, Ludwig-Maximilians-Universität München, Germany — [3]SPECS GmbH, Voltastr. 5, D-13355 Berlin, Germany

An amorphous carbon layer was prepared on Ru(0001) by chemical

vapor deposition of ethylene at about 650 K. High-Temperature Scanning Tunneling Microscopy (HTSTM), Low Energy Electron Diffraction and Temperature Programmed Desorption measurements were used to characterize the layer and its formation. The obtained carbon layer then served as amorphous precursor in an ordering transition towards graphene. At temperatures between 920 and 950 K the layer transformed into graphene which was indicated by the evolving moiré pattern. The ordering was monitored *in situ* by HTSTM. The observations revealed a unique mechanism involving mobile, small topographic holes that move through the disordered carbon layer leaving graphene behind. The transport of carbon monomers mediated by these holes opens a low-energy pathway for the ordering transition. In a dense packed graphene layer this mechanism is impossible which can explain the problems of healing defects in chemically synthesized graphene.

HL 78.6 Thu 11:45 H17

***In situ* LEEM Investigations of the Growth of Graphene on Ni(111)-Films** — •Patrick Zeller[1], Michael Weinl[2], Florian Speck[3], Markus Ostler[3], Thomas Seyller[3], Matthias Schreck[2], and Joost Wintterlin[1] — [1]Department Chemie, Ludwig-Maximilians-Universität München — [2]Institut für Physik, Universität Augsburg — [3]Department für Physik, FAU Erlangen-Nürnberg

We report about low energy electron microscopy (LEEM), scanning tunneling microscopy (STM), auger electron spectroscopy (AES) and x-ray photoelectron spectroscopy (XPS) investigations of graphene grown on single-crystalline Ni(111) films. The films, which may provide an easy and economical way towards a scalable graphene synthesis, consist of 150 nm thick, heteroepitaxially grown Ni(111) layers on a Si(111) wafer with a YSZ-buffer layer. Monolayer graphene was grown by chemical vapor deposition of ethylene and *in situ* LEEM investigations of the graphene growth were performed. Also the formation of nickel carbide and its transformation into graphene were observed. Furthermore we noticed an involvement of the bulk during the reaction. At the beginning of the ethylene dosing the C atoms dissolve in the bulk, and after nucleation segregation of C atoms starts. We could also observe the healing of rotated graphene towards aligned, high quality graphene in a small temperature range. Also a temperature dependent formation and healing of dislocation lines in the Ni films was observed.

HL 78.7 Thu 12:00 H17

Growth of graphene on a stepped iridium surface: morphology, domains and electronic fingerprints — •Iva Šrut[1], Vesna Mikšić Trontl[1], Petar Pervan[1], Fabian Craes[2], Thomas Michely[2], Carsten Busse[2], and Marko Kralj[1] — [1]Institut za fiziku, Bijenička 46, 10000 Zagreb, Croatia — [2]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany

A promising route for modification of graphene properties is the growth of graphene on a substrate with a periodic arrangement of steps. We have used scanning tunneling microscopy and spectroscopy (STM/STS) and low energy electron diffraction (LEED) to study the growth of graphene on such periodically stepped Ir(332) surface. We have found that graphene continuously extends over iridium terraces and steps. Moreover, new distinctive mesoscopic features of the underlying surface are formed involving large, flat terraces accompanied by groups of narrower steps [1]. These morphologically different regions are also distinctive by their spectroscopic features found in STS. The distribution of the newly formed terraces as well as the contribution of various graphene orientations is sensitive to the preparation temperature. Below 800°C we find that the terrace width distribution is closer to the intrinsic distribution of clean Ir(332) than for higher temperatures. Additionally, graphene grown at low temperatures has a prominent contribution of a domain rotated by 30° with respect to the substrate. We find that the microscopic shape of steps after graphene formation strongly depends on the orientation of graphene.

[1] I. Šrut, et al., submitted

HL 78.8 Thu 12:15 H17

Phonons of graphene on Ir(111) — •Michael Endlich[1], Alejandro Molina-Sánchez[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 phonon dispersion relations of graphene on Ir(111) were determined with angle-resolved inelastic electron scattering. A weak graphene–Ir interaction is inferred from the lifting of the degeneracy of the out-of-plane optical and acoustic dispersion branches at the $\bar{K}$ point of the surface Brillouin zone and from the energy reduction of the out-of-plane optical phonon. Despite this interaction the Kohn anomalies known from graphite of the highest optical phonon branch at $\bar{\Gamma}$ and $\bar{K}$ persist. The experimental dispersion relations are in agreement with density functional calculations.

HL 78.9 Thu 12:30 H17

Support restructuring during graphene growth on Cu foils triggers the formation of non flat membranes — •Jürgen Kraus[1], Sebastian Böcklein[2], Robert Reichelt[1], Benito Santos[3], Tevfik O. Mentes[3], Andrea Locatelli[3], and Sebastian Günther[1] — [1]Technische Universität München Chemie Department, D-85748 Garching — [2]Ludwig-Maximilians-Universität, D-81377 München — [3]Sincrotrone Trieste, I-34149 Trieste - Basovizza

Meanwhile the growth of single crystalline graphene flakes on Cu foils at a mm-length scale can be achieved, which provides a potential source for high quality graphene. On the other hand, the g-Cu system still suffers from certain inherent defects: during graphene growth sequences of inclined Cu facets form which are visible in scanning electron microscopy (SEM) images as stripes and which have been observed as well applying atomic force microscopy (AFM) and scanning tunneling microscopy (STM). Since the graphene follows the morphology of the underlying Cu foil the support restructuring leads to the formation of so called nanorippled graphene which persists even if the graphene is transferred on a flat Si wafer. In our study, we identified a sequence of such Cu facets after graphene growth on a Cu foil using low energy electron microscopy (LEEM) and show why the graphene cannot flatten when removed from the support. In addition, we were able to prepare graphene membranes by the local electrochemical removal of the Cu foil underneath the grown graphene. We show that the resulting membranes are exact replicas of the former morphology of the Cu foil during growth, i.e. they are non flat membranes.

HL 78.10 Thu 12:45 H17

Graphene on Rh(111) and Ru(0001): combined STM/NC-AFM and DFT studies — •Yuriy Dedkov[1], Torben Haenke[1], Oliver Schaff[1], Andreas Thissen[1], Elena Voloshina[2], and Mikhail Fonin[3] — [1]SPECS Surface Nano Analysis GmbH, Voltastraße 5, 13355 Berlin, Germany — [2]Physikalische und Theoretische Chemie, Freie Universität Berlin, 14195 Berlin, Germany — [3]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

The electronic and crystallographic structure of graphene moiré on Rh(111) and Ru(0001) is studied via combination of density-functional theory calculations and scanning tunneling and noncontact atomic force microscopy (STM and NC-AFM). Whereas the principal contrast between hills and valleys observed in STM does not depend on the sign of applied bias voltage, the contrast in atomically resolved AFM images strongly depends on the frequency shift of the oscillating AFM tip. The obtained results demonstrate the perspectives of application atomic force microscopy/spectroscopy for the probing of the chemical contrast at the surface.

HL 78.11 Thu 13:00 H17

Epitaxial graphene nanoflakes on Au(111): Structure, electronic properties and manipulation — •Mikhail Fonin[1], Philipp Leicht[1], Lukas Zielke[1], Elena Voloshina[2], and Yuriy S. Dedkov[3] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Institut für Chemie und Biochemie - Physikalische und Theoretische Chemie, Freie Universität Berlin, 14195 Berlin, Germany — [3]SPECS Surface Nano Analysis GmbH, 13355 Berlin, Germany

Graphene nanoribbons and graphene dots have been proposed to exhibit such peculiar phenomena like localized edge states or edge magnetism. The aim of the present study is the investigation of structural and electronic properties of epitaxial graphene nanoflakes on the Au(111) surface.

Upon in situ preparation, we observe a formation of two types of nanoflakes, which are either embedded in the gold surface or sit directly on top of Au(111). In all cases, flakes reveal a moiré contrast, which is modulated by the herring-bone reconstruction of the Au(111) surface with the moiré period depending on the orientation of the graphene sheet in relation to the substrate. We show that quasi-free-standing graphene nanoflakes can be easily manipulated by the STM tip regardless of the flake size. The details of the structure and electronic properites of such quasi-free-standing flakes are discussed upon comparison with graphene dots on Ir(111).

HL 79: Focus Session: Frontiers of electronic structure theory VI (O, jointly with HL, TT)

Time: Thursday 10:30–13:15 Location: H36

Topical Talk HL 79.1 Thu 10:30 H36

Atomic-scale design of energy materials — •Karsten W. Jacobsen — CAMD, DTU Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

The design of new materials for more efficient production and use of sustainable and clean energy is of utmost importance for the standard of living all over the World the coming years. In the talk I shall describe some computational efforts to design new materials related to solar energy in particular to the conversion of light into hydrogen fuel through water splitting. We have employed computational screening to search for stable semiconductor materials with an appropriate bandgap, band edge alignment, and with sufficient stability to be relevant for light-induced water splitting. In particular we have focused on materials in the cubic perovskite structure but also more generally materials in the ICSD database. The screening of bandgaps is performed using the so-called GLLB-functional which is shown to give reasonable estimates of light absorption for a number of different systems. The stability of the materials towards dissolution in water is investigated through the construction of Pourbaix diagrams combining DFT calculations and experimental information about solution energies.

The talk will also cover some recent efforts in using machine-learning techniques to develop new electronic density functionals. The functional construction uses Tikhonov regularization to obtain smooth functionals and employs bootstrapping to avoid overfitting. The new functionals are named Bayesian Error Estimation Functionals (BEEF) because they automatically offer error estimation on calculated results.

HL 79.2 Thu 11:00 H36

A new computational screening approach for co-catalysts for water splitting:
Disentangling electron and proton transfer. — •Harald Oberhofer, Daniel Berger, Ran Jia, and Karsten Reuter — TU München, Germany

Recently, computational screening techniques have made great progress in the identification and classification of promising new materials for (photo-)catalytic water splitting. Yet, contributions of so called co-catalysts—nano-sized particles enhancing the reaction kinetics—have so far not been addressed. In our contribution we present a novel first-principles thermodynamic approach based on earlier work by Nørskov and Rossmeisl [J. Phys. Chem. B **108**, 17886 (2004)] to gauge the efficiency of co-catalyst particles and search for favourable combinations of catalyst surface and co-catalyst particle. Additionally, we study reaction pathways other than the commonly assumed proton-coupled electron transfer. Our results show that these uncoupled paths can lead to new, unexpected behaviour: Catalysts predicted to have a good reactivity considering only coupled mechanisms might actually get stuck in charged intermediates, while others can be much more reactive than anticipated.

HL 79.3 Thu 11:15 H36

An extended Pareto approach to computational materials design — •Kurt Lejaeghere[1], Stefaan Cottenier[1,2], and Veronique Van Speybroeck[2] — [1]Center for Molecular Modeling, Ghent University, Zwijnaarde, Belgium — [2]Department of Materials Science and Engineering, Ghent University, Zwijnaarde, Belgium

Because of competing design criteria, it is often hard to decide on one particular material as the best solution for a given need. A multidimensional optimization strategy can already narrow down the initial large set of candidates to a much smaller number of promising materials, the Pareto-optimal set. Quite often, however, this set contains more materials than can be afforded for further systematic examination. An ordering within this set, highlighting the most promising candidates, would be very useful to expedite the design process. Conventional Pareto approaches cannot offer such a ranking. We present an algorithm to do exactly this.

This procedure is applied to a set of binary tungsten alloys to look for a candidate first-wall material for nuclear fusion purposes. Because of the harsh operating conditions inside (future) fusion reactors, materials selection is a critical aspect there. Tungsten is a promising first-wall material, but several issues, such as room-temperature brittleness, are still to be resolved. Alloying tungsten with other elements is one possible way of overcoming these problems. By combining a computational screening study (at the DFT-PBE level) with our extended Pareto analysis, a select number of alloys is presented as most promising candidates for further experimental investigation.

HL 79.4 Thu 11:30 H36

Automated system for massive sets of first-principles calculations — •Atsushi Togo and Isao Tanaka — Department of Materials Science and Engineering, Kyoto University, Yoshida-honmachi, Sakyo-ku, Kyoto, Japan

Large systematic sets of first principles calculations can provide information that cannot be obtained merely by a single calculation. Computation of phonon, cluster expansion, and data mining are typical examples that require massive sets of calculations. If each of single calculation is independent to the others, it is trivial to handle massive calculations consecutively. However it is annoying if a calculation has to wait for the previous calculations to finish. We have been developing an automated system. This system is composed of an automation algorithm and interfaces for a first-principles calculation code (VASP) and a batch-queuing system (grid engine). Small tools are prepared to handle crystal symmetry and dynamical properties. As an application, an algorithm for crystal structure search is implemented. The automation algorithm is as follows. We define 'task'. A task is made of 'task elements', where each task element is designed to be also a task. A task may be composed of a series of task elements. In this case, each task element waits for the previous task element to finish. A task may be composed of task elements that are mutually independent. In this case, all task elements are distributed into computers at the same time. By describing each kind of task in a similar manner, a task is easily built into the other task as a task element.

HL 79.5 Thu 11:45 H36

Bandgap Engineering via Nanoporosity in ZnO — Ilker Demiroglu[1], Sergio Tosoni[1], Francesc Illas[1], and •Stefan Bromley[1,2] — [1]Departament de Química Física and Institut de Química Teòrica i Computacional, Universitat de Barcelona (IQTCUB), 08028 Barcelona, Spain — [2]Institució Catalana de Recerca i Estudis Avançats (ICREA), 08010 Barcelona, Spain

Following previous studies [1-3], we have mined databases of 4-connected nets to generate novel nanoporous ZnO structures. Using density functional theory and GW calculations, we calculate the energetic stability and band gaps of >80 distinct nanoporous ZnO solids. We find that the degree and type of nanoporosity is inextricably linked with band gap magnitude. Increasing the degree of nanoporosity tends reduce energetic stability and increase the band gap. Within this tendency, we also find significant variations in band gap (˜0.5 eV) for structures with very similar densities or energetic stabilities but different types of nanoporosity (e.g. pore size). We estimate that altering the degree/type of nanoporosity could allow tailored band gap values up to ˜4.2 eV. This proposed nanomorphological approach to band gap engineering potentially opens the door to optoelectronically tunable sensors, solar cells and other unforeseen devices which could take advantage of this versatile combination.

[1] J. Carrasco, F. Illas and S. T. Bromley, PRL 99, 235502 (2007). [2] M. A. Zwijnenburg, F. Illas and S. T. Bromley, PRL 104, 175503 (2010). [3] D. Stradi, F. Illas, S. T. Bromley, PRL 105, 045901 (2010).

HL 79.6 Thu 12:00 H36

Phonon-mediated quantum processes in materials — •Emmanouil Kioupakis — University of Michigan, Ann Arbor, MI, USA

Higher-order quantum processes enabled by the coupling of charge carriers to lattice vibrations can play an important role in the operation of modern electronic and optoelectronic devices. First-principles calculations based on density functional theory can provide insight into the fundamental nature of phonon- assisted quantum processes in materials and their impact on device performance. In this talk, I will discuss our recent work on phonon-assisted quantum processes with first-principles techniques. I will show how phonon- assisted Auger recombination gives rise to the observed efficiency loss in nitride light-emitting diodes. Moreover, I will demonstrate that first-principles techniques can accurately reproduce the phonon-assisted optical absorption spectrum of silicon. Last, I will show that phonon-mediated

free-carrier absorption leads to optical loss in transparent conducting oxides and semiconductor lasers. The developed techniques are general and can be applied to study phonon-assisted quantum processes in any material. This work was done in collaboration with C. G. Van de Walle, P. Rinke, K. Delaney, A. Schleife, F. Bechstedt, D. Steiauf, H. Peelaers, J. Noffsinger, S. G. Louie, and M. L. Cohen.

HL 79.7 Thu 12:15 H36

Electron-hole puddles in the absence of charged impurities — •Marco Gibertini[1,2], Andrea Tomadin[2], Francisco Guinea[3], Mikhail I. Katsnelson[4], and Marco Polini[2] — [1]Theory and Simulations of Materials, École Polytechnique Fédérale de Lausanne, Station 12, 1015 Lausanne, Switzerland — [2]NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, I-56126 Pisa, Italy — [3]Instituto de Ciencia de Materiales de Madrid (CSIC), Sor Juana Inés de la Cruz 3, E-28049 Madrid, Spain — [4]Radboud University Nijmegen, Institute for Molecules and Materials, NL-6525 AJ Nijmegen, The Netherlands

It is widely believed that carrier-density inhomogeneities ("electron-hole puddles") in single-layer graphene on a substrate such as quartz are due to charged impurities located close to the graphene sheet. In this talk we demonstrate by using a Kohn-Sham-Dirac density-functional scheme that corrugations in a real sample are sufficient to determine electron-hole puddles on length scales that are larger than the spatial resolution of state-of-the-art scanning tunneling microscopy.

HL 79.8 Thu 12:30 H36

Ab-initio transport calculations of functionalized graphene flakes — •Michael Walz, Alexei Bagrets, and Ferdinand Evers — Institut für Nanotechnologie, Karlsruher Institut für Technologie (KIT), D-76021 Karlsruhe, Germany

These days, nanoelectronics is focused on molecular systems such as single organic molecules, graphene ribbons, functionalized graphene flakes, carbon nanotubes.

In our project, we calculate the transmission and the local current density in graphene flakes which are functionalized by adsorbed atoms. We are especially interested in current patterns associated with the functionalized carbon atoms and the role of quantum interference effects.

Performing such calculations starting from first principles is challenging because of high computational costs. On this account, we work with the parallelized *ab-initio* framework FHI-aims, on top of which we implement our own transport calculations using non-equilibrium Green's functions (NEGF) techniques with standard functionals [1,2]. Such *ab-initio* transport studies already exist for the field of Molecular Electronics. Our effort presents a first step towards the broader scope of meso-sized molecular materials in general.

[1] V. Blum *et al.*, Comput. Phys. Commun. **180**, 2175 (2009).
[2] A. Arnold *et al.*, J. Chem. Phys. **126**, 174101 (2007).

HL 79.9 Thu 12:45 H36

Thermionic emission from metal surfaces: A first principles study — •Johannes Voss[1], Sharon Chou[1], Aleksandra Vojvodic[1,2], Igor Bargatin[3], Roger Thomas Howe[1], and Frank Abild-Pedersen[2] — [1]Stanford University, USA — [2]SLAC National Accelerator Laboratory, USA — [3]University of Pennsylvania, USA

The ability to lower the temperatures required for sufficient electronic emission from hot cathodes would lead to more efficient thermionic energy converters and electron guns. Thermionic emission of electrons from metal surfaces is governed by the work function and tunneling probabilities. While the former can be extracted easily from ab initio band structure calculations, for the latter, scattering properties of the surface need to be taken into account.

Here, we present density functional theory calculations of thermionic emission currents based on a non-equilibrium Green's function approach. We compare these results to experiments both for clean and coated metal surfaces. Based on an analysis of interactions in the coating layers, we suggest design pathways for new materials with higher emission current densities.

HL 79.10 Thu 13:00 H36

Comparative computational study of Li, Na, and Mg diffusion in bulk Si: influence of cooperative effects, vibrations, and atom-centered bases — •Sergei Manzhos[1], Oleksandr Malyi[1], and Teck L. Tan[2] — [1]Department of Mechanical Engineering, National University of Singapore, Blk EA #07-08, 9 Engineering Drive 1, Singapore 117576 — [2]Institute of High Performance Computing, A*STAR, 1 Fusionopolis Way, #16-16 Connexis, Singapore 138632

Si is one of the most efficient anode materials for Li ion batteries. At the same time, for bulk storage and/or high energy density applications, Na and Mg are advantageous due to low cost and abundance of Na and high energy density in the case of Mg. Yet the performance of Si as anode material for Na and Mg batteries is still understudied. We present a comprehensive computational study of diffusion barriers of Li, Na, and Mg in Si including cooperative effects (influence of neighboring metal atoms on the barrier). Interactions between metal atoms in Si cause a significant lowering of the diffusion barrier; this effect is increasing when going from Li to Na to Mg. Zero-point vibrations (ZPE) affect migration barriers strongly and differently for different metals, increasing the barrier for Li diffusion, having little effect on Na, and decreasing the barrier for Mg. Most calculations to date for metal ion diffusion in battery electrodes were done using plane-wave based codes. We present an analysis of the effects due to atomic-centered basis selection. To the best of our knowledge, this is the first study of the effects of ZPE and atomic-centered bases on the computed properties of battery electrodes.

HL 80: II-VI-compounds other than ZnO

Time: Thursday 11:45–13:00 Location: H15

HL 80.1 Thu 11:45 H15

Point native defects and p-type conductivity of ZnRh2O4: a first principles study — Oksana Volnianska[1] and •Piotr Boguslawski[1,2] — [1]Institute of Physics PAS, al. Lotnikow 32/46, 02-668 Warsaw, Poland — [2]Institute of Physics, Kazimierz Wielki University, 85-064 Bydgoszcz, Poland

Transparent conducting oxides are the subject of active current research in the context of applications in semiconductor devices and photovoltaics. ZnRh2O4, with the band gap of about 2.2 eV, is a member of this class. It crystallizes in the spinel structure, and exhibits a p-type conductivity. Using the density functional theory within the generalized gradient approximation we calculated the electronic structure and formation energies of point native defects in ZnRh2O4 (vacancies, interstitials, and antisites). In the oxygen-rich conditions, there are two defects with formation energies lower than 1 eV, and therefore expected to occur at high concentrations, namely the zinc vacancy and the zinc antisite. Both defects are shallow acceptors that can be responsible for the observed p-type conductivity of ZnRh2O4. Formation energies of the remaining defects exceed 3 eV, and thus they are not expected to affect properties of ZnRh2O4.

Supported by EU within European Regional Development Fund through grant Innovative Economy (POIG.01.03.01-00-159/08, "InTechFun").

HL 80.2 Thu 12:00 H15

Importance of oxygen vacancies for the two dimensional metallic state at the surface of $SrTiO_3$ — •Juan Shen, Harald O Jeschke, and Roser Valenti — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt am Main

We analyze by means of density functional theory (DFT) the electronic structure of various oxygen-deficient ($SrTiO_3$) surface slabs. We find a significant surface reconstruction after introducing oxygen vacancies and we show that the charges resulting from surface-localized oxygen vacancies -independently of the oxygen concentration- redistribute in the surface region and deplete rapidly within a few layers from the surface suggesting the formation of a two-dimensional electron system (2DES). We also investigate possible oxygen-vacancy clustering effects and discuss our results in the context of recent angle-resolved photoemission spectroscopy observations of a highly metallic 2DES at the (001) vacuum-cleaved surface of $SrTiO_3$.

HL 80.3 Thu 12:15 H15

Towards ion beam synthesis of single CdSe nanocrystal quantum dots in a SiO_2 matrix — •Hans Moritz Mangold[1], Jörg B. Kinzel[1], Helmut Karl[2], Hubert J. Krenner[1], and Achim Wixforth[3] — [1]Emmy Noether Group at Lehrstuhl Experimentalphysik 1, Universität Augsburg, Deutschland — [2]Lehrstuhl Experimentalphysik IV, Universität Augsburg, Deutschland — [3]Lehrstuhl Experimentalphysik I, Universität Augsburg, Deutschland

II-VI compound semiconductor quantum dots (QDs) are a promising class of materials for applications in optical devices in the visible spectral domain. Here we show that in addition to traditional fabrication techniques such as molecular beam epitaxy or chemical synthesis, high fluence ion-beam implantation followed by a rapid thermal annealing step, can be readily applied to synthesize CdSe nanocrystals with superior optical properties within the thermal oxide on a Si wafer. In order to confine the implantation volume we employ chromium masks with arrays of nanoscale aperture openings with diameters smaller than 250nm. We analyzed the such implanted and annealed samples by scanning electron microscopy and micro-photoluminescence spectroscopy. We observe a pronounced broadening and blue shift of the nanocrystal emission when decreasing the aperture diameter to $< 1000\,\mathrm{nm}$. We attribute this behavior to a reduction of the mean nanocrystal size but increase of its size distribution. For the smallest aperture sizes used we observe a pronounced shell-filling behavior characteristic for single quantum dot nanoemitters.

HL 80.4 Thu 12:30 H15

Blue lasing and strong coupling in ZnSe monolithic microcavities — •Kathrin Sebald, Moritz Seyfried, Sebastian Klembt, Carsten Kruse, Detlef Hommel, and Jürgen Gutowski — Institute of Solid State Physics, University of Bremen, Germany

Microcavity structures which consist of a cavity located between two distributed Bragg reflectors can be used to study light-matter interaction in the weak and strong coupling regime. In this contribution microcavities with one or three ZnSe quantum wells embedded into the cavity are presented. By increasing the number of implemented ZnSe quantum wells strong coupling was demonstrated to be achieved with a Rabi splitting energy in the order of 19 meV. By excitation density dependent measurements the transition from the strong to the weak coupling regime was observed. In addition, sample areas with a smaller quality factor show already at low excitation densities just the bare cavity emission. This cavity emission reveals a minimal lasing threshold of 5 pJ for the cavity photons. From the integrated intensity of the sample in the strong and weak coupling regime the β factor can be estimated which describes the fraction of spontaneous emission coupled into the cavity mode. As expected, the sample area with the pure cavity emission possesses a small β factor of 0.01 comparable to classical VCSEL structures. In contrast to that the β factor reaches a value of 0.18 in the sample area where the strong coupling regime was observed.

HL 80.5 Thu 12:45 H15

Control of the spontaneous emission of CdTe QDs by means of micropillar cavities — •Tomasz Jakubczyk[1,2], Wojciech Pacuski[1,2], Tomasz Smoleński[1], Matthias Florian[3], Frank Jahnke[3], Carsten Kruse[2], Piotr Kossacki[1], and Detlef Hommel[2] — [1]Institute of Experimental Physics, Faculty of Physics, University of Warsaw, Poland — [2]Institute of Theoretical Physics, University of Bremen, Germany — [3]Institute of Solid State Physics, University of Bremen, Germany

Pillar microcavities containing quantum dots (QDs) represent an excellent tool for exploring and enhancing effects due to the light-matter interaction in semiconductor structures. We present results prooving a significant improvement of the control over the spontaneous emission of CdTe/ZnTe QDs by means of an all-epitaxial ZnTe-based pillar cavity.

We investigated QD's excitonic emission near resonance with the fundamental micropillar cavity mode. Temperature variation of the detuning between the exciton energy and the cavity mode was performed and a significant shortening of the decay time for the QD state was found at zero-detuning. A Purcell factor over 5 was determined and confirmed by the extended transfer matrix method calculations.

HL 81: Focus Session: Extended defects in semi- and nonpolar GaN II

Continuation of the morning session.
Afternoon session: Surfaces, adatomkinetics and indium incorporation in non- and semipolar surfaces / Defect associated luminescence in semipolar GaN / Semipolar InGaN quantum wells and doping of non-polar GaN

Time: Thursday 14:45–18:15 Location: H13

HL 81.1 Thu 14:45 H13

Energetics of step-edges and adatom kinetics on m-plane GaN surfaces: Implications for surface roughening and in-plane growth anisotropy. — •Andrew Duff[1], Liverios Lymperakis[2], and Jörg Neugebauer[2] — [1]Leibniz-Institut für Kristallzüchtung, Berlin — [2]Max-Planck-Institut für Eisenforschung, Düsseldorf

Growth of non-polar m-plane GaN surfaces have attracted considerable interest due to the absence of polarization fields associated with the growth of polar surfaces. Typical m-plane GaN grown by MBE is characterized by a strong in-plane anisotropy in the form of elongated stripes along the [11-20] direction. However, recent growth experiments have demonstrated that atomically smooth m-plane surfaces can be achieved for growth on inclined substrates even under N-rich conditions in contrast to c-plane growth [1]. Full control of the growth of non-polar GaN surfaces requires an atomic-scale understanding of the mechanisms underlying the growth. Hence in the present work, step-edge energetics and adatom kinetics (i.e. Ehrlich-Schwoebel barriers), both in the presence of step-edges as well as on flat terraces, are investigated using density functional theory. Step-edge formation energies are found to be prohibitively large under both N- and Ga-rich conditions, consistent with the achievable smooth growth observed in both N- and Ga-rich regimes. The effect of temperature and the interplay between surface and step-edge energetics and adatom kinetics are addressed with kinetic Monte Carlo simulations, providing physical insight into the anisotropic character of non-polar growth of GaN.

[1] M. Sawicka et al, Phys. Rev. B 83, 245434 (2011).

HL 81.2 Thu 15:00 H13

Electronic states at nonpolar GaN surfaces investigated by photoelectron spectroscopy and optical anisotropy spectroscopy — •Marcel Himmerlich[1], Anja Eisenhardt[1], Jochen Räthel[2], Eugen Speiser[2], Norbert Esser[2], and Stefan Krischok[1] — [1]Institut für Physik and Institut für Mikro- und Nanotechnologien, TU Ilmenau, PF 100565, 98684 Ilmenau, Germany — [2]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Albert-Einstein-Straße 9, 12489 Berlin, Germany

In-situ investigations were carried out on homoepitaxially grown nonpolar m-plane (1-100) and a-plane (11-20) GaN surfaces. Occupied surface states 3.1 and 3.2 eV below the Fermi energy are identified using photoelectron spectroscopy (PES). These states are involved in anisotropic optical transitions at photon energies of 3.2 and 3.3 eV for the m-plane and a-plane configurations, respectively, as confirmed by reflection anisotropy spectroscopy (RAS). Additionally, an optical transition at 4.7 eV was found in RAS. Excitonic and electronic surface band contributions in the RAS measurement were disentangled by comparing spectra of clean and oxidized surfaces. The experimental results are compared to calculated surface band structures from the literature. Furthermore, the influence of oxidation on the surface electronic properties and the correlated optical properties was also investigated. Besides degradation of the initial surface states, a reduction of the upward bend bending by 0.4 eV is found for both cases.

HL 81.3 Thu 15:15 H13

Comparative study on Si and Ge doping in a- and c-plane GaN — •Matthias Wieneke[1], Hartmut Witte[1], Stephanie Fritze[1,2], Armin Dadgar[1], Jürgen Bläsing[1], and Alois Krost[1]

— [1]Otto-von-Guericke-Universität Magdeburg, FNW/IEP, Universitätsplatz 2, 39106 Magdeburg — [2]present address: LayTec AG, Seesener Str. 10-13, 10709 Berlin

The doping efficiencies of Si and Ge were studied by simultaneous growth of n-type doped a-plane and c-plane GaN. For this purpose undoped a-plane and c-plane GaN templates were grown by low pressure metal-organic vapor phase epitaxy (MOVPE) on 2 inch r-plane and c-plane sapphire substrates, respectively. After cleaving into half wafers one template of each orientation was re-loaded into the MOVPE system. Thus, in each case the Si- and Ge-doped GaN layers were grown at identical conditions on the a-plane and c-plane GaN templates using trimethylgallium (TMGa), ammonia (NH_3), silane (SiH_4) and germane (GeH_4) as precursors. The electrical properties of the undoped templates and the doped GaN layers were investigated by conductivity and Hall-effect measurements. By doping with germane the electron concentration in nonpolar a-plane GaN is typically about 50 times higher than in c-plane GaN, while it is nearly identical when using silane doping. Thus, the Ge incorporation is drastically enhanced in the case of a-plane GaN and is consequently strongly dependent on the crystal orientation of the GaN. In our contribution we will discuss possible origins of the different doping efficiencies.

HL 81.4 Thu 15:30 H13

Anisotropy of the optical response of nonpolar GaN in spectroscopic ellipsometry — •Karsten Lange, Christian Lidig, Martin Feneberg, Matthias Wieneke, Hartmut Witte, Armin Dadgar, Jürgen Bläsing, Alois Krost, and Rüdiger Goldhahn — Institut für Exp. Physik Otto-von-Guericke-Universität Magdeburg

A-plane Ge or Si doped GaN layers with electron concentrations between 7×10^{18} cm^{-3} and 2×10^{20} cm^{-3} were grown by metal-organic chemical vapour desposition. On these layers spectroscopic ellipsometry is carried out in order to determine both the ordinary and extraordinary dielectric tensor components. The infrared studies yield optical phonon frequencies influenced by plasmon-phonon coupling, opening a possibility to systematically determine the anisotropy of GaN. Thus, an experimental measure of the electron effective mass anisotropy is obtained. Furthermore, we will discuss first results of the related anisotropic shifts of the absorption edge around the fundamental band gap.

Coffee break

HL 81.5 Thu 16:00 H13

Defects of polar, semipolar and nonpolar (In)GaN - a comparison — •Lukas Schade[1,2], Tim Wernicke[3], Kamran Forghani[4,5], Jens Rass[3], Simon Ploch[3], Lutz Kirste[2], Markus Weyers[6], Michael Kneissl[3,6], Ferdinand Scholz[4], and Ulrich Schwarz[1,2] — [1]Department of Microsys tems Engeneering, IMTEK, University Freiburg — [2]Fraunhofer Institute for Applied Solid State Physics — [3]Institute of Solid State Physics, Technical University Berlin — [4]Institute for Optoelectronics, University Ulm — [5]University of Wisconsin, Madison, USA — [6]Ferdinand-Braun-Institute, Berlin

The GaN/InGaN material system is used to realize light emitting diodes from UV-A to the green-yellow spectral region. However, even on quasi bulk GaN substrates threading dislocations (TDs) are present with a density of 10^7 cm^{-2}. Here, we examine the influence of TDs on the luminescence intensity and transition energy. The impact caused by nonradiative recombination centers and strain fields is analyzed by micro photoluminescence and white light interferometry. We compare TDs in differently oriented GaN layers and InGaN QWs. Three types of burgers vectors are typically observed in GaN: a, c and a+c. When the surface orientation is changed from (0001) c-plane to $(10\bar{1}0)$ m-plane, their character changes from edge to screw type and vice versa. We studied TDs and V-defects associated to them in polar, semipolar and nonpolar GaN and InGaN QWs. Additionally, we will present the effect of Si doping onto the strain field in (0001) GaN edge dislocations. In undoped GaN, the strain around such a dislocation forms a symmetric dipole. With Si doping, the strain dipole becomes asymmetric.

HL 81.6 Thu 16:15 H13

Investigation of defect related luminescence features in semipolar AlGaN layers on GaN — •Ingo Tischer[1], Matthias Hocker[1], Manuel Frey[1], Robert A.R. Leute[2], Ferdinand Scholz[2], Willem van Mierlo[3], Johannes Biskupek[3], Ute Kaiser[3], and Klaus Thonke[1] — [1]Institut für Quantenmaterie, Gruppe Halbleiterphysik, Universität Ulm, 89081 Ulm — [2]Institut für Optoelektronik, Universität Ulm, 89081 Ulm — [3]Materialwissenschaftliche Elektronenmikroskopie, Universität Ulm, 89081 Ulm

For nitride-based laser diodes and LEDs high quality AlGaN electron blocking layers are required. With increasing Al content the lattice mismatch between GaN and AlGaN leads to a modified strain situation and to the introduction of structural defects. In this study, we investigate the luminescence features of such AlGaN on GaN layers. Spatially resolved cathodolumenescence (CL) recorded at temperatures below 10K using a scanning electron microscope (SEM) performed on cross sections allows to determine the spatial and spectral distribution of luminescence features contributing to the global emission spectra. Micrographs and energy dispersive X-ray spectroscopy (EDX) maps recorded in a transmission electron microscope (TEM) at the same sample area allow the direct assignment of optical bands to structural features like defects and regions with different Al content.

HL 81.7 Thu 16:30 H13

Correlation of microscopic optical properties and defect structures of semipolar GaN on pre-patterned sapphire substrates by cathodoluminescence — •Sebastian Metzner[1], Frank Bertram[1], Thomas Hempel[1], Tobias Meisch[2], Stephan Schwaiger[2,3], Ferdinand Scholz[2], and Jürgen Christen[1] — [1]Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg — [2]Institute of Optoelectronics, University of Ulm — [3]now with OSRAM Herbrechtingen

Spatially and spectrally resolved cathodoluminescence(CL) microscopy has been used to analyze the local luminescence characteristics of semipolar (11-22)GaN stripes grown out of trenches exhibiting c-plane-like sapphire sidewalls. The micro structure has been etched into a (10-12)sapphire substrate yielding an inclination angle of 58° towards (0001)sapphire which enables a planar semipolar (11-22) surface for the coalesced triangularly shaped GaN stripes. Local CL spectra reveal a distinct contribution of structural defects like basal plane stacking faults(BSF), prismatic stacking faults(PSF), and partial dislocations(PD) to the CL emission at the region where the GaN is grown into -c direction after leaving the trench. In complete contrast, the main part grown into +c exhibits pure donor-bound exciton emission interrupted by bundled and bended threading dislocations. Due to a delayed coalescence process the defect structures run into a void and, thus are prevented from propagating further through the coalesced layer. The optical properties of InGaN QW structures grown on top of this SF-free semipolar GaN surfaces are going to be discussed.

HL 81.8 Thu 16:45 H13

Structural and luminescence properties of defects in silicon doped a-plane GaN — •Gordon Schmidt, Peter Veit, Frank Bertram, Sebastian Metzner, Silke Petzold, Matthias Wieneke, Armin Dadgar, Alois Krost, and Jürgen Christen — Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Germany

We present a correlation of the optical properties with the crystalline real structure of a silicon doped nonpolar GaN layer by means of highly spatially resolved cathodoluminescence spectroscopy (CL) performed in a scanning transmission electron microscope (STEM).

Using metal-organic vapor-phase epitaxy the structure was grown under a silane flow rate of 3.5 sccm on an r-plane sapphire substrate with an AlGaN seeding layer resulting in an a-plane GaN layer with a typically high basal plane stacking fault (BSF) as well as partial dislocation (PD) density.

The STEM-CL plan view images clearly resolve the BSF and their terminating PD at the surface of the nonpolar GaN layer. The comparison of the annular dark field images in STEM mode with the simultaneously recorded monochromatic CL intensity mappings directly identifies the BSF I_1 as the dominating emission. Furthermore, we observe a luminescence within 363 - 372 nm in the vicinity of the PD/BSF.

Coffee break

HL 81.9 Thu 17:15 H13

Determination of In mole fraction and strain state in semi- and nonpolar InGaN layers by XRD — •Martin Frentrup, Simon Ploch, Tim Wernicke, and Michael Kneissl — TU Berlin, EW 6-1, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin, Germany

In wurtzite semiconductor heterostructures with semi- and nonpolar

orientation the anisotropic lattice mismatch leads to a triclinic distortion. The distortion can be described by introduction of two new lattice parameters δ_1 and δ_2 describing the deviation of the basis angles α (β) and γ from 90° and 120° respectively. This must be taken into account for the determination of ternary alloy composition by XRD.
In this paper, we will compare different XRD algorithms to determine the composition. With the method of Young et al.[1] the position of the symmetric reflection is used to estimate the strain state and composition, assuming a relaxation mechanism by layer tilt.
Alternatively one can determine all parameters of the triclinic lattice (a, c, δ_1, δ_2) by measurement of several X-ray reflexes in ω-2θ-scans. This method is more accurate, since the exact strain state can be determined without making assumptions on the specific mechanism.
We will discuss the advantages and disadvantages of both methods regarding the determination of stoichiometry for $(20\bar{2}1)$ oriented InGaN. These results will be used for comparison of the In incorporation efficiencies and relaxation in $(11\bar{2}2)$ and (0001) orientated InGaN layers.
[1] E. Young, A. Romanov, J. Speck; APEX, 4 (2011), 061001

HL 81.10 Thu 17:30 H13

Growth Studies on Submicrometer-sized GaN Stripes with Semipolar QWs — •Robert Anton Richard Leute, Junjun Wang, Tobias Meisch, and Ferdinand Scholz — Institute of Optoelectronics, Ulm University, 89081 Ulm, Germany

Nanoimprint technology is used to pattern dielectric masks on c-oriented GaN templates grown on two-inch sapphire substrates. Selective epitaxy of GaN and InGaN results in submicrometer-sized GaN stripes with semipolar side facets. The stripes have triangular cross-section and form a 1D grating with a 260 nm periodicity. Stripes aligned $\parallel m$ and $\parallel a$ resulting in $\{11\bar{2}2\}$ and $\{10\bar{1}1\}$ facets respectively are studied. Growth is optimized to create sharp ridges (below 10 nm wide). Quantum wells emitting in the blue to cyan spectral range are deposited on the side surfaces. The effect of embedding as well as the inclusion of InGaN pre-wells and AlGaN claddings is investigated.

HL 81.11 Thu 17:45 H13

Influence of the semipolar GaN template on the charge carrier dynamics in an active InGaN layer — •Jan Wagner, Sarah Schröder, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen and Research Center SCoPE, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

The growth on semipolar GaN is in the focus of many research studies for several years now since the influence of the Quantum Confined Stark Effect (QCSE) on an active region grown on these planes is significantly reduced. This leads to superior charge carrier dynamics, enhanced emission efficiency and increased indium incorporation with respect to an active region grown on c-plane GaN. As the production of native semipolar substrates with adequate crystalline quality is still difficult and expensive other growth techniques have to be considered. In this work we use the facets of three-dimensional grown GaN pyramids as semipolar templates for active InGaN quantum wells. The pyramids are grown by epitaxial lateral overgrowth (ELO). Since the pyramid facets serve as growth template for the active region, their crystalline quality directly affects the emission efficiency and carrier dynamics of the InGaN layer. Therefore, GaN pyramids of different sizes grown on the same sample were examined by time dependent photoluminescence measurements.

HL 81.12 Thu 18:00 H13

Microphotoluminescence studies on the effect of V-pits and the surface orientation on the indium incorporation within InGaN quantum wells on free standing polar GaN — •Sebastian Bauer[1], Benjamin Neuschl[1], Ingo Tischer[1], Manuel Frey[1], Matthias Hocker[1], Robert A.R. Leute[2], SK. Shaid-Ur Rahman[2], Martin Klein[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

During the growth of *c*-plane GaN by hydride vapor phase epitaxy, occasionally large "V-pits" and different surface facets are formed. When such bulk-like thick free standing layers are overgrown by metal organic vapor phase epitaxy with a GaN layer containing multiple InGaN quantum wells, different indium content and quantum well thicknesses result on different facets and facet transition regions.

We investigate such samples in detail by spatially resolved microphotoluminescence and cathodoluminescence at different temperatures. An effect of the surface orientation on the incorporation of indium can be clearly observed.

HL 82: Quantum dots and wires: Cavities and photons

Time: Thursday 15:00–17:45 Location: H2

HL 82.1 Thu 15:00 H2

Qubit-cavity entanglement created with surface-acoustic waves — •Ralf Blattmann[1], Hubert Krenner[1], Sigmund Kohler[2], and Peter Hänggi[1] — [1]Institut für Physik, Universität Augsburg, 86159 Augsburg, Germany — [2]Instituto de Ciencia de Materiales de Madrid, CSIC, 28049 Madrid, Spain

We study the quantum dynamics of an exciton qubit in a quantum dot coupled to an optical nano cavity defined in a two-dimensional photonic crystal membrane. The effective interaction between these two systems depends on the cavity length. A surface-acoustic wave (SAW) renders this interaction time-dependent, such that the qubit-oscillator setup experiences an ac driving. Close to an avoided crossing of the adiabatic spectrum, the induced qubit excitations can be transferred via Landau-Zener transitions to the cavity, which allows one to entangle and disentangle cavity and qubit. We investigate the influence of higher harmonics of the SAW as well as decoherence due to photon losses. Additionally, we identify regimes with maximal entanglement and discuss the experimental feasibility. Work supported by SFB 631.

HL 82.2 Thu 15:15 H2

Triggered photon pair emission from semiconductor quantum dots via resonant two-photon absorption — •Markus Müller, Klaus D. Jöns, Samir Bounouar, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

As single-photon emitters with narrow spectral linewidths, semiconductor quantum dots have various application possibilities, e.g., for linear optical quantum computation, quantum communication or quantum information processing. To fully exploit their outstanding properties in a deterministic way, a coherent resonant excitation scheme is required. A two-photon absorption process allows us to coherently populate the biexciton state of a single In(Ga)As/GaAs quantum dot. Setting the energy of the excitation laser pulses between the exciton and biexciton transition will resonantly excite the quantum dot within a two-photon absorption process, without the disadvantage of having the pump and the detection light on the same wavelength. In autocorrelation measurements a full suppression of multi-photon-events is observed, with one of the cleanest single-photon emission reported in semiconductor quantum dots ($g^2(\tau) < 0.02$). In addition, this resonant excitation scheme is increasing the coherence time of the emitted light compared to non-resonant excitation processes.

HL 82.3 Thu 15:30 H2

Electrically driven quantum dot single-photon source at 2 GHz excitation repetition rate — •Fabian Hargart, Christian Kessler, Thomas Schwarzbäck, Elisabeth Koroknay, Susanne Weidenfeld, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart, Allmandring 3, 70569 Stuttgart

Single-photon sources (SPSs) are key components for future applications in the field of quantum information technology such as quantum key distribution or linear optical quantum computing. Electrically driven semiconductor quantum dots (QDs) offer tailorable emission energy, narrow linewidth and an easy excitation scheme. Thus, they are promising candidates for such SPSs.

We investigated the influence of the bias voltage on the emission properties of a red emitting InP/GaInP QD based SPS. Under pulsed electrical excitation we can manipulate the band bending of the p-i-n diode with the applied bias voltage and thus the charge carrier escape

by quantum tunneling. This leads to control over this non-radiative decay channel and allows carrier escape times as low as 40 ps, effectively reducing the time jitter of the photon emission. We realized high excitation repetition rates of up to 2 GHz while autocorrelation measurements with $g^{(2)}(0)$-values of 0.27 proof triggered single-photon emission.

HL 82.4 Thu 15:45 H2

Free-space quantum key distribution over 500 m using electrically triggered quantum dot - micropillar single photon sources — •Sebastian Unsleber[1,5], Tobias Heindel[1,5], Markus Rau[2], Christian Schneider[1], Martin Fürst[2,3], Sebastian Nauerth[2,3], Matthias Lermer[1], Henning Weier[2,3], Stephan Reitzenstein[1,5], Alfred Forchel[1], Sven Höfling[1], Harald Weinfurter[2,4], and Martin Kamp[1] — [1]Technische Physik, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Fakultät für Physik, Ludwig-Maximilians-Universität, 80799 Munich, Germany — [3]qutools GmbH, 80539 Munich, Germany — [4]Max-Planck-Institut für Quantenoptik, 85748 Garching, Germany — [5]Present address: Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany

In 1984, Bennett and Brassard proposed a secret key-distribution protocol (BB84) that uses the quantum mechanical properties of single photons to avoid the possibility of eavesdropping on an encoded message. So far, most quantum key distribution (QKD) experiments have been performed with strongly attenuated lasers due to the lack of efficient single photon sources (SPS). First experiments utilizing optically pumped solid state based SPSs affirmed the great potential of QKD but still suffered from the drawbacks of this excitation scheme. In this work we report on a free-space QKD experiment over 500 m using electrically triggered quantum dot - micropillar SPSs. These devices generate sifted key rates of up to 16.8 kBits/s at a quantum bit error rate of 5.9 % and $g^{(2)}(0)$-values down to 0.39.

HL 82.5 Thu 16:00 H2

Electrically driven adiabatic AlAs/GaAs Micropillar cavities — •Matthias Lermer[1], Stephan Kuhn[1], Niels Gregersen[2], Jesper Mørk[2], Christian Schneider[1], Alfred Forchel[1], Sven Höfling[1], and Martin Kamp[1] — [1]Technische Physik 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

Adiabatic Micropillar (MP) cavities are excellent testbeds for pronounced cavity quantum electrodynamic (cQED) effects. Due to the positive influence of the adiabatic mode transition in a taper region, this sort of MP cavities provide both, high Q factors and small mode volumes at the same time allowing e.g. for the observation of low threshold lasing and strong Quantum Dot (QD) - cavity coupling [1]. Moreover, for MP cavities in general, an elegant contacting routine is established [2] paving the way for daily use devices e.g. efficient single photon sources under electrical excitation [3]. We have carefully implemented a doping scheme for pin-Diode like, adiabatic MPs. High Q factors exceeding 10,000 have been measured in Photoluminescence (PL) and Electroluminescence (EL) and a distinct Purcell enhancement of a single QD line has been determined in a detuning experiment both in PL and EL. [1] M. Lermer et al., Physical Review Letters 108, 057402 (2012) [2] C. Böckler et al., Applied Physics Letters 92, 091107 (2008) [3] T. Heindel et al., Applied Physics Letters 96, 011107 (2010)

Coffee break

HL 82.6 Thu 16:30 H2

On-Chip Quantum Optics with Quantum Dot Microcavities — •Tobias Heindel[1], Erik Stock[1], Caspar Hopfmann[1], Ferdinand Albert[2], Matthias Lermer[2], Christian Schneider[2], Sven Höfling[2], Alfred Forchel[2], Martin Kamp[2], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany — [2]Technische Physik and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

The prospect of studying quantum optics in solid state systems has triggered enormous efforts in the development of microcavity structures with embedded quantum dots. The success story in this field of modern optics includes the observation of fundamental light-matter interaction in the cavity quantum electrodynamics regime and the realization of novel nonclassical light sources. Up till now, the respective research has focused almost exclusively on individual microcavities excited optically by rather bulky external laser systems.

In this contribution, we demonstrate a novel approach for on-chip quantum optics using an integrated electrically driven whispering gallery mode microlaser. The latter allows for the observation of Purcell enhancement for an integrated, in-plane pumped quantum-dot microcavity system [1].

[1] E. Stock et al., Adv. Mater. 2012, DOI: 10.1002/adma.201202778

HL 82.7 Thu 16:45 H2

Photocurrent spectroscopy on single quantum dots in micropillar cavities - coherent optical manipulation and cavity quantum electrodynamics effects — •Peter Gold[1], Manuel Gschrey[2], Matthias Lermer[1], Christian Schneider[1], Sven Höfling[1], Alfred Forchel[1], Martin Kamp[1], and Stephan Reitzenstein[2] — [1]Technische Physik, Universität Würzburg, Am Hubland, D-97074 Würzburg — [2]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, D-10623 Berlin

We report on photocurrent (PC) studies of single quantum dots (QDs) in electrically contacted micropillar cavities. The PC response originates from the tunneling of strictly resonantly excited charge carriers in the QDs. Here, we demonstrate coherent optical manipulation of an exciton qubit by exciting a single QD inside a micropillar cavity with picosecond laser pulses. The coherent interaction with the pulsed laser field leads to Rabi oscillations in the population dynamics of the excitonic ground state, which are monitored by the corresponding PC signal. Moreover, we study cavity quantum electrodynamics (cQED) effects in coupled QD-microcavity systems under electrical readout. We find a strong anticorrelation between radiative recombination and nonradiative tunnel escape of photoexcited carries which can be controlled by cQED effects in the Purcell regime. In fact, cavity enhanced radiative emission from a QD results in a weaker photocurrent signal which reflects the cQED controlled competition between radiative and nonradiative recombination at the single emitter level [1].
[1] Gold et al., Phys. Rev. B **86**, 161301(R) (2012)

HL 82.8 Thu 17:00 H2

Nonlinear emission characteristics of quantum dot - micropillar lasers in the presence of polarized optical feedback — •Caspar Hopfmann[1], Ferdinand Albert[2], Christan Schneider[2], Sven Höfling[2], Martin Kamp[2], Alfred Forchel[2], Ido Kanter[3], 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]Minerva Center and Department of Physics, Bar-Ilan University, Ramat Gan, 52900 Israel

Cavity quantum electrodynamics in high quality quantum dot (QD) microcavities has been subject of extensive research interest in recent years. In this field, nonlinear light-matter interaction and dynamical processes are of particular interest. We report on electrically pumped QD microlasers in presence of polarized external self-feedback. These high-β micropillar lasers feature Q-factors of up to 20000 and threshold currents of about 1 μA. Moreover, the lasers have two orthogonal linearly polarized fundamental modes which are coupled by the common few QD gain medium. This gain coupling is reflected in pronounced anti-correlations in the current dependence of the two mode components with respect to the output power, the coherence time and the second order photon autocorrelation function. By applying polarized self-feedback we are able to effectively control these emission characteristics. Additionally, self-feedback provides an attractive tool for inspection of light-matter interaction properties (i.e. Purcell factor and exciton lifetime) of the QDs at high excitation conditions.

HL 82.9 Thu 17:15 H2

Gain competition enhanced intensity fluctuations in bimodal quantum dot – micropillar lasers — •Heinrich A. M. Leymann, Mikayel Khanbekyan, Alexander Foerster, and Jan Wiersig — Institut für Theoretische Physik, Universität Magdeburg, Postfach 4120, D-39016 Magdeburg, Germany

In the last decade intense research on the physics of microcavity lasers based on semiconductor quantum dots has been performed due to their high potential for ultralow threshold lasing [1]. For lasers with a spontaneous emission factor close to unity the onset of lasing can be more reliably monitored by means of the photon statistics.

In this contribution, we present a theoretical study of a quantum-dot-based microcavity laser where two nearly degenerate high-Q modes are involved in the laser dynamics. To analyze the coupled carrier-photon system we have extended a single mode microscopic semiconductor theory [2] to the case of two modes and have also taken the crosscorrelation functions into account.

Our theoretical results show that the mode which loses the mode competition exhibit super-thermal photon bunching ($g^{(2)}(0) > 2$). This interesting feature is traced back to mode coupling induced by the gain medium. Calculations of the photon cross-correlations reveal that the two modes are strongly entangled.

[1] J. Wiersig et al., Nature 460, 245 (2009).
[2] C. Gies et al., Phys. Rev. A 75, 013803 (2007).

HL 82.10 Thu 17:30 H2

Quantum limit of nuclear spin polarization in semiconductor quantum dots — •Julia Hildmann[1], Eleftheria Kavousanaki[2], Hugo Ribeiro[1], and Guido Burkard[1] — [1]Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — [2]Femtosecond Spectroscopy Unit, Okinawa Institute of Science and Technology, Graduate University, Okinawa, 904-0412 Japan

Since the original proposal by Loss and DiVincenzo to use single electron spins confined in quantum dots (QDs) as quantum bits (qubits) [1], a lot of effort has been made to perform coherent control of electron spins in QDs. One of the challenges for using electron spins as qubits remains decoherence due to hyperfine interaction with the nuclear spin bath of the host material (III-V semiconductors). Among various proposals to extend coherence times, there is the possibility to polarize the nuclear spins to a high degree (close to 100% [2]). A recent experiment, which relies on spin-forbidden transitions between heavy holes and positive trions, shows the highest until now reported polarization of about 65% [3]. Simple rate equations describing the pumping mechanism fail to describe the observed saturation predicting a fully polarized nuclear state and not constituting an appropriate description of the nuclear spin bath dynamics. We present a full quantum mechanical approach to this particular problem and show that the pumping saturation is a consequence of the collective nuclear spin quantum dynamics. [1] D. Loss and D. P. DiVincenzo, Phys Rev. A 57, 120 (1998). [2] W. A. Coish and D. Loss, Phys. Rev. B 70, 195340 (2004). [3] E. A. Chekhovich et al, Phys. Rev. Lett. 104, 066804 (2010).

HL 83: Transport I

Time: Thursday 15:00–16:30 Location: H16

HL 83.1 Thu 15:00 H16

Electrical properties of InAs nanowires and their interband tunneling across Si heterojunctions for future FET devices — •Pascal Wittlich[1], Stefanie Morkötter[1], Tao Yang[1], Julian Treu[1], Simon Hertenberger[1], Verena Hintermayr[1], Philipp Geselbracht[1], Max Bichler[1], Gerhard Abstreiter[1,2], and Gregor Koblmüller[1] — [1]Walter Schottky Institut and Physik Department, TU München, Garching, Germany — [2]TUM Institute for Advanced Study, Garching, Germany

We present recent results on the electrical transport characteristics of MBE grown InAs nanowires on Si substrate. Several investigations in different NW device geometries are performed, either as vertical free-standing NW devices for all-surround gate NW-FET configurations or as transferred nanowires for fabrication of both back- and top-gated NW-FETs in horizontal geometry. For the latter, we show dependencies of growth parameters, microstructure, contact metal, and surface passivation schemes (high-k dielectrics) on the total NW-FET resistance as well as transconductance and electron mobility. For vertical devices directly integrated on Si, we report a detailed study of interband tunneling across p-type Si/n-InAs heterojunctions as a function of substrate doping level and NW diameter. For large doping levels we find the possibility for large tunnel currents and Esaki-type tunneling with explicit negative differential resistance in thin NWs [1]. These results open viable routes for future high-performance III/V-on-Si tunnel-FET devices.

[1] T. Yang et al, Appl. Phys. Lett. 101, 233102 (2012).

HL 83.2 Thu 15:15 H16

Increased Stability of Solution Processed ZnO TFTs by Selectively Bonded Diketones — •Marlis Ortel, Nataliya Kalinovich, Gerd Röschenthaler, and Veit Wagner — Research Center for Functional Materials and Nanomolecular Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

10nm thick nano-crystalline ZnO layers were deposited by spray pyrolysis in TFT configuration in order to investigate the impact of surface states on the TFT performance. Surface trap states are known to have significant influence on mobility, hysteresis and operational stability of transistors. Diketone molecules were applied to the surface, which are known to bind selectively to zinc ions in order to reduce the trap state density. It was found that the electronic structure of the semiconductor was tuned depending on the functional groups attached to the diketone. Transistors coated with 4,4,4-trifluoro-1-phenylbutane-1,2-dione were found to stabilize the TFT performance even under long term gate bias stress. Furthermore the mobility was significantly increased by 30% to 9cm2V-1s-1 after few seconds of exposure to the chemical compound. Hence diketones are concluded to be suitable materials to minimize trapping process in zinc oxide which leads to strongly improved device characteristics.

HL 83.3 Thu 15:30 H16

Influence of boron cluster states on the transport properties of (B,Ga)P — •Steve Petznick[1], Kathleen Klinkmüller[1], Kerstin Volz[2], and Peter J. Klar[1] — [1]Institute of Experimental Physics I, Justus-Liebig University, Giessen, Germany — [2]Structure & Technology Research Laboratory (STRL), Philipps-Universität, Marburg, Germany

The influence of boron incorporation in n-type $B_xGa_{1-x}P$:Y (with $0.9 \leq x \leq 1.9\,\%$ and Y = Te, Si) layers on the transport properties has been studied. The 500 nm thick (B,Ga)P layers were grown by metal-organic vapor phase epitaxy (MOVPE) on semi-insulating (001) GaP substrates. Transport measurements at ambient and hydrostatic pressure were performed at different temperatures between 1.6 and 280 K in Van der Pauw geometry and in applied magnetic fields up to 10 T.

Boron is an isovalent impurity in GaP yielding to a density of localized states in the vicinity of the conduction band edge. These localized states act as scattering centers and have a severe impact on the transport behavior of this n-type material.

Hydrostatic pressure allows one to tune the band structure while the composition stays exactly the same. Therefore measurements under hydrostatic pressure were performed to examine the interplay of boron cluster states and the conduction band edge states. The impact on magneto-resistance, resistivity, carrier mobility and concentration, and their temperature and pressure dependence will be discussed.

HL 83.4 Thu 15:45 H16

Magnetotransport measurements on nanostructured $Bi_{1-x}Sb_x$ alloys — •Matthias T. Elm[1], Christian H. Will[1], Bernadette Landschreiber[2], Ekrem Güneş[2], Sabine Schlecht[2], and Peter J. Klar[1] — [1]I. Physikalisches Institut, Justus-Liebig-Universität, Heinrich-Buff Ring 16, 35392 Gießen — [2]Institut für Anorganische und Analytische Chemie, Heinrich-Buff-Ring 58, 35392 Gießen

A series of nanostructured $Bi_{1-x}Sb_x$ alloy samples were prepared by cold pressing of Bi and Sb nanoparticles, which were synthesized by mechanical alloying. The Sb content in the alloys varied between 0% to 50%. Increasing the Sb content strongly influences the band structure resulting in a change of the transport behavior from semi-metallic to semiconducting behavior with a maximum band gap of 41.5 meV at a Sb concentration of around 14% determined from temperature-dependent resistivity measurements. At even higher Sb concentrations the transport behavior becomes semi-metallic again. The change of the band structure was investigated by magnetotransport measurements at a temperature of 30 K in magnetic fields up to 10 T. Using a three band model and taking into account the influence of the magnetic field on the band structure it was possible to describe the magnetic-field induced changes of the magnetoresistance as well as the Hall-constant of the different samples.

HL 83.5 Thu 16:00 H16

Resonant cavity enhanced telecommunication wavelength light detection by resonant tunneling — •Andreas Pfenning, Fabian Hartmann, Fabian Langer, Dirk Bisping, Sven Höfling, Martin Kamp, Alfred Forchel, and Lukas Worschech — Technische Physik, Physikalisches Insitut, Universität Würzburg and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Am Hubland, D-97074 Würzburg, Germany

We have fabricated GaAs based resonant tunneling diodes (RTD) with a nearby and lattice matched quaternary GaInNAs absorption layer for light detection at the telecommunication wavelength $\lambda = 1.3$ μm. The RTD photodetector was embedded in an optical cavity consisting of alternating GaAs/AlAs distributed Bragg reflectors (DBR) with a resonance wavelength at $\lambda = 1.29$ μm. RTD mesas with ring shaped contacts and an aperture for optical excitation of charge carriers were fabricated with diameters from 12 μm down to 1 μm. At room temperature resonant tunneling was found with a peak-to-valley ratio of 1.3. Photocurrent measurements of the RTD photodetector showed sensitivities of 31 kA/W for resonant optical excitation and a quantum efficiency enhancement of 10 compared to off resonance excitation. The photodetector shows a resolution down to single photons.

HL 83.6 Thu 16:15 H16

Effects of defects near source or drain contacts of carbon nanotube transistors — •Neng-Ping Wang[1] and Xiao-Jun Xu[2] — [1]Physics Department, Science Faculty, Ningbo University, Fenghua Road 818, Ningbo 315211, P.R. China — [2]Information Faculty, Ningbo City College of Vocational Technology, Xuefu Road 9, Ningbo 315100, P.R. China

In field-effect transistors, charge trapping in the gate oxide is known to cause random telegraph signals (RTSs) in the drain current. We calculate the amplitude of the RTS due to a single charged defect in a long-channel p-type carbon nanotube field-effect transistor, using the nonequilibrium Greens function method in a tight-binding approximation. We find that in the turn-on regime, the amplitude of the RTS due to a positive charge increases with the distance of the charge from the source (or drain) contact, and in the middle of the channel the RTS amplitude reaches about 100%. The amplitude of the RTS caused by a positive charge close to the source (or drain) contact increases with the applied gate voltage and drain voltage. In the on-state, a positive charge located at the nanotube-oxide interface and close to the source (or drain) contact may cause large RTSs about 50%. Similar amplitudes of RTSs have been observed in recent experiments [F. Liu, etal, Appl. Phys. Lett., 86 (2005) 163102].

HL 84: Graphene: Theory (HL, jointly with O, TT)

Time: Thursday 15:00–17:30 Location: H17

HL 84.1 Thu 15:00 H17

Influence of non-local exchange-correlation and spin-orbit interaction on electronic and optical properties of graphene, silicene, germanene, and tinene — •Lars Matthes[1], Olivia Pulci[2], Paola Gori[3], and Friedhelm Bechstedt[1] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena — [2]Dipartimento di Fisica, Università di Roma "Tor Vergata", via della Ricerca Scientifica 1, 00133 Rome, Italy — [3]CNR-ISM, Via Fosso del Cavaliere 100, 00133 Rome, Italy

We present first-principles studies of the optical absorbance of the group-IV honeycomb crystals graphene, silicene, germanene, and tinene. We account for many-body effects on the optical properties by using the non-local hybrid functional HSE06. The optical absorption peaks are blue-shifted due to quasi-particle corrections, while the influence on the low-frequency absorbance remains unchanged and reduces to the universal value $\pi\alpha$,[1,2] where α is the Sommerfeld fine-structure constant. However, in silicene, germanene and tinene an electronic band gap arises at the Dirac-point due to spin-orbit splitting and parabolic bands with a very small effective mass emerge. Consequently, the low-frequency absorbance is modified due to the spin-orbit induced fundamental absorption edge. We demonstrate numerically that the absorbance increases at the fundamental absorption edge.

[1] A. Geim et al., Science 320, 1308 (2008)

[2] F. Bechstedt, L. Matthes et al., Appl. Phys. Lett. 100, 261906 (2012)

HL 84.2 Thu 15:15 H17

Generalized Hubbard models for two dimensional hybrid 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, Universität Bremen, D-28359 Bremen, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [3]1. Institut für Theoretische Physik, Universität Hamburg, D-20355 Hamburg, Germany — [4]Radboud University Nijmegen, Institute for Molecules and Materials, NL-6525 AJ Nijmegen, The Netherlands

We present effective generalized Hubbard models for the description of novel two dimensional materials. The local and non-local partially screened Coulomb interaction as well as hopping integrals are calculated from first principles for silicene and graphene on a metallic substrate. We consider interactions up to the 6th nearest neighbor in real space and investigate the long range behavior of the dielectric function in k-space. We compare the resulting silicene Hubbard model to the corresponding model for pure graphene. Thereby we find values of $U/t \approx 4.0$ eV for the on-site and $V/t \approx 2.4$ eV for the nearest neighbor partially screened Coulomb interaction in silicene, which are slightly bigger than in freestanding graphene. We further show that the ratio of the local to the non-local Coulomb interaction can be controlled by a metallic substrate, which efficiently screens non-local Coulomb terms.

HL 84.3 Thu 15:30 H17

Subgap conductivity in gated bilayer graphene — •Maxim Trushin — University of Konstanz, 78457 Konstanz

In the present work [1], the subgap electron transport has been investigated in gated bilayer graphene [2] within the two-band effective model using the finite-size Kubo formula. The conductivity does not vanish even though the temperature is set to zero and the chemical potential gets into the middle of the band gap. In contrast to the universal subgap conductivity observed in the 2D topological insulators [3], the subgap conductivity in bilayer graphene turns out to be sensitive to the band gap size and disorder strength.

The effect can be explained in terms of the quantum mechanical interband coherence which turns out to be important for the chiral carriers. At finite temperature, a competition between the temperature-dependent interband decoherence and thermal activation processes results in the non-monotonic conductivity vs. temperature dependence. The non-monotonicity can be seen as a signature of the interband entanglement responsible for the difference between the transport and spectral gaps. The effect can be observed in gapped bilayer graphene sandwiched in boron nitride where the electron-hole puddles and flexural phonons are strongly suppressed.

[1] M. Trushin, Europhys. Lett. **98**, 47007 (2012). [2] E. McCann, Phys. Rev. B **74**, 161403 (2006). [3] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. **82**, 3045 (2010).

HL 84.4 Thu 15:45 H17

Lattice dynamics of few-layer graphene after ultrashort laser excitation — •Naira Grigoryan, Eeuwe S. Zijlstra, and Martin E. Garcia — Universität Kassel, Kassel, Germany

Femtosecond laser pulses may induce striking structural effects in solids via electronic excitation. Here we studied the phonon dynamics on the 10 ps timescale in thin graphite films as a function of its thickness after laser interaction using ab initio molecular dynamics simulations including a Van der Waals force correction term to the local density approximation. We implemented the coupling of the hot electrons with the so-called strongly coupled optical phonons (SCOPs) [T. Kampfrath et al., PRL 95, 187403 (2005)] in a semiempirical way . From our simulations we could determine the decay of the SCOPs into other phonon modes, in particular, the out-of-plane lattice vibrations.

HL 84.5 Thu 16:00 H17

RKKY Interaction in a Graphene Bilayer — •Nicolas Klier, Sam Shallcross, and Oleg Pankratov — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

RKKY interaction in doped graphene monolayer ($k_F \neq 0$) shows Friedel oscillations decaying as $1/r^2$ [1]. In this work we consider the RKKY interaction in AA- and AB-stacked bilayer graphene using exact low energy Green's functions. Apart from the common site-to-site interaction we discuss impurities located at the bond centers as well as impurities at the center of the hexagonal plaquettes and intercalant-type impurities located in-between the two carbon layers. Similarly to the monolayer case, we find an oscillatory $1/r^2$ decay for on-site impurities in AA-stacked bilayer graphene. The exchange integral separates into the product of an energy dependent oscillation and an additional modulation resulting from the interlayer coupling. Interestingly, for on-site impurities in AB-stacked bilayer graphene this additional modulation vanishes at low Fermi energies. Moreover, due to the interference of the neighboring site-to-site interactions, at high Fermi energies the RKKY interaction between two plaquette impurities shows a $1/r^3$ behavior.

[1] M. Sherafati and S. Satpathy, Phys. Rev. B 84, 125416, 2011

Coffee break

HL 84.6 Thu 16:30 H17

***Ab initio* calculations of functionalized graphene nanoribbons** — •Christian Till, Nils Rosenkranz, Christian Thomsen, and Janina Maultzsch — TU Berlin, Institut für Festkörperphysik, Hardenbergstraße 36, 10623 Berlin

Since nearly 30 years the discovery and subsequent research on fullerenes, carbon nanotubes, and graphene fuel expectations on carbon-based nanoelectronics. In this context, thin stripes of the two-dimensional material graphene, so-called graphene nanoribbons (GNRs), draw broad interest as well. In this work, we present a comprehensive ab initio study of the structural, electronic and vibrational characteristics of a 7-armchair GNR with hydroxyl functionalized edges. Our results show AGNRs with increasing hydroxyl saturation to be particularly stable. In addition, we find a variation of the ribbon geometry under functionalization. An increasing degree of functionalization leads to a compression perpendicular to the ribbon axis. As a consequence we find a linear shift of the band gap with growing edge hydroxylation. With regard to a possible experimental determination of the degree of functionalization, we indicate fingerprint vibrational modes of the hydroxyl groups as well as a substantial shift of Raman active phonons.

N. Rosenkranz, C. Till, C. Thomsen, and J. Maultzsch, Phys. Rev. B **84**, 195438 (2011).

HL 84.7 Thu 16:45 H17

Phonon dispersions of AB- and ABC-stacked graphene trilayers and multilayers — •Bart Verberck[1,2], Karl H. Michel[1], and Björn Trauzettel[2] — [1]Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium — [2]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Recently, it was experimentally confirmed that the electronic structure of graphene multilayers crucially depends on how they are stacked. The simplest multilayer for which different stackings can be realised is the trilayer. The ABA variant features both linearly and quadratically dispersed electronic bands near the K-point, while the ABC variant has cubic electronic dispersion. At the same time, the difference between the phonon dispersions for ABA and ABC trilayer graphene is less well established. Detailed knowledge of the phonon spectra is, however, essential for understanding double-resonant Raman scattering experiments, offering a simple means for characterising multilayer graphene samples (number of layers and stacking sequence). Here we present a theoretical study of the phonon dispersions of AB- and ABC-stacked multilayers based on a phenomenological force-constants model. We find that the difference between the phonon spectra for the two variants is much less apparent than the difference between the respective electronic band structures; the main distinction concerns the low-energy phonon modes around the K-point. We argue that the observed difference in double-resonant Raman scattering signals for ABA and ABC trilayers mainly originates from the different electronic dispersions.

HL 84.8 Thu 17:00 H17

Optical selection rules in graphene quantum dots — •Eleftheria Kavousanaki and Keshav Dani — Femtosecond Spectroscopy Unit, Okinawa Institute of Science and Technology, Graduate University, Okinawa, Japan

We theoretically study the optical absorption of graphene quantum dots for different shapes, sizes and edge types. We calculate the single particle energy spectrum using the tight-binding Hamiltonian and the Dirac-Weyl equation and show that dots with zigzag edges exhibit a degenerate shell of zero energy states, in agreement with previous results. Using standard group theoretical tools, we identify the optical selection rules for triangular and hexagonal quantum dots and discuss the role of light polarization on the absorption spectrum. Finally, we calculate the oscillator strengths and absorption spectra for different quantum dot sizes and identify the contribution of the zero energy states therein.

HL 84.9 Thu 17:15 H17

Electronic reflection for a single layer graphene quantum well — •Abir Mhamdi[1,2], Emna Ben Salem[1], and Sihem Jaziri[3] — [1]Laboratoire de Physique de la Matière Condensée, Faculté des Sciences de Tunis, Tunisia — [2]Institut für Theoretische Physik, Georg-August Universität Göttingen, Germany — [3]Laboratoire de Physique des Matériaux, Faculté des Sciences de Bizerte, Tunisia

We address the problem of Dirac fermions' graphene quantum well (GQW) and we focus on the low energy approximation for the Hamiltonian of the system where the former can be described by a Dirac-like Hamiltonian. Interesting relations are obtained and used to discuss the influence of the spin-orbit coupling, which induces an effective mass-like term, on the transport properties of single-layer graphene quantum well. It is found that the reflection probability of incident electrons is sensitive to the effective mass-like term. This can be explained by the dependence of reflection coefficient R on the incident electrons' direction and their energies. Notably, we found that the reflection probability for massive fermions with a very small angle, i.e. the wave-vector along the transport direction is zero in the GQW, can be greatly suppressed.

HL 85: Topological insulators (TT, jointly with DS, HL, MA)

Time: Thursday 15:00–18:00 Location: H18

Topical Talk HL 85.1 Thu 15:00 H18

Correlation Effects in Quantum Spin Hall Insulators — •Martin Hohenadler — Theoretische Physik I, Universität Würzburg, 97074 Würzburg, Germany

Time-reversal invariant insulating states with topological properties, including topological insulators, have been in the focus of research in recent years. On the theoretical side, electronic correlation effects are of particular interest, as they can both destroy and create topological phases. This talk gives an overview of research on two-dimensional, correlated topological insulators, with a focus on quantum Monte Carlo results for the Kane-Mele-Hubbard model.

HL 85.2 Thu 15:30 H18

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 spectacular phenomena occurring at the surface of 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.

High quality thin films of Bi_2Te_3 were grown on α-$Al_2O_3(0001)$ and $BaF_2(111)$ using Molecular Beam Epitaxy. A two-step growth pro-

cedure provides high quality epitaxial films despite the large lattice mismatch of 9% to Al_2O_3; the mismatch to BaF_2 is less than 1%.

To protect the surface integrity an all in-ultra-high-vacuum study is crucial. This means not only the preparation and characterization by RHEED, LEED, XPS and ARPES, but especially the transport measurements are performed in-ultra-high-vacuum. The results of this study and ongoing work will be presented.

HL 85.3 Thu 15:45 H18

Magnetotransport in MBE-grown topological insulator $(Bi_{1-x}Sb_x)_2Te_3$ thin films — •Christian Weyrich[1], Tobias Merzenich[1], Igor E. Batov[1,2], Gregor Mussler[1], Jörn Kampmeier[1], Yulieth Arango[1], Detlev Grützmacher[1], and Thomas Schäpers[1,3] — [1]Peter Grünberg Institute (PGI-9), Research Centre Jülich GmbH, 52425 Jülich, Germany — [2]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, 142432, Moscow Distr., Russia — [3]II. Physikalisches Institut, RWTH Aachen University, 52056 Aachen, Germany

We report on the magnetotransport study of topological insulator $(Bi_{1-x}Sb_x)_2Te_3$ thin films. The films were grown on a silicon on insulator (SOI) substrate with a Si(111)-layer on top by molecular beam epitaxy. In Bi_2Te_3 samples, we observed a positive magnetoresistance at low magnetic fields with a cusplike minimum at B = 0 (weak antilocalization) as well as positive magnetoresistance in the entire magnetic field range (up to 12 T). The weak antilocalization effect disappears when an in-plane field is applied, showing the anisotropy between the transport parallel and perpendicular to the quintuple-layers. The estimated phase coherent lengths up to 250 nm at low temperatures are comparable to those previously obtained for Bi_2Te_3. The magnetotransport measurements were also performed on MBE-grown films of Sb_2Te_3 (p-doped) as well as on the ternary compound $(Bi_{1-x}Sb_x)_2Te_3$ ($0<x<1$). A transition from n- to p-doping depending on x has been seen in the measurements.

HL 85.4 Thu 16:00 H18

Surface state contribution to thermoelectric transport in Bi_2Te_3 — •Nicki F. Hinsche[1], Florian Rittweger[1], Peter Zahn[3] und Ingrid Mertig[1,2] — [1]Martin-Luther-Universität, Institut für Physik, Von-Seckendorff-Platz 1, DE-06120 Halle — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, DE-06120 Halle — [3]Helmholtz-Zentrum Dresden-Rossendorf, P.O. Box 51 01 19, DE-01314 Dresden

Bulk Bi_2Te_3 and related heterostructures are well known as efficient thermoelectric materials [1,2]. Recent research revealed Bi_2Te_3 to be a strong topological insulator, i.e. its bulk is insulating, while its surface is metallic due to the presence of robust gapless surface states [3]. While the spin structure and the low-temperature electrical transport gained much attention, the physics of the thermoelectric transport is still under debate. To contribute on this, we studied the electronic structure of the Bi_2Te_3 surface with a fully relativistic screened Korringa-Kohn-Rostoker Green's function method. The thermoelectric transport properties were calculated within the relaxation time approximation of the Boltzmann theory. The influence of temperature and doping on the thermoelectric properties of the surface state were analysed in detail.

[1] T. M. Tritt *et al.*, MRS bulletin **31**, 188 (2006)
[2] N. F. Hinsche *et al.*, Phys. Rev. B **86**, 085323 (2012)
[3] H. Zhang *et al.*, Nature Phys. **5**, 438 (2009)

HL 85.5 Thu 16:15 H18

Quasi-ballistic transport of Dirac fermions in a Bi_2Se_3 nanowire — •Joseph Dufouleur — IFW-Dresden, Dresden, Germany

Quantum coherent transport of Dirac fermions in a mesoscopic nanowire of the 3D topological insulator Bi_2Se_3 is studied in the weak-disorder limit. At very low temperatures, many harmonics are evidenced in the Fourier transform of Aharonov-Bohm oscillations, revealing the long phase coherence length of surface states. Remarkably, from their exponential temperature dependence, we infer an unusual 1/T power law for the phase coherence length. This decoherence is typical for quasi-ballistic fermions weakly coupled to the dynamics of their environment.

15 min. break

HL 85.6 Thu 16:45 H18

Quasi-ballistic transport of Dirac fermions in a Bi_2Se_3 nanowire — •Joseph Dufouleur[1], Louis Veyrat[1], Andreas Teichgräber[1], Stephan Neuhaus[1], Christian Nowka[1], Silke Hampel[1], J érôme Cayssol[2,3], Joachim Schumann[1], Barbara Eichler[1], Oliver Schmidt[1], Bernd Büchner[1], and Romain Giraud[1,4] — [1]Leibniz Institute for Solid State and Materials Research, IFW Dresden, 01171 Dresden, Germany — [2]LOMA, University Bordeaux 1, F-33045 Talence, France — [3]Max-Planck-Institut für Physik Komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany — [4]CNRS - Laboratoire de Photonique et de Nanostructures, Route de Nozay, 91460 Marcoussis, France

Quantum coherent transport of Dirac fermions in a mesoscopic nanowire of the 3D topological insulator Bi_2Se_3 is studied in the weak-disorder limit. At very low temperatures, many harmonics are evidenced in the Fourier transform of Aharonov-Bohm oscillations, revealing the long phase-coherence length of surface states. Remarkably, from their exponential temperature dependence, we infer an unusual $1/T$ power law for the phase coherence length $L_\varphi(T)$. This decoherence is typical for quasi-ballistic fermions weakly coupled to the dynamics of their environment.

HL 85.7 Thu 17:00 H18

Magnetotransport in disordered HgTe ribbons — •Sven Essert and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

HgTe quantum wells allow the realization of 2D topological insulator structures. They feature edge states which are protected from backscattering by time-reversal symmetry leading to dissipationless transport in the presence of non-magnetic disorder. We perform transport calculations using the four-band BHZ model to investigate the lifting of this protection by an external magnetic field. We find that the edge state transport is very robust to the application of a perpendicular magnetic field as long as the transport is still in the quasi-one dimensional regime, i.e. as long as the system is far from a topological phase transition to the topologically trivial insulating phase. However, by gating parts of the system to the metallic regime and thereby allowing for true 2d transport, the effect of the magnetic field can be drastically increased.

HL 85.8 Thu 17:15 H18

Probing the Band Topology of Mercury Telluride through Weak Localization and Antilocalization — •Viktor Krueckl and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg

We investigate the effect of weak localization (WL) and weak antilocalization (WAL) in the diffusive transport through HgTe/CdTe quantum wells. Our results reveal different transitions between WL and WAL depending on the Fermi energy as well as the band topology [1]. If spin-orbit interactions from bulk and structure inversion asymmetry can be neglected, the magnetoconductance of a system with inverted band ordering features a transition from WL to WAL and back. This is a signature of the Berry phase arising for inverted band ordering and not present in heterostructures with conventional ordering. In presence of strong spin-orbit interaction both band topologies exhibit WAL, which is distinctly energy dependent solely for quantum wells with inverted band ordering. This can be explained by an energy-dependent decomposition of the Hamiltonian into two blocks.

[1] V. Krueckl and K. Richter, Semicond. Sci. Technol. **27**, 124006 (2012)

HL 85.9 Thu 17:30 H18

Robustness of edge states in non-centrosymmetric superconductors — •Raquel Queiroz und Andreas P. Schnyder — Max Planck Institut für Festörperforschung, 70569 Stuttgart, Germany

Nodal superconductors without inversion symmetry have non-trivial topological properties, manifested by topologically protected flat-band edge states [1-3]. Since the bulk is not fully gapped, the edge states of nodal superconductors can in principle be susceptible to impurities, which break translational symmetries. Using recursive Green's function techniques we study the robustness of these edge states against both magnetic and non-magnetic disorder. We show that for weak and dilute non-magnetic impurities, a finite number of mid-gap edge states remains at zero-energy. We compute the zero bias conductance of a junction between a normal lead and a non-centrosymmetric superconductor as a function of disorder strength. It is found that the flat-band edge states give rise to a nearly quantized zero-bias conductance even

in the presence of non-magnetic impurities.

[1] A. P. Schnyder and S. Ryu, Phys. Rev. B 84, 060504(R) (2011)
[2] P. M. R. Brydon, A. P. Schnyder, and C. Timm, Phys. Rev. B 84, 020501(R) (2011)
[3] A. P. Schnyder, P. M. R. Brydon, and C. Timm, Phys. Rev. B 85, 024522 (2012)

HL 85.10 Thu 17:45 H18

The Kondo cloud in helical edge states — •Thore Posske and Björn Trauzettel — Institute for Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany

The Kondo cloud is one of the last left unobserved phenomena of the Kondo effect. It stands for spatially extended spin-spin correlation between the electrons in the leads and the spin of the impurity in a Kondo system. Attempts to measure the Kondo cloud directly at the impurity usually perturb the system vastly and therefore modify the Kondo cloud. Helical edge states of topological insulators obey a unique coupling of the direction of motion and the spin degree of freedom. This, as we show, allows for the possibility to find signatures of the Kondo cloud far away from its origin by measuring current-current correlations.

HL 86: Organic electronics and photovoltaics V (CPP, jointly with HL, O)

Time: Thursday 15:00–18:45 Location: H34

Invited Talk HL 86.1 Thu 15:00 H34

Quantum coherence controls the charge separation in a prototypical artificial light harvesting system — •C. Lienau[1], S. M. Falke[1], C. A. Rozzi[2], N. Spallanzani[2], A. Rubio[2], E. Molinari[2], D. Brida[3], M. Maiuri[3], G. Cerullo[3], H. Schramm[4], and J. Christoffers[4] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg, Germany — [2]Istituto Nanoscienze - CNR, Centro S3, Modena, Italy — [3]IFN-CNR, Dipartimento di Fisica, Politecnico di Milano, Italy — [4]Institut für Reine und Angewandte Chemie, Carl von Ossietzky Universität Oldenburg, Germany

The efficient conversion of light into electricity or chemical fuels is a fundamental challenge. In artificial photosynthetic and photovoltaic devices this conversion is generally thought to happen on ultrafast time scales in the fs to ps range and to involve an incoherent electron transfer process. In some natural biological systems, however, there is now growing evidence that the coherent motion of electronic wavepackets is an essential primary step, raising questions about the role of quantum coherence in artificial devices. Here we investigate the primary charge transfer process in a supramolecular triad, a prototypical artificial reaction center. Combining high time-resolution femtosecond spectroscopy and time-dependent density functional theory, we provide compelling evidence that the driving mechanism of the photoinduced current generation cycle is a correlated wavelike motion of electrons and nuclei on a timescale of few tens of femtoseconds. We highlight the fundamental role of the interface between chromophore and charge acceptor in triggering the coherent wavelike electron-hole splitting.

HL 86.2 Thu 15:30 H34

Simulations of Electron Transfer in a Fullerene Hexa-Pyropheophorbide-a Complex — •Thomas Plehn, Jörg Megow, and Volkhard May — Humboldt-Universität zu Berlin, Germany

Electron transfer (ET) is studied between electronically excited chromophores and a C60 fullerene forming a highly flexible complex, which is dissolved in a solvent. Such investigations are of particular interest with regard to future artificial photosynthetic reaction centers and respective applications in future components of photovoltaic devices. The whole discussion is based on extended MD-simulations. To obtain reliable ET results three differently advanced theories are used. The first treatment uses the classical Marcus theory. Respective Marcus parameters are obtained from literature [1]. A generalized ansatz can be derived by the Landau-Zener theory [2]. Secondly, a semiclassical surface-hopping method [3] is chosen. For this approach the conformation-dependent free-energy surfaces and Marcus parameters are calculated directly from the MD-trajectory. The third approach uses the dispersed-polaron/spin-boson model [3]. This method enables the approximation of a quantum-mechanical harmonic oscillator bath and thus the treatment of nuclear tunneling. A comparative discussion of the outcome of these three methods also in relation to experiment [1] is given finally.

[1] Regehly M. et al., J. Phys. Chem. B 2007, 111, 998
[2] Hilczer M. et al., J. Photochem. Photobiol. A 2003, 158, 83
[3] Warshel A. et al., Q. Rev. Biophys. 2001, 34, 4, 563

HL 86.3 Thu 15:45 H34

Highly conductive PEDOT:PSS for flexible structured ITO-free solar cells — •Claudia M. Palumbiny[1], Christoph Heller[1], Robert Meier[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, 85747 Garching, Germany — [2]HASYLAB at DESY, Notkestr. 85, 22603 Hamburg, Germany

PEDOT:PSS is widely used as selective intermediate electrode in flexible electronics. The mechanical stability of the electrodes yet play a crucial role and is limited by the instability of the ITO/FTO electrode and the low conductivity of PEDOT:PSS. We investigate a recently developed post treatment method enhancing the conductivity of PEDOT:PSS reaching the order of ITO. For a deeper understanding the nanomorphology is investigated with surface imaging techniques (AFM, SEM) and the inner morphology and crystallinity is addressed with GISAXS and GIWAXS. The morphological changes are consequently related to the electronically changes. Furthermore, we introduce a novel structuring routine for PEDOT:PSS, plasticizer assisted soft embossing [1]. Being able to control the interface between the transparent electrode and the active material, the device efficiency of OPVs under oblique light can be increased. Combining highly conductive PEDOT:PSS with controlled structuring, these results reveal new paths for flexible structured ITO-free solar cells of enhanced efficiency.

[1] R. Meier, C. Birkenstock, C.M. Palumbiny and P. Müller-Buschbaum, Phys. Chem. Chem. Phys., 14, 15088-15098 (2012)

HL 86.4 Thu 16:00 H34

Electropolymerized polythiophenes as contact layers in organic solar cells — •Sidhant Bom and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Electropolymerized thiophene offers additional advantages to solution processable thiophenes because the doping concentration can be controlled with electrical parameters. The in-situ electrochemical doping provides a handle for the optimization of organic solar cells, either as a bulk polymer in the active layer or as an electron blocking layer. Here in this study, thiophenes are grown electrochemically with a standard three electrode system on Indium Tin Oxide (ITO) contacts. Characterization by UV-Vis measurements reflects the tunable final oxidation state of the thiophene layer. Thin layers are used in diode configuration using metal contacts like Au, Ag, Al and Cu. Static IV measurement allows the characterization of the contact according to Schottky model. Impedance measurements are used to determine the doping level of the layer. The doping level is found to be systematically depending on the applied negative bias during growth at the working ITO electrode with respect to the counter electrode. Applying a negative bias for a short interval at the end of the growth results in highly doped layers which are suitable for contact layers in solar cells.

HL 86.5 Thu 16:15 H34

Efficient solution processed p-type doping for OLEDs — •Christian Töpel, Thorsten Umbach, André Joppich, Jeanette Böckmann, Anne Köhnen, and Klaus Meerholz — University of Cologne, Chemistry Department

Organic light emitting diodes (OLEDs) have drawn much attention in science and industry. Application such as new generation lighting and display devices contribute strongly. However, drawbacks are inefficient charge carrier injection into and low conductivity of the organic materials. A promising solution for this problem is molecular doping which is commonly used in vacuum processed OLEDs, yielding in highly efficient luminescent devices (pin concept). In this case, the molecular doping leads to partial redoxchemical doping. As vacuum

deposition is very cost intensive and does not allow high volume processing, researchers focus more and more on solution processing. Here, we present efficient molecular p-type doping using various crosslinkable small-molecule hole transporting materials combined with a range of molecular dopants. Unipolar devices feature an increase in current density by several orders of magnitude compared to the undoped devices at the same voltage. We will also introduce these layers into all-solution-processed multiple-layer OLEDs. These devices are compared with their vacuum-processed counterparts to show the influence of the deposition method and doping ratio on OLED lifetime and device performance.

HL 86.6 Thu 16:30 H34

Degradation induced decrease of the radiative quantum efficiency in organic light-emitting diodes — •Tobias D. Schmidt[1], Daniel S. Setz[2], Michael Flämmich[3], Bert J. Scholz[1], Arndt Jaeger[2], Carola Diez[2], Dirk Michaelis[3], Norbert Danz[3], 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 efficiency decrease during electrical operation of organic light-emitting diodes is a crucial issue for both applied and fundamental research. In order to investigate degradation processes, we have performed an efficiency analysis for phosphorescent state-of-the-art devices in the pristine state and after an accelerated aging process at high current density resulting in a luminance drop to less than 60 % of the initial value. This loss in efficiency can be explained by a decrease of the radiative quantum efficiency of the light-emitting guest/host system from 70 % to 40 %, while other factors determining the efficiency are not affected.

15 min. break

HL 86.7 Thu 17:00 H34

Enhanced light outcoupling from corrugated top-emitting OLEDs — •C. Fuchs[1], T. Schwab[1], A. Zakhidov[1,2], K. Leo[1], M. C. Gather[1], and R. Scholz[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr Str. 1, 01069 Dresden — [2]Fraunhofer COMEDD, Maria-Reiche-Str. 2, 01109 Dresden

We analyse the emission spectra of phosphorescent top-emitting OLEDs grown on corrugated substrates. The corrugation is produced using photolithography. Thereby photoresist, spin-coated on a glass substrate is illuminated by an incoherent UV source across a contact mask with periodic structures in the sub-μm range. The optical microcavity of the OLED grown on top is defined by a thick metallic bottom contact, organic layers following the p-i-n concept, a thin metallic top contact, and an organic capping layer maximizing the outcoupling efficiency. Depending on the periodicity of the substrate, Bragg scattered wave guide modes may interfere constructively or destructively with the cavity mode inside the air light cone, hence enhancing or decreasing light emission with respect to a planar microcavity. Thus, the emission pattern deviates strongly from a Lambertian shape, but the angle-integrated external quantum efficiency can be enhanced by up to a factor of about 1.2 with respect to a fully optimized planar reference. Besides a quantitative assignment of sharp features in the emission spectra, an analysis of Bragg scattering for different periodicities can be used for designing a particular angular emission pattern, e.g. very strong forward characteristics.

HL 86.8 Thu 17:15 H34

Characterization of Gravure Printed Polymer Light-Emitting Electrochemical Cells — •Gerardo Hernandez-Sosa, Ralph Eckstein, Serpil Tekoglu, Florian Mathies, Uli Lemmer, and Norman Mechau — Lichttechnisches Institut, Karlsruher Institut für Technologie , Karlsruhe, Deutschland

In this work we present the fabrication, characterization and ink formulation of gravure printed polymer light-emitting electrochemical cells (LECs). These light emitting devices are fabricated by sandwiching a blend of a semiconducting polymer with a solid polymer electrolyte (SPE) between two electrodes, regardless of their work function. When applying a voltage to the device, the ionic species in the active film will help to form p or n doped layers at the corresponding electrode. Following the injection of carriers, the light emission will come from the semiconductor through the formation and successive recombination of excitons in the intrinsic layer between the p and n doped regions. We correlate the LEC ink formulation to the film quality and device performance. The properties of the formulation are characterized by viscosity and contact angle measurements while the properties of the film are studied by impedance spectroscopy and atomic force microscopy.

HL 86.9 Thu 17:30 H34

Strongly Fluorescent Copper Complexes for Application in OLEDs Using the Singlet-Harvesting Effect — •Rafal Czerwieniec and Hartmut Yersin — Institut für Physikalische und Theoretische Chemie, Universität Regensburg, D-93040, Germany.

A series of strongly luminescent Cu(I) complexes is presented. The emissions cover a broad spectral range from the blue to the orange. The ambient temperature quantum yields are as high as 90 % and the decay times lie in the order of several microseconds. From a detailed analysis of the photophysical behavior, the ambient temperature emission is assigned to a thermally activated delayed fluorescence (TADF). This is in contrast to the situation at low temperatures, e.g. below 100 K, at which the emission stems from the lowest triplet state decaying as long-lived phosphorescence (order of several hundred microseconds). The observed photophysical properties are related to small energy separations between the S_1 (singlet) and T_1 (triplet) excited states. The results demonstrate the high potential for application of these materials as OLED emitters by exploiting the recently reported singlet harvesting mechanism.

Literature:
1. R. Czerwieniec, J. Yu, H. Yersin, Inorg. Chem., 2011, 50, 8293-8301.
2. H. Yersin, A. F. Rausch, R. Czerwieniec, T. Hofbeck, T. Fischer, Coord. Chem. Rev., 2011, 255, 2622-2652.

HL 86.10 Thu 17:45 H34

Insight into the photophysics of photocatalytically active polymeric carbon nitride: an optical quasi-monomer — •Christoph Merschjann[1], Tobias Tyborski[1,2], Steven Orthmann[1,3], Florent Yang[1], Klaus Schwarzburg[1], Michael Lublow[1,4], and Thomas Schedel-Niedrig[1] — [1]Helmholtz-Zentrum-Berlin für Materialien und Energie — [2]Max-Born-Institut für nichtlineare Optik und Kurzzeitspektroskopie, Berlin — [3]Technische Universität Berlin — [4]Leibnitz-Institut für Katalyse, Rostock

A comprehensive investigation of the luminescent properties of photocatalytically active carbon nitride polymers, based on tri-*s*-triazine units, has been conducted for the first time. Steady-state temperature- and excitation-power-dependent as well as time-resolved measurements with near-UV excitation (λ = 325 nm & 405 nm) yield strong photoluminescence, covering the visible spectrum. The spectral, thermal and temporal features of the photoluminescence can be satisfactorily described by the excitation and radiative recombination of molecular excitons, localized at single tri-*s*-triazine units. The discussed model is in accordance with the recently reported absorption features of carbon nitride polymers. Thus, from the point of view of optical spectroscopy, the material effectively behaves as a monomer rather than a classical semiconductor.

HL 86.11 Thu 18:00 H34

Polymer semiconductors for electro chemical measurements in biosensing applications — •Martin Schmid — Helmholtz Zentrum München, Munich, Germany

There is an increasing need in medical diagnosis for reliable fast and simple biosensing devices. Sensors based on organic semiconducting polymers, which are suitable for large-area, low-cost, flexible, and eventually single-use throwaway electronics, provide a unique opportunity in that sense. We report on organic field-effect transistors (OFETs) with regioregular poly(3-hexylthiophene) (P3HT) operable at low-voltages in liquid solutions, suitable for in vitro biosensing applications. Measurements in electrolytes have shown that the performance of the transistors did not deteriorate and they can be directly used as ion-sensitive transducers. Here we show the detection of pH alterations in a wide linear range. With the intention to use the sensors as biosensing devices in biomedical applications, the experiments were performed under physiological conditions and temperature.

HL 86.12 Thu 18:15 H34

Magnetoresistive Field-Effect Transistors based on Spiro-

TAD/Spiro-PFPy Donor/Acceptor-Blends — •Thomas Reichert, Carolin Isenberg, Tobat Saragi, and Josef Salbeck — Macromolecular Chemistry and Molecular Materials (mmCmm), Department of Mathematics and Science and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Strasse 40, 34132, Kassel, Germany.

One promising opportunity for the realization of next generation magnetooptoelectronic devices is the use of the electron spin as an additional control parameter. In organic semiconductors the spin states of quasiparticles can be adjusted with low magnetic fields, which leads to large (up to 20% at 10mT) magnetoresistive effects at room temperature. We show that the sign of magnetoresistance (MR) in organic field-effect transistors (OFETs) can be tuned from positive to negative by simply applying illumination. In darkness an external magnetic-field increases the resistance (positive MR) while a magnetic-field induced resistance decrease (negative MR) can be achieved under illumination. The key aspect of this promising effect is the application of co-evaporated Spiro-TAD/Spiro-PFPy blends as the charge transport layers in OFETs. Due to the hole (electron) stabilizing properties of Spiro-TAD (Spiro-PFPy) a mixed donor/acceptor blend is formed, which leads to the observed photoinduced MR sign change. This effect can pave the way to future multifunctional spintronic devices.

HL 86.13 Thu 18:30 H34

In-wire device: combination of organic semiconductors with electrodes in an individual nanowire — •Chengliang Wang, Huaping Zhao, Liaoyong Wen, Yan Mi, and Yong Lei — Fachgebiet 3D-Nanostrukturierung, Institut fur Physik & IMN MacroNano* (ZIK), Technische Universitaet Ilmenau, Prof. Schmidt Str. 26, 98693 Ilmenau, Germany

One-dimensional wires constituted with kinds of segments attracted much attention due to the their potential application in nanogaps obtained from on-wire lithography, plasmonic disk arrays, optimized Raman *hot spots* and heterojuction structures1. Here, we will talk about the in-wire device, which combined the organic semiconductor and the electrodes in an individual nanowire, based on anodic alumina oxide (AAO) template2-3. This kind of nanodevice could be applied in organic diodes, transistors or memories, which attracted extensive attention due to the flexibility, the ease to be functionalized, the colorful and the low cost4.

Reference:

[1] S. J. Hurst, E. K. Payne, L. Qin, C. A. Mirkin, Angew. Chem. Int. Ed. 2006, 45, 2672.

[2] Y. Lei, S. Yang, M. Wu, G. Wilde, Chem. Soc. Rev. 2011, 40, 1247.

[3] Y. Lei, W. Cai, G. Wilde, Progress in Materials Science 2007, 52, 465.

[4] C. Wang, H. Dong, W. Hu, Y. Liu, D. Zhu, Chem. Rev. 2012, 112, 2208.

HL 87: Goup IV elements and their compounds II

Time: Thursday 15:45–17:30 Location: H15

HL 87.1 Thu 15:45 H15

Indirect to direct gap transition in strained and unstrained group-IV semiconductor alloys — Christian Eckhardt, •Kerstin Hummer, and Georg Kresse — University of Vienna, Computational Materials Physics, Sensengasse 8/12, 1090 Vienna, Austria

The basic problem of the well established Si technology is the indirect nature of the fundamental band gap of the elemental group-IV semiconductors resulting in inefficient light absorption and emission. To overcome these limitations, advanced (opto)electronic device design concentrates on strategies to transform materials consisting of group-IV elements from indirect into direct gap semiconductors. One promising route established is the introduction of strain either by alloying or by growing heterostructures/superlattices. Besides the extensively investigated Si/Ge system, the Sn_xGe_{1-x} alloy turned out to be very promising [1].

In this work, we focus on Sn_xGe_{1-x} and C_xGe_{1-x} random substitutional alloys. The transition from an indirect to a direct gap semiconductor in strained and unstrained alloys as a function of the Sn/C content between $0 \leq x \leq 0.5$ is investigated within density functional theory by means of both, a supercell approach and the Virtual Crystal Approximation. Accurate band structures are obtained with the modified Becke-Johnson exchange potential in combination with LDA correlation [2].

[1] H. Lin et al., Appl. Phys. Lett. **100**, 102109 (2012)

[2] F. Tran and P. Blaha, Phys. Rev. Lett. **102**, 226401 (2009)

HL 87.2 Thu 16:00 H15

Defect states at c-Si/a-$Si_3N_xH_y$ interfaces — •Leif Eric Hintzsche[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

Amorphous silicon nitrides are deposited on crystalline silicon as antireflection and passivating coatings. Up to date detailed knowledge about the interfaces is largely lacking. We have investigated the electronic and structural properties of c-Si/a-$Si_3N_xH_y$ interfaces obtained by large scale ab initio molecular dynamics simulations. Over 500 independent samples have been generated for each considered stoichiometry to perform a reliable defect analysis. While the classes of dominant defect states coincided with previous bulk calculations, we found a considerably increased defect density at the interface. By applying an energy and spatially resolved defect analysis, we observed that most of the defect states originate from the first silicon nitride layer at the interface. Additionally, we examined passivation effects of hydrogen at the interface which play an important role to increase the efficiency of modern solar cells.

HL 87.3 Thu 16:15 H15

First stages of 4H-SiC crystal growth: *ab initio study* — •Elwira Wachowicz[1,2] and Adam Kiejna[1] — [1]Institute of Experimental Physics, University of Wroclaw, Wroclaw, Poland — [2]Interdisciplinary Centre for Mathematical and Computational Modelling, University of Warsaw, Warsaw, Poland

The wide band-gap semiconductor silicon carbide has attracted a great interest during the past decades because of number of properties which make it very attractive for many applications in electronic devices. For electronic applications purposes hexagonal 4H-SiC is the preferred polytype. One of the main problems in the development of the SiC-based electronics is still poor quality of the SiC crystals. Therefore, it is necessary to understand the interaction of basic building bricks like Si, C, Si_2C and SiC_2 with the surface. Since hexagonal SiC crystals grow along <0001> direction the interaction of Si, C and Si_2C interaction with Si- and C-terminated {0001} surfaces is examined within DFT framework. The most favourable adsorption sites are identified. Qualitative *ab initio* molecular dynamic simulations show that molecules bind to both examined surfaces without dissociation. It is confirmed by quantitative DFT studies showing that there is no barrier for the molecule adsorption. Moreover, a possible mechanism of Si_2C on-surface dissociation is examined.

HL 87.4 Thu 16:30 H15

Reactive Ion Etching of Nano- and Ultrananocrystalline Diamond Films for Fabrication of Nanopillars — Christo Petkov, Emil Petkov, Florian Schnabel, Wilhelm Kulisch, Johann Peter Reithmaier, and •Cyril Popov — Institute of Nanostructure Technologies and Analytics, Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

One-dimensional diamond nanostructures, namely diamond nanopillars, have been prepared using nano- and ultrananocrystalline diamond films (NCD and UNCD, respectively) as starting materials. The fabrication process of arrays of nanopillars with diameters from 200 nm to 1000 nm consisted of their definition by electron beam lithography (EBL) applying gold or silica as a hard mask and subsequent inductively coupled plasma reactive ion etching (ICP-RIE) with oxygen. The major ICP-RIE parameters, like ICP power, RF power, working pressure, oxygen flow, etc. were optimized with respect to the quality

of the nanopillars and the etching rate, which was monitored in situ with an interferometer. Furthermore, the influence of the hard mask material and pillar diameter on the geometry of the nanostructures was studied. The fabricated diamond nanopillars, especially those from NCD, can be used as photonic devices for integration of NV centers during the film growth or by follow-up ion implantation.

HL 87.5 Thu 16:45 H15

Dephasing in Ge/SiGe quantum wells measured by means of coherent oscillations — •Kolja Kolata[1], Niko S. Köster[1], Alexey Chernikov[1], Michael J. Drexler[1], Eleonora Gatti[2], Stefano Cecchi[3], Daniel Chrastina[3], Giovanni Isella[3], Mario Guzzi[2], and Sangam Chatterjee[1] — [1]Philipps-Universität Marburg — [2]L-NESS, Università di Milano Bicocca — [3]L-NESS, Polo di Como

In general, all coherent effects in optically excited materials depend crucially on the dephasing of the addressed states. Therefore, knowing the duration of the coherence and understanding the dephasing mechanisms is mandatory in order to interpret coherent effects correctly. Dephasing mechanisms are often summarized in the dephasing time which is also used as a phenomenological damping parameter in theoretical descriptions. Ge/SiGe heterostructures as a material system are especially interesting for dephasing studies since they exhibit strong nonlinear coherent responses such as the giant dynamical Stark effect. We present a dephasing time analysis of the three lowest excitonic resonances in Ge/SiGe quantum well samples for the temperatures down to 7K by coherent oscillations spectroscopy (COS). The results are compared to the line widths of the excitonic resonances determined by linear absorption measurements. Strikingly, the lowest direct-gap transition in the best quality sample is dominated by homogeneous broadening over the entire investigated temperature range. This is explained by the fast inter-valley scattering of the electrons which leads to intrinsically short dephasing times of merely 300 fs as an upper limit.

HL 87.6 Thu 17:00 H15

Photonic crystal microcavities for the luminescence enhancement of Si/Ge-Quantum dots around 1550nm wavelength — •Viktoriia Rutckaia[1], Benjamin Koehler[1], Vadim Talalaev[2], Frank Heyroth[3], and Joerg Schilling[2] — [1]Martin-Luther University, Halle (Saale), Germany — [2]Centre for Innovation Competence SiLi-nano, Halle (Saale), Germany — [3]Interdisciplinary Center of Materials Science, Halle (Saale), Germany

Defects in two dimensional photonic crystal slabs represent microcavities with small mode volumes and can exhibit large Q-factors. This can lead to a large enhancement of spontaneous emission rate causing an overall enhancement of radiative recombination efficiency. This was also already observed for the photoluminescence of Ge quantum dots in Si [1]. The aim of this work is to show how the Q-factor of certain defect modes can be altered by adjusting the geometry of the pores adjacent to the cavity. This involves changing their diameter and variation of their positions. We present band gap and defect resonance calculations for 2D photonic crystal cavities using MIT mpb program [2], and COMSOL multiphysics. From the field distribution the mode volume is determined and theoretically possible Purcell factors are obtained. Experimental studies of the luminescence enhancements in the micro cavities involve micro-photoluminescence measurements on Ge quantum dots embedded in Si. Defect resonances are observed and their Q-factors were obtained from the luminescence spectra. [1] J.S.Xia,Y.Ikegami, and Y.Shiraki, Appl.Phys.Let.89,201102(2006),[2] Steven G.Johnson and J.D.Joannopoulos, Opt.Exp.8,3,173-190(2001)

HL 87.7 Thu 17:15 H15

Side-wall damage analysis of low-k interlayer dielectric from energy-filtered transmission electron microscopy — •Pradeep K. Singh[1], Sven Zimmermann[2], Steffen Schulze[1], Stefan Schulz[2,3], and Michael Hietschold[1] — [1]Chemnitz University of Technology, Institute of Physics, D-09107 Chemnitz, Germany — [2]FraunhoferInstitute for Electronic Nano Systems (Fraunhofer ENAS), Dept. BEOL, D-09107 Chemnitz, Germany — [3]Chemnitz University of Technology, Center for Microtechnologies, D-09107 Chemnitz, Germany

The continues shrinkage in device dimensions leads towards the inevitable replacement of the conventional SiO2 material as an inter-layer dielectric with lower dielectric constant (low-k) material. Several low-k dielectric materials were developed for this purpose. Among these, the organosilicate glasses are of preferred choice due to their excellent properties as an inter-layer dielectric. The organosilicate glasses consist of the methyl groups doped inside the SiO2 networks. One of the major challenges to incorporate the low-k dielectric materials in device production is the side-wall damage of these materials. The side-wall damage regions were characterized by the energy-filtered transmission electron microscopy. The etch and ash plasma used in the standard processes, damaged the side-walls in the 10th of nano-meter region. The side-walls were found to be depleted from carbon and hence behave more like SiO2 material.Due to the higher dielectric constant of SiO2 as compared to the low-k dielectric materials, the effective dielectric constant of the low-k material increases by the plasma treatment.

HL 88: Focus Session: Frontiers of electronic structure theory VII (O, jointly with HL, TT)

Time: Thursday 16:00–19:00 Location: H36

HL 88.1 Thu 16:00 H36

Determination of the one-body Green's function: freedom and constraints — Giovanna Lani[1,4], •Pina Romaniello[2,4], and Lucia Reining[3,4] — [1]Forschungszentrum Jülich, Jülich, Germany — [2]Laboratoire de Physique Théorique-IRSAMC, CNRS, Université Paul Sabatier, Toulouse, France — [3]Laboratoire des Solides Irradiés, Ecole Polytechnique, CNRS, CEA-DSM, Palaiseau, France — [4]European Theoretical Spectroscopy Facility (ETSF)

The one-particle Green's function G plays a key role in many-body physics due to the wealth of physical information that it contains. In this work we go beyond the standard methods to calculate G, which are plagued by various shortcomings, and we use an approximate set of functional differential equations relating the one-particle Green's function to its functional derivative with respect to an external perturbing potential [1]. We show that this set of equations has, in principle, multiple solutions, but that only one is well behaved - this is the physical solution. We give the formally exact family of solutions, which depends on an auxiliary quantity q, for which we find stringent exact constraints. Our findings suggest that once q is known, the physical solution is uniquely fixed by the vanishing Coulomb interaction limit [2-3].

[1] L. P. Kadanoff and G. Baym, Quantum Statistical Mechanics (W.A. Benjamin Inc., New York, 1964)
[2] G. Lani, P. Romaniello, and L. Reining, New Journal of Physics, 14, 013056 (2012)
[3] G. Lani, P. Romaniello, and L. Reining, in preparation

HL 88.2 Thu 16:15 H36

Restoring piecewise linearity in density-functional theory — •Ismaila Dabo[1], Andrea Ferretti[2], Matteo Cococcioni[3], and Nicola Marzari[4] — [1]Ecole des Ponts ParisTech, Marne-la-Vallee, France — [2]CNR-Istituto Nanoscienze, Modena, Italy — [3]University of Minnesota, Minneapolis, USA — [4]EPFL, Lausanne, USA

Electronic-structure calculations based upon density-functional theory (DFT) have been fruitful in diverse areas of condensed matter physics. Despite their exceptional success, it can hardly be denied that a range of fundamental electronic properties fall beyond the scope of current DFT approximations. Many of the failures of DFT calculations take root in the lack of piecewise linearity of approximate functionals, which reverberates negatively on the electronic-structure description of systems involving fractionally occupied and spatially delocalized electronic states, including but not restricted to dissociated molecules, adsorbed species, charge-transfer complexes, and semiconducting compounds. In this talk, I will present a novel class of first-principles methods that restores the piecewise linearity of the total energy by imposing Koopmans' theorem to DFT approximations. The Koopmans-compliant approach is apt at describing full orbital spectra within a few tenths of an electron-volt relative to experimental direct and inverse photoemission data. This level of accuracy is comparable to the predictive performance of accurate many-body perturbation theory methods at a fraction of their computational cost, and with the additional benefit of providing accurate total energies for systems with fractional occupations.

HL 88.3 Thu 16:30 H36

Self-interaction-corrected and Koopmans-compliant functionals: from molecules to solids — •Giovanni Borghi[1], Linh Nguyen[1], Andrea Ferretti[2], Ismaila Dabo[3], and Nicola Marzari[1] — [1]Theory and Simulation of Materials, EPFL, Lausanne — [2]CNRNANO, University of Modena and Reggio Emilia — [3]Ecole des Ponts ParisTech, Université Paris-Est

We present an overview of the performance of self-interaction corrected, orbital-density dependent functionals as applied to the calculation of the electronic structure of atoms, molecules and solids.

In particular, we show how orbital-dependent corrections of Koopmans' compliant functionals are able to restore not only the correct ionization energies, but also the eigenvalues of low-lying single-particle states with an accuracy comparable or better to that of many-body perturbation theory, while retaining a variational principle which grants the possibility to optimize geometries and bond lengths.

The outcome of these orbital-density dependent calculation remain, even in the thermodynamic limit, Wannier-like orbitals, that localize thanks to a condition related to the Edmiston-Ruedenberg criterion. These localized functions can be used as Wannier interpolators of band structures, allowing to discuss the performance of the functionals in the solid-state limit.

HL 88.4 Thu 16:45 H36

Lattice density functional theory at finite temperature with strongly density-dependent exchange-correlation potentials — •Stefan Kurth[1], Gao Xianlong[2], A-Hai Chen[2], and Ilya Tokatly[1] — [1]Univ. of the Basque Country UPV/EHU, San Sebastian, Spain and IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — [2]Zhejiang University, Jinhua, China

The derivative discontinuity of the exchange-correlation (xc) energy of density functional theory (DFT) at integer particle number is absent in many popular local and semilocal approximations. In lattice DFT, approximations exist which exhibit a discontinuity in the xc potential at half filling but due to convergence problems of the Kohn-Sham (KS) self-consistency cycle, the use of these functionals is mostly restricted to situations where the local density is away from half filling. Here a numerical scheme for the self-consistent solution of the lattice KS Hamiltonian with a local xc potential with rapid (or quasi-discontinuous) density dependence is suggested. The problem is formulated in terms of finite-temperature DFT where the discontinuity in the xc potential emerges naturally in the limit of zero temperature. A simple parametrization is suggested for the xc potential of the uniform 1D Hubbard model at finite temperature obtained from the thermodynamic Bethe ansatz. The feasibility of the numerical scheme is demonstrated by application to a model of fermionic atoms in a harmonic trap. The corresponding density profile exhibits a plateau of integer occupation at low temperatures which melts away for higher temperatures.

HL 88.5 Thu 17:00 H36

Kohn-Sham equations beyond the single-determinant approximation — Nektarios N. Lathiotakis[1], •Nicole Helbig[2,3], Nikitas I. Gidopoulos[4], and Angel Rubio[3,5] — [1]Theoretical and Physical Chemistry Institute, NHRF, Athens, Greece — [2]Peter-Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, Jülich, Germany — [3]Nano-Bio Spectroscopy group and ETSF Scientific Development Centre, Dpto. Física de Materiales, Universidad del País Vasco, CFM CSIC-UPV/EHU-MPC and DIPC, San Sebastián, Spain — [4]ISIS, STFC, Rutherford Appleton Laboratory, HSIC, Didcot, United Kingdom — [5]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

We describe a new method for the optimization of the total energy in reduced density matrix functional theory (RDMFT) which reduces the computational costs to the costs of a density functional calculation within the optimized effective potential method. Within this method the natural orbitals are restricted to be solutions of a single-particle Schrödinger equation with a local effective potential which in addition to reducing the computational costs also provides an energy eigenvalue spectrum connected to the natural orbitals. This energy spectrum is shown to reproduce the ionization potentials of different atoms and molecules very well. In addition, the dissociation limit is well described without the need to break any spin symmetry, i.e. this attractive feature of RDMFT is preserved.

HL 88.6 Thu 17:15 H36

Initial stages of time-evolution of excitations in Fermi liquids and finite systems — •Yaroslav Pavlyukh[1], Jamal Berakdar[1], and Angel Rubio[2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany — [2]Nano-Bio Spectroscopy Group and ETSF Scientific Development Centre, Dpto. de Física de Materiales, Universidad del País Vasco, CFM CSIC-UPV/EHU-MPC and DIPC, Av. Tolosa 72, E-20018 San Sebastián, Spain

A particle-hole excitation in a many-body system is not an eigenstate and, thus, evolves in time. The evolution at short times after an excitation with the energy ϵ was created is the quadratic decay with the rate constant $\sigma^2(\epsilon)$. Later, after some set-in time $\tau(\epsilon)$, the exponential decay develops. It is governed by another rate constant $\gamma(\epsilon)$.

We study the electron-boson model for the homogenous electron gas and use the first order (in boson propagator) cumulant expansion of the electron Green's function. In addition to a quadratic decay in time upon triggering the excitation, we identify non-analytic terms in the time expansion similar to those found in the Fermi edge singularity phenomenon.

Finite systems (J. Chem. Phys., **135**, 201103 (2011)) give an opportunity to test the conjectured behavior numerically as an exact solution of a many-body problem is feasible. We propose a simple model for the electron spectral function that links together all three aforementioned parameters and give a prescription how the energy uncertainty $\sigma^2(\epsilon)$ can be computed within the many-body perturbation theory.

HL 88.7 Thu 17:30 H36

Real-structure effects from *ab-initio* calculations — •Andre Schleife — Condensed Matter and Materials Division, Lawrence Livermore National Laboratory, Livermore, CA, USA

By harnessing the power of supercomputers, *computational materials science* is becoming a field that enables insight into fundamental materials physics. It is inevitable to further push *ab-initio* approaches, allowing them to account for effects that are important at the forefront of experimental research.

I will present the solution of the Bethe-Salpeter equation as a recent theoretical-spectroscopy technique and how it is extended and used to understand real-structure effects in oxide and nitride semiconductors. This talk will illustrate the success of our modification of this framework to describe the interplay of free electrons and excitonic effects in n-doped ZnO. Combining a cluster expansion scheme and electronic-structure calculations allows to explore the potential for band-gap tailoring in oxide and nitride alloys. These material systems are a driving force of current semiconductor technology, e.g. for solar cells and solid-state lighting; understanding fundamental effects will help to overcome performance limits.

In addition, computational materials science can *replace* dangerous experiments, e.g. in the context of radiation damage: I will present large-scale simulations of non-adiabatic electron-ion dynamics based on real-time time-dependent density functional theory that explain electronic stopping as an important mechanism responsible for radiation damage when fast H or He ions penetrate aluminum.

HL 88.8 Thu 17:45 H36

Specwer: an efficient first-principle program for electronic structures and spectroscopic simulations of nanomaterials — •Bin Gao — Center for Theoretical and Computational Chemistry, Department of Chemistry, University of Tromso, N-9037 Tromso, Norway

Although nanomaterials have been routinely synthesized and analyzed in various laboratories around the world, they still present great challenges for theoretical studies using the ab initio and/or first-principle methods due to the simple fact that they are too large to handle for the conventional theoretical approaches. Various linear-scaling methods have been proposed in recent decades to circumvent this difficulty. In this talk, I will present our recently developed program Specwer and its applications for electronic structures and spectroscopic simulations of different nanomaterials. For large-scale molecules, Specwer program employs the reduced single-electron density matrix and divide-and-conquer method. I will show its applications in the ground and excited states of nanomaterials at various density functional theory levels, in which the information of excited states is obtained via solving the so-called Liouville-von Neumann equation. I will also highlight the importance of including the spin-orbit coupling in some cases, for instance, the L-edge X-ray absorption spectroscopy, and the electron transport in double-stranded DNA molecules.

HL 88.9 Thu 18:00 H36

Generalized incomplete-basis-set correction applied to EXX-

OEP — •Markus Betzinger, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We recently derived [1] an incomplete-basis-set correction (IBC) for all-electron response functions within the full-potential linearized augmented plane-wave (FLAPW) method as realized in the FLEUR code [2]. The IBC utilizes the potential dependence of the LAPW basis functions whose response is calculated explicitly by solving radial Sternheimer equations in the spheres. While in the original formulation of the IBC [1] only spherical perturbations of the potential have been taken into account, we show here an extension to non-spherical perturbations, replacing the single radial Sternheimer equation for each angular momentum ℓ by a set of equations coupling different angular momenta. Likewise, the response of the core electrons is computed. We demonstrate that this generalized IBC improves further the convergence in terms of basis-set size and number of unoccupied states. We apply the generalized IBC to the exact-exchange (EXX) optimized-effective-potential (OEP) approach. While for simple semiconductors and insulators the original IBC already leads to a physical and stable local EXX potential, we show that for more complex materials like NiO, whose band gap is formed by d states, the generalization of the IBC is crucial to obtain a well-converged local optimized potential.

[1] M. Betzinger *et al.*, Phys. Rev. B **85**, 245124 (2012)
[2] http://www.flapw.de

HL 88.10 Thu 18:15 H36

One particle spectral function and analytic continuation for many-body implementation in the exact muffin-tin orbitals method — •Andreas Östlin[1], Liviu Chioncel[2,3], and Levente Vitos[1,4,5] — [1]Department of Materials Science and Engineering, Applied Materials Physics, KTH Royal Institute of Technology, Stockholm SE-100 44, Sweden — [2]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany — [3]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [4]Department of Physics and Astronomy, Division of Materials Theory, Uppsala University, Box 516, SE-751210, Uppsala, Sweden — [5]Research Institute for Solid State Physics and Optics, Wigner Research Center for Physics, Budapest H-1525, P.O. Box 49, Hungary

We investigate one of the most common analytic continuation techniques in condensed matter physics, namely the Padé approximant. Aspects concerning its implementation in the exact muffin-tin orbitals (EMTO) method are scrutinized with special regard towards making it stable and free of artificial defects. We discuss the difference between the **k**-integrated and **k**-resolved analytical continuations, as well as describing the use of random numbers and pole residues to analyze the approximant. It is found that the analytic properties of the approximant can be controlled by appropriate modifications. At the end, we propose a route to perform analytical continuation for the EMTO + dynamical mean field theory (DMFT) method.

HL 88.11 Thu 18:30 H36

Core-electron forces within the FLAPW method — •Daniel Aaron Klüppelberg, Markus Betzinger, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

The full-potential linearized augmented-plane-wave method (FLAPW) is an all-electron electronic-structure method based on density functional theory (DFT). Characteristic to the method is that space is divided into spheres around the atoms, so called 'muffin-tins', and an interstitial region in between. Local orbitals can be used to describe semicore states within the valence-state formalism. It is established as an accurate tool for describing many properties of complex materials.

We address the occurrence of contributions to the forces due to core electrons described by wave functions having tails exceeding the muffin-tin boundary. Accurate forces are needed not only for relaxing the atomic structure to its ground state, but also in order to calculate precise phonon spectra via the finite-displacement method. We present a core-tail correction to the Pulay force term found by Yu *et al.* [1], implemented into the FLEUR code [2], which deals with the core electrons. This addition extends the known formula over the whole unit cell and therefore includes the complete force contribution coming from core states that extend beyond their muffin-tin. In this talk, we will present examples on the performance of this addition in comparison to the inclusion of local orbitals and the adjustment of the muffin-tin radii.

[1] R. Yu, D. Singh, and H. Krakauer, Phys. Rev. B **43**, 6411 (1991)
[2] www.flapw.de

HL 88.12 Thu 18:45 H36

The linearized augmented lattice-adapted plane wave basis — •Gregor Michalicek and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The full-potential linearized augmented plane wave method (FLAPW) is an all-electron electronic structure method that provides density functional results for complex solids with very high precision, irrespective of the chemical element of the solid. For this purpose the Kohn-Sham wavefunctions are expanded into LAPW basis functions. These are plane waves in an interstitial region (IR) that are augmented by atom-centered functions in non-overlapping spheres around each atom. The LAPW basis features many desirable properties that are a key component to the high precision of the FLAPW method.

In this talk we show that the capability of the FLAPW method can be kept with a modification of the basis-set that is numerically more efficient. We argue that the required plane-wave cut-off of the interstitial part of the LAPW basis results mostly from mathematical conditions and the efficiency of the LAPW description can be increased by incorporating more physics into the construction of this part of the basis. We propose a linearized augmented lattice-adapted plane wave basis ((LA)^{2}PW) that replaces the plane waves in the IR by smart linear combinations of plane waves, show how to realize an efficient implementation of such a basis, and provide a construction principle for the linear combination of plane waves. The so constructed basis is evaluated in terms of precision and calculation runtime performance.

HL 89: Transport II

Time: Thursday 16:45–18:00 Location: H16

HL 89.1 Thu 16:45 H16

Non-equilibrium Polaritonics - Non-linear Effects and Optical Switching — •Regine Frank — Institut für Theoretische Physik, Universität Tübingen

A microscopic electronic non-equilibrium effect, highly nonlinear polaritonics, is proposed to mediate an ultrafast all-optical switching. The electronic band structure within the switching material shall be modified by external laser light, namely the Franz-Keldysh effect, and the modified electronic density of states within the Au grains are coupled to a single mode photonic waveguide. Using this microscopic polaritonic coupling without ever including any macroscopic influences due to the geometric arrangement a strong transmission reduction originating from the established quantum interference is derived. The lifetime of the coupled states is heavily dependent on the Fano resonance type binding and the amplitude of the applied electric field. Besides the Fano signatures the microscopic coupling photon-electron-photon leads to a modified gaped electronic density of states within the switching material. On site interaction as well as finite temperature effects are considerd.

HL 89.2 Thu 17:00 H16

Analytical and numerical transistor models for carbon nanotubes under strain — •Christian Wagner[1], Jörg Schuster[2], and Thomas Gessner[1,2] — [1]Center for Microtechnologies, Chemnitz University of Technology, Chemnitz, Germany — [2]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany

Carbon nanotubes (CNTs) are objects attracting high interest in research and applications. While the physics of CNTs is understood quite well, the quantitative description of their properties within an application-environment is of huge interest.

Piezoresistive acceleration sensors are first upcoming applications of CNTs, where they are ideal candidates due to their mechanical strength

and their outstanding piezoresistive response. In experiments, these kinds of sensors need an applied gate voltage to adjust the working point which may change i.e. due to adsorbed molecules on the CNT.

Therefore, we calculate the resistance of infinite CNTs under strain — with respect to different gate and drain-source voltages, but without regard to contacts. The Landauer approach is used and condensed into an analytical model. This yields a simplified description of the characteristics based on the band gaps of strained CNTs described in [1,2]. The different levels of theory – analytical and numerical – are investigated. This ends up in a fully parametric description of a CNT device. One of the results is that the sensing regime can be adjusted by the gate- and drain-source voltage.

[1] Yang, L. and Han, J., *Phys. Rev. Lett. 85*, p. 154, **2000**
[2] Wagner, C. et al., *Phys. Stat. Sol. C*, **2012**, doi: 10.1002/pssb.201200113

HL 89.3 Thu 17:15 H16

All-electrical measurements of direct spin Hall effect in GaAs with Esaki diodes — •Markus Ehlert[1], Mariusz Ciorga[1], Cheng Song[1,2], Martin Utz[1], Dominique Bougeard[1], and Dieter Weiss[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, D-93040 Regensburg, Germany — [2]Laboratory of Advanced Materials, Department of Material Science & Engineering, Tsinghua University, Beijing 100084, China

We present measurements of direct spin Hall effect (DSHE) in lightly doped n-GaAs channels (2×10^{16} cm^{-3}) employing ferromagnetic (Ga,Mn)As/GaAs Esaki diode structures as spin detecting contacts. This setup, similar to the one used in [1], allows us to efficiently probe the low level spin polarization generated by DSHE even in channels with low conductivities (below 2000 Ω^{-1}m^{-1}). In our experiments [2] we investigate bias and temperature dependence of the measured spin Hall signal and evaluate the value of total spin Hall conductivity and its dependence on channel conductivity and temperature. From the results, we determine skew scattering and side-jump contribution to the total spin Hall conductivity, which we compare to both theory [3] and experiments performed with higher conductive n-GaAs channels [1]. We conclude that both skewness and side jump contribution cannot be treated as fully independent of the conductivity of the channel. This work was supported by DFG SFB689 and DFG SPP1285.

[1] E. S. Garlid *et al.*, Phys. Rev. Lett. **105**, 156602 (2010).
[2] M. Ehlert, M. Ciorga *et al.*, Phys. Rev. B **86**, 205204 (2012).
[3] H. A. Engel *et al.*, Phys. Rev. Lett. **95**,166605 (2005).

HL 89.4 Thu 17:30 H16

Electron spin dynamics in Gd-implanted GaN — •Jörg Rudolph[1], Jan Heye Buss[1], Stepan Shvarkov[2], Andreas D. Wieck[2], and Daniel Hägele[1] — [1]AG Spektroskopie der kondensierten Materie, Ruhr-Universität Bochum, Bochum, Germany — [2]Angewandte Festkörperphysik, Ruhr-Universität Bochum, Bochum, Germany

Dilute magnetic semiconductors (DMS) are a prerequisite for the development and realization of a spin-based electronics. GaN-based DMS have attracted strong interest in the last years, with a special focus on Gd-doped GaN after reports of ferromagnetism with Curie temperatures far above room-temperature [1]. Experimental evidence for high-temperature ferromagnetism in Gd:GaN was, however, always based on integral measurements of the magnetization by SQUIDs, while complementary methods like x-ray magnetic dichroism or magnetic resonance techniques could not corroborate the claimed ferromagnetism [2]. We measure the electron spin dynamics in GaN implanted with different Gd densities as well as coimplanted with Si by time-resolved magneto-optical Kerr-rotation spectroscopy. We find strongly increased electron spinlifetimes for an intermediate Gd concentration. This strong increase is, however, shown to be a consequence of the high defect density created during the ion implantation, and not a consequence of a magnetic effect of the Gd ions.

[1] S. Dhar *et al.*, Phys. Rev. Lett. **94**, 037205 (2005)
[2] A. Ney *et al.*, J. Magn. Magn. Mat. **322**, 1162 (2010)

HL 89.5 Thu 17:45 H16

Exchange Interaction of Phosphorus Donors and Interface Defects at the Si/SiO_2 Interface — •Max Suckert[1], Felix Hoehne[1], Lukas Dreher[1], Hans Huebl[2], Martin Stutzmann[1], and Martin S. Brandt[1] — [1]Walter Schottky Institut, Garching, Germany — [2]Walther-Meißner-Institut, Garching, Germany

Electrically detected magnetic resonance (EDMR) has been established as a versatile tool to investigate the properties of paramagnetic defects. The method involves the formation of spin pairs whose symmetry determines the transport properties resulting in a resonant current change when spins are flipped by microwave irradiation.

We apply the method of electrically detected double electron–electron resonance (EDDEER), recently added to the EDMR toolbox, to determine the coupling between phosphorus donors ^{31}P and dangling bonds P_{b0} at the Si/SiO_2 interface quantitatively. This spin pair is of particular interest for the electrical readout mechanism allowing for the detection of coherent spin manipulation of the ^{31}P and decoherence introduced by the P_{b0} to the ^{31}P spins. By modelling the exchange interaction numerically and comparing the result to the EDDEER time evolution, we assign the typical coupling strength of 600 kHz observed to a distribution of ^{31}P–P_{b0} spin pairs with distances in the range from 14 to 20 nm.

The work was supported by DFG (Grant No. SFB 631, C3 and Br 1585/8-1) and BMBF.

HL 90: Poster Session: Quantum information systems; Optical properties; Ultrafast phenomena

Presenters are kindly asked to be near their posters at least 17:00–18:00 or to leave a note at the poster indicating a time period of availability for discussions. — Beverages will be served starting at 18:00.

Time: Thursday 16:00–20:00 Location: Poster A

HL 90.1 Thu 16:00 Poster A

Strong bipartite and multipartite entanglement from planar microcavities — •Daniel Pagel[1], Holger Fehske[1], Jan Sperling[2], and Werner Vogel[2] — [1]Institut für Physik, Ernst-Moritz-Arndt-Universität Greifswald, 17487 Greifswald, Germany — [2]Institut für Physik, Universität Rostock, 18051 Rostock, Germany

The emission of entangled light from planar semiconductor microcavities is studied. In doing so, their nonclassical correlations are analyzed and quantified. Entanglement arises due to phase matching of the intracavity scattering dynamics of polaritons for multiple pump beams or pulses. We show, how parametric processes involving the lower polariton branch only, give rise to 2^N-partite entangled photons in W states, being the equal-weighted superposition of all pure states with one excited qubit and $2^N - 1$ qubits in the ground state. A second scenario that involves both polariton branches can generate multiple pairs of photons which are frequency entangled. By a decomposition into two parties, their nonclassical correlations can be identified as a bipartite entanglement, which is quantified by Schmidt number witnesses. We discuss to which extent the resources of the originally strongly entangled light field are diminished by dephasing in propagation channels.

HL 90.2 Thu 16:00 Poster A

Optical superresolution microscopy of individual spin defects in diamond — •Matthias Pfender, Nabeel Aslam, Gerald Waldherr, Philipp Neumann, and Jörg Wrachtrup — 3. Physikalisches Institut, Universität Stuttgart, Germany

The nitrogen-vacancy defect center in diamond is one of the major candidates for a room temperature quantum processor. By optical microscopy the quantum state of individual defects can be readout and initialized. This includes charge states as well as electron and nuclear spin states. As the spins associated with the NV center possess favorable coherence properties first quantum information tasks have already been implemented. In addition to quantum information processing this spin system is also applied for metrology purposes (i.e. nanoscale sensing of magnetic and electric fields as well as temperature). When the average distance of NV centers in these quantum devices is decreased below the diffraction limit individual addressing becomes challenging. Here we demonstrate a novel method for farfield optical superresolution imaging of NV centers with a resolution below

10 nm which is applicable to dense clusters of defects. Our method exploits recent novel insight into the charge state dynamics of this defect. Furthermore, additional spin manipulation allows for further resolution improvements and nanoscale metrology without the need for scanning probe techniques.

HL 90.3 Thu 16:00 Poster A

Temperature dependent dielectric function of yttria stabilized zirconia and alumina — •Tobias Lühmann, Tammo Böntgen, Helena Franke, Rüdiger Schmidt-Grund, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstraße 5, 04103 Leipzig

We present the dielectric function (DF) of yttria stabilized zirconia (YSZ) and Al_2O_3 thin films in the spectral range 1 - 7.5 eV for temperatures between 10 K and room temperature. The DF spectra of the pulsed laser deposited thin films where obtained by means of spectroscopic ellipsometry with subsequent layer model analysis using model dielectric functions. Special attention is devoted to differences in the absorption properties in the near band gap spectral range for films grown at low and high temperature, respectively. It was found that the structural properties, and thus the absorption properties, differ considerably. The low temperature grown materials are found to be amorphous whereas the high temperature grown films are nano-crystalline.

The near band gap absorption properties of these materials have great impact on the usability of these materials for dielectric mirrors, so-called distributed Bragg reflectors, which are used in ZnO-based microcavities [1].

[1] H. Franke, C. Sturm, R. Schmidt-Grund, G. Wagner, and M. Grundmann, New J. Phys. **14**, 013037 (2012).

HL 90.4 Thu 16:00 Poster A

THz-Transmission Spectroscopy of Charge Carriers in Surface Electric Fields — •Shovon Pal, Nathan Jukam, and Andreas D. Wieck — Applied Solid State Physics, Ruhr University Bochum, Germany

Intersubband transitions take place between quasi-two-dimensional 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 absorption maxima at intersubband resonance (ISR) frequencies. The absorption wavelength of accumulation and inversion layers lie in the THz domain and hence THz-transmission spectroscopy of these 2D charge carriers serves as an effective tool. A lot of work has been done on intersubband transitions with metallic Schottky gates. But these gates suffer from low breakdown voltages, low transmittance and fails to grow lattice-matched and epitaxially on most compound semiconductors. Epitaxial, complementary doped gates open the possibility to control the charge carrier density to observe the ISR with better optical access. The experimental set-up is being built, which uses a Bruker IFS 113V spectrometer. Semiconductor heterostructures were grown by molecular beam epitaxy (MBE). In the beginning, deposition of a 5 nm semi-transparent gold gate was accomplished by means of UV-photolithography and metallization techniques. The deposition of complementary p-doped gates were performed inside the MBE. The characterization of the heterostructures was done by Hall measurement technique at 300 K and 4.2 K.

HL 90.5 Thu 16:00 Poster A

Phase resolved near field measurements on surface plasmons — •Lena Simone Fohrmann, Jens Ehlermann, Jan Siebels, and Stefan Mendach — Institute of Applied Physics, University of Hamburg, Germany

As Surface plasmons can be confined to small nanostructure sized areas - much smaller than the wavelength of the exciting free space photons - they are thought to combine the benefits of photonics and microelectronics, i.e. high frequency and small dimensions, in future integrated devices [1].

Scanning near field optical microscopy is an outstanding tool to investigate the interaction of surface plasmons with nanostructures prepared on metal films. In combination with heterodyne detection it is possible to directly detect the amplitude and phase of near field distributions on sample surfaces [2][3].

Here we present phase resolved near field measurements of surface plasmons propagating on gold films and their interaction with plasmonic nanostructures.

We gratefully acknowledge financial support of the Deutsche Forschungsgemeinschaft via the Graduiertenkolleg 1286.

[1] D. Chang et al., Nature Physics, 3, 807-812 (2007)
[2] M.L.M. Balistreri et al., Phys. Rev. Lett. 85, 294 (2000)
[3] A. Nesci et al., Optics Letters, 26, 208-210 (2001)

HL 90.6 Thu 16:00 Poster A

Photocapacitance of metal-bilayer oxide-semiconductor capacitors — •Varun John[1], Danilo Bürger[1,2], Ilona Skorupa[2], Gyyörgy.J. Kovacs[2], Martin Schuster[3], Oliver G. Schmidt[4], and Heidemarie Schmidt[1] — [1]University of Technology Chemnitz, Faculty of Electrical Engineering and Information Technology, 09107 Chemnitz, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf e.V., Institute of Ion Beam Physics and Materials Research, Germany — [3]NaMLab gGmbH, 01187 Dresden, Germany — [4]Institute for Integrative Nanosciences, IFW Dresden, 01069 Dresden, Germany

Photocapacitance-voltage measurements have been performed on metal-VO2/SiO2-p-Si semiconductor capacitors under illumination in the spectral range from 300 nm to 800 nm. For depletion and inversion bias mode we observe that for energies smaller than 2.5 eV, i.e. for energies below the transition energy between a set of oxygen 2p orbitals and the Fermi energy of VO2 [1], the photocapacitance is larger than the capacitance without illumination. Furthermore, the photocapacitance has a broad maximum in the spectral range from 650 nm to 750 nm. For the accumulation bias mode the photocapacitance equals the capacitance without illumination. The drift of photogenerated charge carriers is used to discuss the observed photocapacitance effects in SiO2 single layer and VO2/SiO2 bilayer semiconductor capacitors with varying thickness of the PLD grown VO2 [2] and the thermally grown SiO2 layers. [1] C.N. Berglund and H.J. Guggenheim, Phys. Rev. 185 (1969); [2] György J. Kovács, D. Bürger et al., J. Appl. Phys. 109 (2011)

HL 90.7 Thu 16:00 Poster A

Effects of reduced symmetry on the Raman spectra of Cu_xO_y — •Christian Reindl, Thomas Sander, Christian Heiliger, and Peter J. Klar — I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen

Raman spectra of copper oxide make it possible to clearly indentify the three individual phases Cu_2O, Cu_4O_3, and CuO. These assignments are in good aggreement with results of X-ray diffraction measurements performed. Each copper oxide phase possesses a different crystal symmetry leading to typical unique Raman modes. However, in the particular case of Cu_2O, the spectra obtained reveal modes being forbidden in the perfect crystal.

The presented Raman spectra of copper oxide were recorded with a Renishaw InVia Raman microscope using excitation lasers of 325 nm, 532 nm, and 633 nm, respectively. The samples were grown by sputter deposition, CVD, and MBE. Group theory considerations show that reduction of symmetry, originating from vacancies and interstitials within the crystal lattice, leads to a relaxation of selection rules making forbidden modes allowed. This will be discussed with respect to the modes observed.

Furthermore DFT calculations for Raman modes of Cu_2O with various defects such as copper vacancies support this idea.

HL 90.8 Thu 16:00 Poster A

Imaging interferometry of excitons in two-dimensional structures — •Heinrich Stolz, Maria Kaupsch, Dirk Semkat, and Günter Manzke — Institut für Physik, Universität Rostock, 18051 Rostock

Recently, spontaneous coherence of excitons in two-dimensional systems has been claimed from measurements of interference contrast using different setups like double slit, shift and mirror interferometers [1,2]. Using the theory of imaging with partial coherent light, we derive general expressions for these setups. We show that in all cases the interference patterns depend not only on the point spread function of the imaging setup but also strongly on the spatial emission pattern of the sample. Taking the experimentally observed emission patterns into account, we can reproduce at least qualitatively all the observed interference structures, which have been interpreted as signatures for spontaneous long range coherence of excitons, already for incoherent emitters. This requires a critical reexamination of the previous work.
[1] High A. A.; Leonard J. R.; Remeika M.; Butov L. V.; Hanson M.; Gossard A. C. *Nano Lett.* **12**, 2605 (2012). [2] High A. A.; Leonard J. R.; Butov L. V.; Gossard A. C. *Nature* **483**, 584 (2012). [3] Semkat, D.; Sobkowiak, S.; Manzke, G.; Stolz, H. *Nano Lett.* **12**, 5055 (2012).

HL 90.9 Thu 16:00 Poster A

Interferometric measurements of luminescence from Bose-Einstein condensates of trapped excitons in Cu_2O — •Maria Kaupsch, Rico Schwartz, Frank Kieseling, Gerd Rudlof, and Heinrich Stolz — Institut für Physik, Universität Rostock, D-18051, Rostock, Germany

Recent measurements of the luminescence from Cu_2O at ultra low temperatures show strong evidences of an excitonic Bose-Einstein condensation (BEC) [1,2]. One direct proof of the BEC is the spatial coherence of the luminescence. First measurements were realised with a Michelson interferometer, whereby the image is superimposed with the flipped one. The measurements were made at different cw-excitation powers and temperatures. We observe a rather complicated interference pattern, which depends critically on the optical delay. The results already support the assumption that the luminescence differs from that of a thermal light source. There are also first theoretical approaches for describing the imaging interferometry of ultracold exciton gases [3] which stress the importance of maximum spatial resolution. We discuss first experiments using an aspheric lens close to the Cu_2O sample inside the mixing chamber of the used $^3He/^4He$ dilution cryostat.

[1] R. Schwartz, N. Naka, F. Kieseling, and H. Stolz, New J. Phys, 14, 023054 (2012); [2] H. Stolz, R. Schwartz, F. Kieseling, S. Som, M. Kaupsch, S. Sobkowiak, D. Semkat, N. Naka, Th. Koch, and H. Fehske, New J. Phys. 14, 105007 (2012); [3] D. Semkat, S. Sobkowiak, G. Manzke, and H. Stolz, Nano Lett. 12, 5055 (2012)

HL 90.10 Thu 16:00 Poster A

Feedback loop for in-situ reflection measurement analysis and optimization during material processing of fs-laser structured silicon — •Anna Lena Baumann[1], Wolfgang Schippers[1], Thomas Gimpel[1], Stefan Kontermann[1], and Wolfgang Schade[1,2] — [1]Fraunhofer Heinrich Hertz Institute, EnergieCampus, Am Stollen 19B, 38640 Goslar, Germany — [2]Clausthal University of Technology, EFZN, EnergieCampus, Am Stollen 19B, 38640 Goslar

Through femtosecond-laser pulse processing the absorption of silicon can be increased considerably and through incorporation of sulfur also extended in the infrared wavelength range. The increase in absorption in the visible wavelength range is due to a decrease in reflection of the surface structures that arise through the laser process. A setup for spot-by-spot femtosecond-laser scanning and realtime reflection measurement analysis is designed. Using a two axis stage system, a continuous wave laser reflection for feedback and a genetic algorithm for signal analysis, the optimal pulse shape for a tailored sample reflection can be found.

HL 90.11 Thu 16:00 Poster A

Strong light-matter coupling between photons and several excitonic states in ZnO-based microcavities — •Martin Thunert, Hannes Krauss, Helena Franke, Chris Sturm, Rüdiger Schmidt-Grund, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig

We report on the observation of strong coupling between cavity-photons and free single particle excitonic states as well as bound or free exciton-complex states in ZnO-based microcavities via PL and reflectivity measurements. While the coupling to the free exciton states is present in each case, the coupling to the two types of complex excitonic structures seems to be present in two situations:

1.) In the case of a low-temperature grown but annealed cavity we have observed the additional coupling of the cavity-photon to the donor bound excitons (D^0,X), which are strongly localized.

2.) In a cavity grown at high temperature, we have observed coupling to exciton-phonon complexes. Each of both contributions to the polaritons are observed by an additional branch in the polariton dispersion. While the coupling to the (D^0,X) has a low coupling strength due to its low density in the cavity, the coupling strength for the exciton-phonon complexes is found to be similar to that for the free excitons.

The different excitonic contributions could be ascribed to different crystal quality of the cavity material for the two types.

HL 90.12 Thu 16:00 Poster A

Ultrafast Dynamics of the Phase Transition in GST Phase Change Materials — •Lutz Waldecker[1], Simon Wall[2], and Ralph Ernstorfer[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]ICFO - Institut de Ciències Fotòniques, Castelldefels (Barcelona), Spain

The fast and reversible optically induced switching between amorphous and crystalline states of $Ge_xSb_yTe_z$ (GST) and similar compounds has found numerous applications in modern data storage technology. However, the microscopic mechanism of the switching process is still subject to debate. By applying two different pump-probe techniques, we investigate the ultrafast optical as well as structural properties of GST as the phase transition occurs. Combining femtosecond transient reflectivity spectroscopy and time-resolved electron diffraction allows for investigating the correlation between structure and function in phase change materials as well as for addressing the question whether the phase transition is thermally or non-thermally driven.

HL 90.13 Thu 16:00 Poster A

Studying Ultrafast Quasiparticle Dynamics by Inelastic Scattering of Electromagnetic Waves: Part 1 Visible Light — •André Bojahr, Marc Herzog, Jevgenij Goldshteyn, Steffen Mitzscherling, Lena Maerten, and Matias Bargheer — Intstitut für Physik und Astronomie, Universität Potsdam, Germany

Collective excitations in crystalline materials lead to complex physical phenomena such as metal-insulator or magnetic phase transitions. Phonons often have a participating or driving role in such transitions. Therefore studying phonons and their coupling among each other and to other subsystems of the material is very important for the understanding of the underlying physics. Here we show new experiments which support a generalized view on scattering of electromagnetic waves from quasiparticles. In particular we study phonons and phonon-polaritons in different perovskite oxides such as SrTiO3 or LiNbO3. We use three different excitation schemes to generate ultrashort quasi-monochromatic phonons and phonon-polaritons. After excitation we probe the quasiparticle dynamics in real time by Brillouin- and Raman scattering. We discuss the experiments in a unified view, where the pump- and probe-process are disentangled and the inelastic aspect of the scattering is emphasized. We observe the quasiparticle dynamics including the phonon damping and nonlinear interaction in real time, and compare the results to simulations in a nonlinear masses-and-springs model.

HL 90.14 Thu 16:00 Poster A

Studying Ultrafast Quasiparticle Dynamics by Scattering of Electromagnetic Waves: Part 2 X-rays — •Marc Herzog[1], André Bojahr[1], Daniel Schick[1], Roman Shayduk[2], Hengameh Navirian[2], Jevgenij Goldshteyn[2], Wolfram Leitenberger[1], Peter Gaal[2], and Matias Bargheer[1,2] — [1]Institut für Physik und Astronomie, Universität Potsdam, Potsdam, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany

Materials exhibiting different types of collective physical phenomena such as metal-insulator transitions or (multi)ferroic behavior are of particular physical and technological interest. The related phase transitions are often mediated by the lattice and can in many cases be transiently triggered by ultrashort laser pulses. A thorough understanding of the ultrafast structural dynamics after laser excitation is therefore crucial for the optical control of material properties.

In general, a suitable experimental method to study ultrafast structural dynamics is the scattering of electromagnetic waves. This contribution summarizes the investigation of laser-induced coherent acoustic phonons in metal-insulator heterostructures by time-resolved scattering of hard x-rays. We use different excitation schemes and sample geometries to generate high-amplitude sub-THz quasi-monochromatic phonons in $SrTiO_3$. We observed linear and nonlinear propagation effects which can be accurately simulated by an anharmonic linear chain model.

HL 90.15 Thu 16:00 Poster A

Ab-initio MD-simulation of large TiO_2 supercells after fs-laser excitation — •Sergej Krylow, Fairoja Cheenicode Kabeer, Eeuwe S. Zijlstra, and Martin E. Garcia — Theoretical Physics, University of Kassel, Heinrich-Plett-Str. 40, 34132 Germany

Using the computer program CHIVES(Code for Highly-excited Valence Electron Systems), which is based on electronic temperature dependent density functional theory, pseudopotentials and localized atom centered basis functions, we performed MD-simulations of TiO_2 in order to determine its structural response to intense fs-laser excitation. We pay particular attention to different types of electronic forces driving the coherent phonons as well as to their decay as a function of time due to phonon-phonon interactions. We compare our results to recent experiments.

HL 90.16 Thu 16:00 Poster A

Nonlinear Phononics — •Matthias Gohlke, André Bojahr, and Matias Bargheer — Department of Physics and Astronomy, Potsdam University, Germany

This contribution discusses simulations of nonlinear phononics in SrTiO3 (STO) crystals using realistic parameters. These parameters were derived from ultrafast Brillouin scattering experiments, where a thin metallic film was excited by femtosecond laser pulses to generate large-amplitude hypersound waves[1]. Using the anharmonic linear chain model tested in this publication, we investigate realistic scenarios for nonlinear phononics in full analogy to photonics: We demonstrate second harmonic generation (SHG) as well as difference and sum frequency mixing (DFG and SFG) of quasi-monochromatic phonons synthesized by optical multipulse excitation. We discuss potential applications of such nonlinear techniques, e.g. for the fundamental analysis of phonon-phonon interaction.

[1] A. Bojahr et al., Calibrated real time detection of nonlinearly propagating strain waves, Phys. Rev. B 86,144306 (2012)

HL 90.17 Thu 16:00 Poster A

Difference in structure and sulfur content of silicon, structured with shaped double femtosecond-laser pulses — •Anna Lena Baumann[1], Kay-Michael Guenther[2], Thomas Gimpel[1], Stefan Kontermann[1], and Wolfgang Schade[1,2] — [1]Fraunhofer Heinrich Hertz Institute, EnergieCampus, Am Stollen 19B, 38640 Goslar, Germany — [2]Clausthal University of Technology, EFZN, EnergieCampus, Am Stollen 19B, 38640 Goslar

Double femtosecond-laser pulses of different pulse distances, shaped by a phase-only pulse shaper, were used to structure the surface of silicon under sulfur hexafluoride atmosphere. When using only one pulse per sample spot (pink silicon), the morphology changes decrease with growing pulse distance, as does the sulfur content in the sample. The absorption changes from single to double pulses, but stays the same in the visible and near infrared range for all investigated pulse distances. The relative sulfur content dependence is investigated with SIMS measurements, which indicate a dependence correlated with the morphology changes. Samples irradiated with 5 pulses per sample spot show a greater dependence on the double pulse distance in the visible as well as in the infrared wavelength range.

HL 90.18 Thu 16:00 Poster A

Generating squeezed phonons by repeated ultrafast excitations of a quantum dot — •Daniel Wigger[1], Doris E. Reiter[1], Vollrath Martin Axt[2], and Tilmann Kuhn[1] — [1]Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [2]Theoretische Physik III, Universität Bayreuth, 95440 Bayreuth

We study theoretically squeezing properties of phonon wave-packets generated by ultrafast optical excitations of a semiconductor quantum dot (QD). We model the QD in the strong confinement limit as an electronic two-level system coupled to longitudinal acoustic (LA) phonons via deformation potential. An ultrashort laser pulse creates an exciton in the QD, which leads to a shift of the equilibrium position of the lattice ions. Thus, a static lattice deformation in the QD area builds up forming a polaron state. Due to the rapid contraction of the lattice an additional strain pulse leaves the QD. Manipulating the exciton with a second laser pulse another phonon wave packet is emitted. Depending on the time delay and relative phase between the two laser pulses the fluctuation properties of the second wave packet can fall below their vacuum limit, i.e., squeezing may occur. In contrast to optical phonons, which are confined to the QD, here the squeezing feature is imprinted to the second traveling wave packet and leaves the QD.

HL 91: Poster Session: Quantum dots and wires: preparation & characterization & optical properties & transport properties

Presenters are kindly asked to be near their posters at least 17:00–18:00 or to leave a note at the poster indicating a time period of availability for discussions. — Beverages will be served starting at 18:00.

Time: Thursday 16:00–20:00 Location: Poster A

HL 91.1 Thu 16:00 Poster A

Fabrication and characterization of site-controlled quantum dots grown on pre-patterned GaAs substrates — •Patrick Krawiec, Muhammad Usman, Mohamed Benyoucef, and Johann Peter Reithmaier — Nanostructure Technologies and Analytics, CINSaT, University of Kassel, Heinrich-Plett-Strasse 40, 34132 Kassel, Germany

Semiconductor quantum dots (QDs) are attractive building blocks for scalable quantum information processing systems. In the last years, there has been an increasing need for the investigation of site-controlled QDs, which can be used as active elements in quantum devices such as single-photon sources. In this work, we present the growth of site-controlled InAs QDs on pre-patterned GaAs substrates using electron beam lithography, wet-chemical etching and molecular beam epitaxy. Large QD arrays with periodicities ranging from 0.5 μm to 8 μm were achieved. The single QDs obtained in this study present a high optical quality, which have been evaluated by micro-photoluminescence.

HL 91.2 Thu 16:00 Poster A

MBE-Growth of self-assembled uncapped InAs quantum dots on GaAs (001) surface — •Thomas Jost[1], Eddy P. Rugeramigabo[1,2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Abteilung Nanostrukturen, Leibniz Universität Hannover, Deutschland — [2]QUEST Centre for Quantum Engineering and Space-Time Research, Leibniz Universität Hannover, Deutschland

InAs quantum dots (QDs) are well known nanostructures which can be grown by molecular beam epitaxy (MBE). The electronic properties of an InAs QD depend on the form, external fields and the charges accumulated in the dot. For self-assembled uncapped InAs QDs we have studied the growth conditions to get well defined and reproducible parameters of QDs like: diameter, density of QDs and inter-dot distance.

To produce the InAs QDs we have grown two monolayers of InAs on a GaAs (001) surface under different conditions. We have shown that the density and inter-dot distance of QDs depends on the growth-rate and the annealing. The diameter of the QDs showed a dependence on annealing. Now we are able to produce QDs with a diameter of 50 nm, inter-dot distance of 70 nm and a density of around $2{\cdot}10^{10}$ QDs/cm^2, which will be used in transport experiments.

HL 91.3 Thu 16:00 Poster A

Growth of GaAs nanowires on GaAs (111)B substrates induced by focused ion beam — •Rüdiger Schott[1], Dirk Reuter[2], Arne Ludwig[1], and Andreas D. Wieck[1] — [1]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum — [2]Arbeitsgruppe für optoelektronische Materialien und Bauelemente, Universität Paderborn

Semiconductor nanowires are a promising system for applications in the areas of electronics and photonics as well as for exploring phenomena at the nanoscale. There are several approaches to grow nanowires at predetermined sites on the wafer. We report about growing GaAs nanowires on GaAs (111)B substrates via the vapor-liquid-solid (VLS) mechanism in an ultra-high-vacuum (UHV)-cluster consisting of a molecular beam epitaxy (MBE) and a focused ion beam (FIB) system. Our idea is to implant metal seeds for the nanowire growth using FIB. Due to the UHV transfer between the FIB and the MBE chamber, no further cleaning step of the substrate surface is necessary. We were able to grow single nanowires in user defined patterns on the wafer. Nanowire diameters below 20 nm were observed. The structural and optical properties of the nanowires were investigated by SEM, TEM and photoluminescence spectroscopy.

HL 91.4 Thu 16:00 Poster A

Correlation of electrical and structural parameters of single GaAs nanowires grown by MBE onto silicon substrate — •Genziana Bussone[1,2], Heiko Schäfer-Eberwein[3], Emmanouil Dimakis[4], Andreas Biermanns[2], Lutz Geelhaar[4], Pe-

ter Haring-Bolívar[3], and Ullrich Pietsch[2] — [1]ESRF, Grenoble, France — [2]Festkörperphysik, Universität Siegen, Germany — [3]Hochfrequenztechnik & Quantenelektronik, Universität Siegen, Germany — [4]PDI, Berlin, Germany

Semiconductor nanowires are possible candidates for future electronic application. Most of their properties strongly depend on structural parameters such as phase purity or lattice strain. Here we report on the correlation between electrical properties of single GaAs nanowires (NWs) grown by MBE on a highly doped silicon substrate (111) and their particular structural properties. Various single NWs, freestanding in their as-grown geometry onto the substrate, were measured using micromanipulators in a Focused Ion Beam (FIB) system at Siegen University (Germany), providing individual Current-Voltage characteristics. In order to understand the origin of the different electrical responses, the structure of the same nanowires were then investigated using a nano-focused beam of synchrotron radiation at beamline ID01 at the ESRF in Grenoble (France). All the NWs show mainly zincblende (ZB) structure units separated by stacking faults. The size of perfectly stacked ZB units differs among the measured NWs and correlates well with the differences of the respective Current-Voltage characteristics.

HL 91.5 Thu 16:00 Poster A

Structural and electronic and optical properties of Si_xGe_{1-x} alloy nanocrystals embedded in SiO_2: First-principles calculations — •Kaori Seino[1], Peter Kroll[2], Moritz Laubscher[1], and Friedhelm Bechstedt[1] — [1]nstitut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Jena, Germany — [2]Department of Chemistry and Biochemistry, University of Texas at Arlington, Arlington, TX, USA

Silicon-Germanium (SiGe) technology is the driving force behind the explosion in low-cost, personal communication devices. Combining two major semiconductors, these alloys allow tailoring of the band gap and fundamental properties that depends on it in both bulk systems and nanocrystals (NCs). Recent advances in Group-IV semiconductor NCs have demonstrated their promise for optoelectronic and photovoltaic applications. Current developments of photonic devices focus on size control and ordered arrangements of NCs embedded in a SiO_2.

Our understanding of SiGe alloy NCs embedded in SiO_2 is, however, limited. Therefore, in this study we provide theoretical investigations of such systems. We study structural and electronic properties of Si_xGe_{1-x} alloy NCs with well-defined sizes embedded in silica glass by means of first-principles calculations. We investigate their electronic and optical properties and how their depends on the compositional parameter x of Si_xGe_{1-x} alloys.

HL 91.6 Thu 16:00 Poster A

Growth of InAs/InGaAs nanowires on GaAs(111)B substrates — •Sven Scholz[1], Rüdiger Schott[1], Dirk Reuter[2], Arne Ludwig[1], and Andreas D. Wieck[1] — [1]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum — [2]Arbeitsgruppe für optoelektronische Materialien und Bauelemente, Universität Paderborn

To investigate the structure and behavior of individual 1D-quantum structures, so called nanowires, we have grown single localized Au seeded InAs/InGaAs nanowires on GaAs(111)B substrate by molecular beam epitaxy. The Au-seeds are implanted by focused ion beam (FIB) technology. We developed a AuGa-LMIS to avoid the beam spread induced by using a Wien-Filter, which allows us to reduce the spot size of the focused ion beam and as consequence the number of implanted ions necassary to seed a wire. At present the growth of InAs nanowires is not fully understood and we have been working on optimizing the process. We identified an optimal growth temperature and arsenic to indium ratio for nanowire growth. Further investigations also aim at analyzing the influence of the growth rates and growth directions. We studied the morphology of the nanowires by SEM imaging and the optical properties with photoluminescence spectroscopy.

HL 91.7 Thu 16:00 Poster A

Compressive strain in MBE grown GaAs nanowires induced by an Al_2O_3 shell prepared by atomic layer deposition — •Torsten Jörres[1,2], Torsten Rieger[1,2], Andreas Biermanns[3], Ullrich Pietsch[3], Detlev Grützmacher[1,2], and Mihail Ion Lepsa[1,2] — [1]Peter Grünberg Institut - 9, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology — [3]Universität Siegen, Festkörperphysik, Walter-Flex-Str. 3, 57072 Siegen, Germany

In the processing of nanowire (NW) based electronic devices, high-κ dielectrics are used to passivate the surface or as gate oxides for field effect transistor applications. In this sense, Al_2O_3 films prepared by atomic layer deposition (ALD) represent an alternative because it allows a precise control of the layer thickness and dielectric properties by choosing appropriate deposition conditions. However, at such a scale, any difference in thermal expansion coefficients might induce strain in the NW and therefore affect their electronic properties. Here, we show recent results on MBE grown GaAs NWs with diameter of 75 nm encapsulated in a 30 nm thick Al_2O_3 shell. High resolution XRD measurements were performed at the P08 beamline at the PETRA III synchrotron in Hamburg in order to measure the shell-induced strain in the NWs. A small, but measurable compressive strain in the GaAs NWs of 0.05% was observed. High resolution transmission electron microscopy images of these nanowires show the conformal deposition of the Al_2O_3 shell as well as a very small roughness.

HL 91.8 Thu 16:00 Poster A

Tunability of the confining potential of Quantum Point Contacts — •Jakob Schluck, Bernd Schüler, Mihai Cerchez, and Thomas Heinzel — HHU Düsseldorf

The energy spacing of allowed states for a particle confined in one dimension depends on the form of the confining potential. Well known cases are the equidistant spacing of the harmonic oscillator or the parabolic spacing in a hard wall confinement.

We tune the confining potential of a one-dimensional, ballistic quantum wire produced by AFM lithography on a Ga[Al]As heterostructure via a combination of in-plane gates and self-aligned top gates, also produced with an AFM. [1]

The level spacing is then determined by differential transconductance measurements allowing us to determine the shape of the confinement potential. [2]

[1] M. Sigrist, A. Fuhrer, T. Ihn, and K. Ensslin, Appl. Phys. Lett. 85, 3558 (2004)

[2] K. S. Pyshkin, C. J. B. Ford, R. H. Harrell, M. Pepper, E. H. Linfield, and D. A. Ritchie, Phys. Rev. B 62 15842 (2000)

HL 91.9 Thu 16:00 Poster A

Radical formation by photo-generated carriers at GaN nanowires - electrolyte interfaces — •Jan Martin Philipps, Gesche Mareike Müntze, Pascal Hille, Jörg Schörmann, Jörg Teubert, Detlev Michael Hofmann, and Martin Eickhoff — I. Physikalisches Institut, JLU Giessen, Germany

We investigated the transfer of photogenerated carriers from GaN nanowires into an electrolyte environment by electron paramagnetic resonance (EPR) and fluorescence-spectroscopy. Using 5,5-dimethyl-1-pyrroline-N-oxide (DMPO) as a spin trap and a neutral electrolyte (pH = 7) the formation of hydroxide radicals dominates, while for an electrolyte with a pH of 13.5 the superoxide formation becomes detectable. We explain this asymmetry for the two processes in the frame of the surface band bending model considering the redox potentials in the electrolyte and the conduction and valence band positions of the semiconductor.

HL 91.10 Thu 16:00 Poster A

Raman characterization of electrically biased polymer quantum dot composites — •Prahlad M Mohandas[1], Daniel Lehmann[1], Ovidiu D Gordan[1], Istvan S Todor[2], Christian Spudat[3], Jörg Martin[3], Michael Thomas Müller[4], Thomas Gessner[3], and Dietrich R. T. Zahn[1] — [1]Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany — [2]Department of Solid State Physics, Faculty of Physics, Babes-Bolyai University, Cluj-Napoca, Romania — [3]Fraunhofer-Institut für Elektronische Nanosysteme, Technologie-Campus 3, D-09126 Chemnitz, Germany — [4]Leibniz-Institut für Polymerforschung Dresden e.V., Polymerreaktionen und Blends, Hohe Straße 6, D-01069 Dresden, Germany

Thin films of a polymer/quantum dot composite are characterized using Raman and photoluminescence spectroscopy under electrically biased conditions in order to investigate the effect of voltage on the quantum dot charging behaviour. The quantum dots are CdSe/ZnS core/shell quantum dots, mixed homogeneously in polymethylmethacrylate (PMMA) polymer. The PMMA-CdSe/ZnS composite film was deposited on a glass substrate using spin-coating technique. The polymer quantum dot composites were biased between +48V and -48V. Peaks corresponding to CdSe longitudinal optical (LO) phonon and ZnS LO phonon were observed at 206 cm-1 and 272 cm-1, respectively. Quenching of phonon bands due to charging

of quantum dots by the applied voltage is observed. The effect of quenching depends and varies based on the sign of the applied voltage.

HL 91.11 Thu 16:00 Poster A

Study of excitonic states in single InAs quantum dots by low-temperature SNOM — •Alexander Senichev[1], Vadim Talalaev[1,2], Jörg Schilling[2], George Cirlin[3,4,5], and Peter Werner[1] — [1]Max-Planck-Institut, Halle, Germany — [2]Martin-Luther-Universität, ZIK "SiLi-nano", Halle, Germany — [3]A. F. Ioffe Physico-Technical Institute, St. Petersburg, Russia — [4]St. Petersburg Physics and Technology Center for Research and Education, St. Petersburg, Russia — [5]Institute for Analytical Instrumentation, St. Petersburg, Russia

We report on near-field optical spectroscopy on InAs quantum dots embedded in a GaAs matrix. Quantum dot samples are grown by molecular beam epitaxy in different configuration of the active region. Sharp spectral lines corresponding to optical recombination in single quantum dots are selected. The spectral width of most resonances is quite narrow and comparable with the resolution of our monochromator (0.1 meV). Varying the excitation power density from 2W/cm2 to 300W/cm2 power dependence of photoluminescence (PL) parameters is investigated. For spatial PL imaging (spatial resolution 300 nm), the fiber probe is scanned across the sample surface, and a full PL spectrum is recorded at every pixel. The intensity of the observed emission lines shows approximately linear power dependence and saturate at the power of 100W/cm2. The results are discussed in respect to the capability of SNOM and provide a better understanding of the exciton behavior of individual QDs.

HL 91.12 Thu 16:00 Poster A

Temperature dependence of hole spin coherence measured by spin echo andspin mode locking in an ensemble of (In,Ga)As quantum dots — •Steffen Varwig[1], Alexandre René[1], Alex Greilich[1], Dmitri R. Yakovlev[1], Dirk Reuter[2], Andreas D. Wieck[2], and Manfred Bayer[1] — [1]Experimentelle Physik II, TU Dortmund, D-44221 Dortmund, Germany — [2]Angewandte Festkörperphysik, Ruhr- Universität Bochum, D-44780 Bochum, Germany

Electron and hole spins confined in quantum dots (QDs) are promising candidates for implementing qubits in semiconductors. One of the spin's most important properties for quantum information processing is its coherence time T_2. For electrons in (In,Ga)As QDs, T_2 is determined to be around $3\,\mu$s [1]; for holes it is in the order of $1\,\mu$s [2]. Although for electron spins the coherence time is mainly limited by hyperfine interactions with the QD's nuclei, for hole spins it is known that the coupling constant is about ten times weaker [3].

To study the hole spin coherence in QDs we performed optical time-resolved pump-probe ellipticity measurements on the hole spin polarization in (In,Ga)As QDs. In particular we investigated the temperature dependence of the coherence time T_2, making use of the spin mode-locking effect, demonstrated in reference [2], and spin echo techniques similar to those in reference [4].

[1] A. Greilich et al., Science 313, 341 (2006)
[2] S. Varwig et al., Phys. Rev. B 86, 075321 (2012)
[3] E. A. Chekhovich et al., Phys. Rev. Letters 106, 027402 (2011)
[4] A. Greilich et al., Nat. Phys. 5, 262-266 (2009)

HL 91.13 Thu 16:00 Poster A

Shape dependence of excitonic states in self-assembled GaAs/AlGaAs quantum dots — •Andreas Graf[1], David Sonnenberg[1], Andrei Schliwa[2], Christian Heyn[1], and Wolfgang Hansen[1] — [1]Institut für Angewandte Physik, Universität Hamburg, 20355 Hamburg, Germany — [2]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany

Local droplet etching (LDE) allows for a molecular beam epitaxy compatible self-assembled patterning of semiconductor surfaces. Using LDE with aluminum droplets, nanoholes with a defined depth up to 100 nm are drilled in AlGaAs surfaces. With the arsenic flux and the temperature during the LDE the shape, depth and density of the nanoholes are controlled [1]. Partial filling of the nanoholes with GaAs provides highly uniform strain-free quantum dots (QD). Their shape is defined by the nanohole profile and the GaAs-filling level [2]. We study the QD shape dependence of the excitonic states with single-dot photoluminescence spectroscopy and compare the results with calculated transition energies. For the calculation, a basis of single-particle wave functions is determined with $\boldsymbol{k}\cdot\boldsymbol{p}$ theory, and configuration interaction is used to determine excitonic states [3].

[1] Sonnenberg et al., APL **101**, 143106 (2012)
[2] Heyn et al., APL **94**, 183113 (2009)
[3] Schliwa et al., PRB **76**, 205324 (2007)

HL 91.14 Thu 16:00 Poster A

Excitons in double quantum dots: Phonon effects and spin-orbit coupling — •Jonas Daniels[1], Paweł Machnikowski[2], and Tilmann Kuhn[1] — [1]Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [2]Institute of Physics, Wrocław University of Technology, 50-370 Wrocław, Poland

We investigate theoretically excitons in a double quantum dot system. As a function of an external electric field, the absorption spectrum exhibits various anticrossings. These can be attributed to different coupling mechanisms such as tunnel-coupling, Coulomb interaction or spin-orbit coupling. The linewidth of the exciton transitions depends on the interaction of the excitons with the phononic environment, which causes phonon-assisted relaxation as well as phonon-assisted tunneling especially at an anticrossing.

We investigate these phenomena for a pair of lens-shaped vertically aligned InAs/GaAs QDs. A variational method is used to calculate single-particle states, while Coulomb interaction is included within configuration-interaction. We calculate phonon-assisted relaxation rates caused by the deformation-potential coupling to longitudinal-acoustic (LA) phonons and the piezoelectric coupling to LA and transverse-acoustic (TA) phonons. Spin-orbit coupling is considered by the Dresselhaus or k^3-term.

HL 91.15 Thu 16:00 Poster A

Impact of longitudinal acoustic phonons on the excitation of quantum dots driven by chirped laser pulses — •Sebastian Lüker[1], Krzysztof Gawarecki[2], Martin Glässl[3], Anna Grodecka-Grad[4], Doris E. Reiter[1], Vollrath Martin Axt[3], Paweł Machnikowski[2], and Tilmann Kuhn[1] — [1]Institut für Festkörpertheorie, WWU Münster, 48149 Münster — [2]Institute of Physics, Wrocław University of Technology, 50-370 Wrocław, Poland — [3]Theoretische Physik III, Universität Bayreuth, 95440 Bayreuth — [4]Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen Ø, Denmark

We theoretically investigate the impact of phonons on the excitation of quantum dots (QD) driven by chirped (frequency-swept) laser pulses, referred to as adiabatic rapid passage (ARP). The QD is modeled in the strong confinement limit as a two-level system, which is coupled to longitudinal acoustic phonons via the deformation potential.

A chirped pulse drives the system adiabatically along the spectral branch of the dressed eigenstates. Without coupling to phonons this results in a robust population of the exciton state for positive as well as for negative chirps. Transitions between the dressed states can occur by emission or absorption of phonons, which reduces the fidelity of the ARP. Because absorption of phonons is negligible at low temperatures, an asymmetry with respect to the sign of the chirp appears.

We calculate the system dynamics using a fourth order correlation expansion and compare our results to a time-convolutionless method and to numerically exact path integral calculations.

HL 91.16 Thu 16:00 Poster A

Carrier multiplication in a multi-level, colloidal quantum dot under the presence of phonons — •Mario Schoth, Franz Schulze, Andreas Knorr, and Marten Richter — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany

Carrier multiplication (CM) in quantum dots (QD) has been proposed as a possible technique to further increase the efficiency of photovoltaic conversion [1,2]. In this process, the Auger-type Coulomb processes of impact ionization and Auger recombination lead to the creation of multiple electron–hole pairs per absorbed high–energy photon. The efficiency of such processes is reduced by competing relaxation channels, such as radiative recombination or relaxation via phonons [3]. In this contribution, we present a microscopically derived, dynamical model of CM in a single, multi-level, colloidal QD, where we consider the electron–electron- as well as the electron–phonon interaction. The finite size of the colloidal QD gives rise to a discretization of phonon modes, which we calculate for a spherical QD [4]. Using this parameter–free approach, we simulate the dynamics of exciton creation and annihilation, and investigate if CM is enhanced or suppressed by phonons.

[1] A.J Nozik, Physica E 14, 115 (2002)
[2] R.D. Schaller and V.I. Klimov, Phys. Rev. Lett. 92, 186601 (2004)
[3] F. Schulze, M. Schoth, U. Woggon, A. Knorr, and C. Weber,

Phys. Rev. B 84, 125328 (2011)
[4] T. Takagahara, J. Lumin. 70, 129 (1996)

HL 91.17 Thu 16:00 Poster A

Time-resolved optical spectroscopy of colloidal quantum dots and gold nanoparticles with dye molecules — •Robert Malinowski, Uwe Kaiser, Mikko Wilhelm, Wolfram Heimbrodt, Faheem Amin, Dorleta Jimenez de Aberasturi, and Wolfgang Parak — Experimental physics of Philipps-University Marburg

We report about the opportunity to do multiplexed detection of different ionic species via ion-sensitive fluorophores. Multiplexed measurements can be made possible by coupling ion-sensitive fluorophores to different types of nanoparticles for biological sensor applications. These nanoparticles exhibit different radiative lifetimes and will act as donor for energy transfer to the ion-sensitive fluorophores as acceptors. As result the ion-sensitive fluorophores will obtain different effective lifetimes and can be read out in parallel via time-resolved detection of fluorescence. We investigate inorganic CdSe/ZnS core-shell quantum dots (QD) and gold nanoparticles (Au-NP) which are coated with amphiphilic polymers and functionalized by dye molecules. Main tasks are time resolved photoluminescence measurements of QD-dye and Au-dye mixtures in different concentrations. Using a laser (355nm) with pulse durations of a few nanoseconds, it is possible to characterize the time behavior of the photoluminescence decay of the dye molecules. By variation of the QD-dye to Au-dye ratio, the decay of the dye photoluminescence shows different behavior. The experimental results can be described and analyzed in the framework of a kinetic model. This opens up the possibility to determine the proportion of QD-dye and Au-dye for unknown mixing ratios by lifetime measurements.

HL 91.18 Thu 16:00 Poster A

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

Applying computational time dependent density functional techniques we analyse small structures of potential quantum dot material. In particular we focus on the absorbtion spectra as function of the cluster size, the composition, ligands and complexation.

HL 91.19 Thu 16:00 Poster A

Spatial resolved optical pH- and bias response of (In, Ga)N nanowires and quantum dots — •Sabrina Darmawi, Jens Wallys, Pascal Hille, Martin Eickhoff, and Peter J. Klar — I. Physikalisches Institut, JLU, Heinrich-Buff-Ring 16, 35392 Gießen

We present photoluminescence (PL) imaging measurements of GaN nanowire ensembles and InGaN quantum dots in electrolyte solutions of different pH in a three electrode setup. By application of external bias the PL intensity and its pH sensitivity can be controlled. A microscope system attached to the measurement chamber transfers a magnified image of the sample onto the slit of a subtractive double spectrometer which acts as a tunable band pass and allows for PL intensity imaging at different emission wavelengths with a CCD system. The response of the PL intensity of the sample to the pH value of the surrounding electrolyte and the applied bias will be discussed.

HL 91.20 Thu 16:00 Poster A

Photoluminescence intensity and lifetime of ordered arrays of GaN nanowires with different diameter and pitch — •Christian Hauswald, Oliver Brandt, Timur Flissikowski, Tobias Gotschke, Raffaella Calarco, Lutz Geelhaar, Holger T. Grahn, and Henning Riechert — Paul-Drude-Institut für Festkörperelektronik, Berlin

Selective-area growth (SAG) of nanowires (NWs) by molecular beam epitaxy constitutes an important step towards uniform III-V NW arrays on Si. Using this approach, the diameter and length distribution of self-induced GaN NWs can be significantly reduced as compared to the growth on non-patterned substrates.

In this work, we study the influence of different diameters and pitches of selectively grown GaN NWs on their optical properties. The NWs have diameters and periods in the range of 110−260 nm and 0.3−1.0 μm, respectively. Time-integrated μ-photoluminescence (μ-PL) spectra at 10 K show a narrow linewidth, while the rather short decay times obtained by time-resolved PL measurements indicate a quite low internal quantum efficiency. We observe a monotonic decrease of the PL intensity with increasing NW diameter, although the PL decay times remain virtually constant. To investigate the origin of this effect, we use finite-element simulations to solve the Maxwell equations for the three-dimensional NW geometry. These simulations allow us to clarify whether the decrease in PL intensity is caused by a systematic change of the electromagnetic coupling to the ordered NW array.

HL 91.21 Thu 16:00 Poster A

Optical properties of organically-linked ZnO nanoparticles — •Carsten Kruska[1], Wolfram Heimbrodt[1], Christine Chory[2], Ingo Riedel[2], and Jürgen Parisi[2] — [1]Philipps-Universität Marburg — [2]Energy and Semiconductor Research, Oldenburg

To improve the efficiency of organic bulk heterojunction solar cells, accurate control of the nanoscale morphology is required. Due to phase segregation, controlling the morphology of normal solution-processed semiconductor blends is difficult. ZnO nanoparticles offer a sufficiently high electron affinity to replace the normal absorber in such systems. This study uses UV-Vis absorption and temperature-dependent photoluminescence measurements to investigate the optical properties of solution-processed three dimensional networks of ZnO nanoparticles. The covalent links between the ZnO nanoparticles and the bifunctional organic molecules could be observed for two different linker molecules. An organically linked network of ZnO nanoparticles was formed. Linking of nanoparticles with organic molecules yields an new material system which is relatively easy to process and have some promising properties as an absorber in semiorganic bulk heterojunction solar cells.

HL 91.22 Thu 16:00 Poster A

Group-IV nanocrystals: Spin-orbit coupling and optical properties from first principles — •Sebastian Küfner, Lars Matthes, Jürgen Furthmüller, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, D-07743 Jena

The electronic structure of materials significantly changes due to spatial confinement. Consequently, nanostructures are interesting objects for manipulating electronic and optical properties. We use density-functional theory within local density approximation to calculate the electronic structure of $\alpha-$Sn, Ge, and Si nanocrystals (NCs). We investigate the spin-orbit splitting of the highest occupied state and show that its size dependence appears to be not monotonic in case of Ge and Sn. We identify the spin-orbit splitted states by the degree of degeneracy and the symmetry of the wave-functions. In addition, we show how the size dependence of the electronic structure influences the optical absorption- and emission properties of the nanodots. Calculating the oscillator strengths, we identify the transitions resulting in the main contributions to the absorption spectra. Applying the ΔSCF method which considers many-body effects and screened Coulomb interaction, we calculate the optical Stokes-shifts depending on the NC-diameter as the difference between the lowest electron-hole excitation and recombination energy. We also give values for the corresponding radiative lifetimes.

HL 91.23 Thu 16:00 Poster A

Quantum emitters in whispering gallery mode resonators — •Assegid Flatae[1], Tobias Grossmann[1], Torsten Beck[1], Thomas Laue[2], Halald Fuchs[2], and Heinz Kalt[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), Wolfgang-Gaede-Str.1. 76131 Karlsruhe, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1. 76344 Eggenstein-Leopoldshafen.

The high Q-factor and the small modal volume of whispering gallery mode resonators play an important role for the study of the interaction between the cavity mode and quantum emitters (e.g. semiconductor quantum dots (QDs)). We fabricated goblet shaped micro-resonators with high Q-factor of ten million using polymers and standard fabrication techniques. We attach QDs to single and coupled resonators using nanotechnological tools (e.g. dip-pen and fountain-pen nanolithography techniques) for the study of weak coupling (Purcell effect), lasing and possibly strong coupling between the emitters and the cavity photons.

HL 91.24 Thu 16:00 Poster A

Single-photon time-delayed feedback: a way to stabilize intrinsic quantum cavity electrodynamics — •Franz Schulze[1], Alexander Carmele[1], Julia Kabuss[1], Stephan Reitzenstein[2], and Andreas Knorr[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany — [2]Institut für Festkörperphysik, Optoelektronik und Quan-

tenbauelemente, Technische Universität Berlin, Germany

The control of non-classical photon states is of great importance in quantum information science and can be addressed, for example, by extrinsic [1] and intrinsic methods. We apply an intrinsic control scheme to cavity quantum electrodynamics (cQED) by utilizing quantum optical time-delayed self-feedback in the single-photon limit. In particular, we investigate theoretically how a single-emitter cavity system, operating initially in the weak coupling regime, is driven into the strong-coupling regime by introducing time-delayed optical self-feedback via an external mirror. This peculiar transition from weak to strong coupling manifests in Rabi oscillations, which start to emerge in the coupled cavity field dynamics. Our method treats the correlation between the external and the internal cavity photon field on a non-Markovian level. This quantum optical approach to time-delayed self-feedback opens new ways to experimentally control features of cQED in the single-photon limit.

[1] X. Zhou *et al.*, Phys. Rev. Lett. **108**, 243602 (2012)

HL 91.25 Thu 16:00 Poster A

Thermoelectric Properties of a Strongly Coupled Double Quantum Dot — •Holger Thierschmann[1], Michael Henke[1], Johannes Knorr[1], Wolfgang Hansen[2], Hartmut Buhmann[1], and Laurens W. Molenkamp[1] — [1]Physikalisches Institut, Experimentelle Physik 3, Universität Würzburg — [2]Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Universität Hamburg

We study the thermoelectric properties of a double quantum dot (DQD) in the low temperature regime under a temperature difference of a few 10 mK. Our sample consists of a lateral DQD system defined electrostatically by gate electrodes on top of a GaAs/AlGaAs-HEMT structure. By measuring the serial conductance of the DQD we yield a stability diagram from which we can extract the charging and coupling energies. We infer that the system is in the strong tunnel-coupling regime. For thermopower measurements we use the current heating technique to establish a temperature difference of approx. 20 mK across the DQD structure [1]. Measuring the thermovoltage across the serial DQD, we obtain a thermopower stability diagram. We find maximum thermovoltage in the corners of each stability region. In the vicinity of a tripel point we observe a strong asymmetry of the thermovoltage signal. This can be traced back to an asymmetric distribution of energy levels with respect to the Fermi-energy in the DQD system which is consistent within a simple DQD model.

[1] L.W. Molenkamp, H. van Houten, C.W.J. Beenakker, R. Eppenga, C.T Foxon, PRL 65, 1052(1990)

HL 91.26 Thu 16:00 Poster A

Time-resolved transconductance spectroscopy: Towards all electrical spectroscopy of a single self-assembled quantum dot — •A. Beckel[1], D. Zhou[1], A. Kurzmann[1], B. Marquardt[1], A. D. Wieck[2], D. Reuter[2], M. Geller[1], and A. Lorke[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany — [2]Chair for Applied Solid State Physics, Ruhr-Universität Bochum, Universitätsstraße 150, 44780 Bochum, Germany

We have shown recently an all electrical preparation and probing of non-equilibrium (i.e. excited) states in an ensemble of self-assembled quantum dots (QDs) using a time-resolved measurement scheme [1,2].

In our high electron mobility transistor structure a two-dimensional electron gas (2DEG) is used as detector and reservoir for the QD states. Using a 2DEG offers sensitive, time-resolved detection via transconductance as well as ideal scaling properties to address a single self-assembled QD.

Electron beam lithography has been applied to process samples containing only ~ 100 QDs. We present devices and measurements which show enhanced energy resolutions, beyond the inhomogeneous broadening of the QD ensemble. The additional information of the time-resolved measurement is used to attribute the measured spectrum to a set of QD sub-ensemble as well as attribute the tunneling processes to the shell structure of the involved QD states.

[1] B. Marquardt et al., Appl. Phys. Lett. **95**, 22113, (2009).
[2] B. Marquardt et al., Nature Commun. **2**, 209 (2011).

HL 91.27 Thu 16:00 Poster A

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] Our sample design allows to simultaneously measure the conductance along two different paths with two quantum dots in each path. The structure is made with local anodic oxidation by AFM on a GaAs/AlGaAs heterostructure. By controlling the potentials quadruple points with all three dots in resonance can be established. [3,4] Using two of the leads as source and one lead as a drain contact, signatures of three dots can be detected in both transport paths. This setup provides the possibility of applying different bias voltages to the sources of the two paths and detecting excited states of the dots. Transport measurements in one path while varying the source-drain voltage on the other path show interesting features and prove interaction between the transport paths. The measurement results are compared with a simulation of the electrostatics of the triple dot system.

[1] M. C. Rogge, et al., Phys. Rev. B 77, 193306 (2008).
[2] P. Hawrylak, et al., Solid State Comm. 136 (2005), pp. 508-512.
[3] L. Gaudreau, et al., PRL 97, 036807 (2006).
[4] M. C. Rogge, et al., New Journal of Physics 11, 113037 (2009).

HL 91.28 Thu 16:00 Poster A

Magnetic field modulation of RKKY interaction between quantum dots — •Alexander W. Heine[1], Katharina Janzen[2], Brendan Coughlan[2], Daniel Tutuc[1], Gertrud Zwicknagl[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Institut für Mathematische Physik, Technische Universität Braunschweig, 38106 Braunschweig, Germany

The spin of a quantum dot is proposed as a possible realization of a qubit in quantum information processes. One possible mechanism to control the spin of a quantum dot beyond the nearest neighbour approach is the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction, an indirect exchange between magnetic moments. To probe the RKKY interaction between two quantum dots, we use the Kondo effect as spectroscopic tool. At low temperatures between 25 mK and 900 mK and high magnetic field of 5 T we measure the differentieal conductance of the quantum dots. In the presence of RKKY interaction we observe a qualitative change of the temperature dependence with variation of the magnetic field.

Modelling our system and calculating the interaction strength by evaluating the Lindhard function yields the variation with magnetic field of the indirect exchange. We theoretically analyze the magnetic-field tuning of the Kondo singlet formation in a double-dot system.

HL 91.29 Thu 16:00 Poster A

Thermal noise measurements of low-dimensional electron gases — •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 in low dimensional mesoscopic systems strongly differ from those of bulk material. We investigate the transport properties in 1D and 2D electron gases in the presence of temperature gradients. We apply Johnson noise thermometry to measure the spectral noise density in GaAs-AlGaAs heterostructures at temperatures below 10 K. The current heating technique allows us to create temperature gradients in 2D electron gases as well as in quantum point contacts. The cross-correlation technique and an improved measurement setup [1] enable a strong reduction of perturbation signals generated in ohmic contacts and leads. Non-local noise measurements on 1D electron gases at low temperatures have shown heat transport which is only carried by electrons. Our findings in local noise measurements differ from the expected Joule's law due to an anomaly in thermal noise as a function of heating current. We observe time dependence of Johnson noise in structures that fulfill certain conditions. We present the results of systematic measurements and discuss possibilities of their physical origin.

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

HL 91.30 Thu 16:00 Poster A

Study of Phase-Coherent Transport in Differently Doped InAs Nanowires — •Thomas Gerster[1], Sebastian Heedt[1], Isabel Wehrmann[1,2], Kamil Sladek[1], Hilde Hardtdegen[1],

Detlev Grützmacher[1], and Thomas Schäpers[1,3] — [1]Peter Grünberg Institut (PGI-9) and JARA-Fundamentals of Future Information Technology, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]OSRAM Opto Semiconductors GmbH, 93055 Regensburg, Germany — [3]II. Physikalisches Institut, RWTH Aachen University, 52056 Aachen, Germany

We report on differently doped InAs nanowires grown epitaxially by selective area metalorganic vapor phase epitaxy. The nanowires are individually contacted with Ω-shaped top-gates using high-k dielectrics to investigate the low-temperature electronic transport properties. The band profile and the carrier concentration of the nanowires can be manipulated by the application of a gate voltage. At small current-bias, phase-coherent transport occurs and gives us the ability to determine the phase-coherence length l_ϕ and the spin relaxation length l_{so}. In our measurement setup, phase-coherent transport is investigated for temperatures down to 30 mK and magnetic fields up to 10 T. To extract l_ϕ and l_{so}, we make use of an analytical model for the low-field quantum conductivity correction. This model considers spin relaxation under linear Rashba and linear and cubic Dresselhaus spin-orbit coupling for diffusive wires with diameters smaller than l_ϕ. The impact of doping on the electron spin lifetime is studied for InAs nanowires fabricated under various doping conditions.

HL 91.31 Thu 16:00 Poster A

Single-particle-reduced entropy for few-electron states in gated semiconductor nanowires — •Jose Maria Castelo[1], Klaus Michael Indlekofer[1], and Joerg Malindretos[2] — [1]RheinMain University of Applied Sciences, IMtech / Faculty of Engineering, D-65428 Rüsselsheim, Germany — [2]Georg-August-Universität Göttingen, IV. Physikalisches Institut, D-37077 Göttingen, Germany

We consider electronic transport within a coaxially-gated nanowire field-effect transistor (FET) in the Coulomb blockade regime by means of a non-equilibrium Green's function technique. Two different approaches are considered for the description of the Coulomb interaction: a many-body multi-configurational technique and a mean-field approximation. This allows us to calculate the single-particle density matrix ρ_1 of the nanowire channel for non-equilibrium conditions. In turn, we derive the single-particle-reduced entropy $S_1 = -Tr(\rho_1 \log_2 \rho_1)$ of the system as a function of the applied bias and gate voltages. S_1 can be interpreted as a measure of deviation from a single Slater-determinant. Within the multi-configurational approach, the numerically obtained entropy diagrams exhibit diamond-shaped structures, resembling the Coulomb diamonds present in the current-voltage characteristics in this transport regime. Finally, we compare the results with those which are obtained within the mean-field approximation.

HL 91.32 Thu 16:00 Poster A

Torque magnetometry on doped semiconductor nanowires — •Susanne Goerke[1], Florian Herzog[1], Marc Wilde[1], Eleonora Russo-Averchi[2], Anna Dalmau-Mallerqui[2], Daniel Rüffer[2], Anna Fontcuberta i Morral[2], and Dirk Grundler[1,3] — [1]Physik.-Dep. E10, TU München, D-85748 Garching — [2]LMSC, IMX, EPF Lausanne, CH-1015 Lausanne — [3]STI, EPF Lausanne, CH-1015 Lausanne

Filamentary semiconductor nanocrystals exhibit novel electronic properties due to their large surface-to-volume ratio and strong one dimensional confinement. We intend to investigate the magnetic properties of ensembles of free-standing GaAs and InAs nanowires, grown on (111) Si substrates by molecular beam epitaxy. Due to doping, the nanowires contain charge carriers. At low temperature, magnetic quantum oscillations (de Haas-van Alphen effect) are expected which allow one to extract scattering times, electron densities, and information on electron-electron interaction. We report on our on-going experiment aiming at torque magnetometry on doped nanowires at 260 mK. Financial support by the DFG via GR1640/3 in SPP 1285, NIM, the SNF, QSIT and the ERC is gratefully acknowledged.

HL 92: Poster Session: Structure and transport in organic photovoltaics; Photovoltaics; Impurities/Amorphous semiconductors; New materials

Presenters are kindly asked to be near their posters at least 17:00–18:00 or to leave a note at the poster indicating a time period of availability for discussions. — Beverages will be served starting at 18:00.

Time: Thursday 16:00–20:00 Location: Poster A

HL 92.1 Thu 16:00 Poster A

Nanostructured metal oxides for hybrid solar cells — •Julian Reindl[1], Jonas Weickert[1], Andreas Wisnet[2], Sophia Betzler[2], Christina Scheu[2], and Lukas Schmidt-Mende[1] — [1]Hybrid Nanostructures, FB Physik, Universität Konstanz — [2]Department of Chemistry and Center for Nanoscience, LMU München

Organic solar cells are an interesting technology to realize low-cost photovoltaics on a large scale. Even though efficiencies beyond 8 % have been achieved with a mixed film of donor and acceptor for thin films of about 100 nm, the unordered inner morphology of the active layer has detrimental effects in thicker layers due to more pronounced charge trapping and charge carrier recombination. A promising approach to realize thicker active layers with accordingly higher absorptivity is the hybrid solar cell concept, where the organic donor is substituted by a wide band gap metal oxide like titania (TiO2). Due to the small exciton diffusion length in organic semiconductors of usually 10-20 nm a structured donor-acceptor interface with this dimension is supposed to support efficient exciton separation and therefore lead to decreased recombination in these devices.

Here we present different approaches of fabricating a structured hybrid solar cell where we use either structured TiO2 wires with controllable dimensions or a structured transparent electrode underneath a thin TiO2 layer. The first attempt provides a crystalline acceptor matrix whereas the latter takes advantage of short pathways for electrons from the donor-acceptor interface to the collecting electrode.

HL 92.2 Thu 16:00 Poster A

Morphology and interdiffusion in organic donor-acceptor blends studied by analytical TEM — •Diana Nanova[1,2,4], Dominik Daume[2,4], Levin Dieterle[1,3,4], Martin Pfannmöller[3,4], Rasmus R. Schröder[3,4], and Wolfgang Kowalsky[1,4] — [1]Institute for High-Frequency Technology, TU Braunschweig, Germany — [2]Kirchhoff-Institute for Physics, Heidelberg University, Germany — [3]CellNetworks, BioQuant, Heidelberg University, Germany — [4]InnovationLab GmbH, Heidelberg, Germany

We present a combined study of the morphology and its relation to function on model devices of organic solar cells. The device characteristics acquired from impedance spectroscopy are correlated with the microstructural properties, obtained from analytical TEM. We found a novel morphology of P3HT:PCBM by applying electron energy loss spectroscopy and electron spectroscopic imaging in the low energy loss region. We observed a mixed-phase at the interface between the PCBM-rich and P3HT-rich phase, which seems to be crucial for efficient charge separation. To study the phase separation kinetics at the donor-acceptor interface, planar heterojunction samples of P3HT/PCBM bi-layer assemblies were prepared and annealed at various temperatures. In order to investigate the formation of a composite phase at the bi-layer interface via TEM, we prepared cross-sections by different methods, e.g. FIB-milling. We observed a change in the interface structure due to recrystallization and interdiffusion during annealing. This process leads to changes in the capacitance of the bi-layer devices, which can be derived from the measured impedance spectra.

HL 92.3 Thu 16:00 Poster A

Scanning Kelvin Probe Microscopy on FIB-milled crosssections of different organic photovoltaic devices — •Christian Müller[1,2,3], Rebecca Saive[1,2,3], Michael Scherer[1,2,3], Michael Kröger[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

Scanning Kelvin Probe Microscopy (SKPM) is a powerful tool to investigate the charge transport in organic devices and has been successfully applied to Organic Field Effect Transistors (OFETs). Conventional SKPM is restricted to the device's surface. Hence we have developed a new method to investigate device's cross-sections by milling with a Focused Ion Beam (FIB) and adjacent Scanning Probe Microscopy (SPM) characterization. We applied this method to organic solar cells and could reveal the potential distribution along the charge transport path. Sample preparation and measurements were performed in-situ in a combined SEM/FIB crossbeam system with an integrated SPM to avoid sample degradation by ambient air.

HL 92.4 Thu 16:00 Poster A

Influence of intercalation on geminate and nongeminate recombination in organic bulk heterojunction solar cells — •Benedikt Allendorf[1], Andreas Zusan[1], Vladimir Dyakonov[1,2], and Carsten Deibel[1] — [1]Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [2]Bavarian Centre for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg

The fundamental understanding of charge carrier generation and recombination is one of the key issues for further optimization of organic photovoltaics. Generation of free charge carriers with a high yield is a crucial step to ensure high power conversion efficiencies. We study how it is influenced by the morphology of the photoactive layer. We processed organic bulk heterojunction solar cells from blends of poly(2,5-bis(3-hexadecylthiophen-2-yl)thieno[3,2-b]thiophene) (PBTTT) with different fullerene acceptors. The blend of PBTTT donor with phenyl-C71-butyric acid methyl ester ($PC_{71}BM$) leads to intercalation of the acceptor molecules between the side chains of the conjugated polymers. In contrast, the bisadduct of phenyl-C61-butyric acid methyl ester (bis-$PC_{61}BM$) as acceptor material does not intercalate due to its larger volume. By means of time delayed collection field (TDCF) measurements we gain insight into the field dependence of polaron pair dissociation as well as into nongeminate recombination. Finally, we discuss the influence of intercalating and non–intercalating acceptors on generation and recombination of free charge carriers in organic solar cells.

HL 92.5 Thu 16:00 Poster A

Modeling disordered morphologies in organic semiconductors — •Tobias Neumann[1], Denis Danilov[1], Christian Lennartz[2], and Wolfgang Wenzel[1] — [1]KIT Campus Nord Gebäude 640 D-76344 Eggenstein-Leopoldshafen — [2]BASF Ludwigshafen

Organic thin film devices are investigated for many diverse applications, including light emitting diodes, organic photovoltaics and organic field effect transistors. Modeling of their properties on the basis of their detailed molecular structure requires generation of representative morphologies for these systems, many of which are amorphous. Because time-scales for the creation of morphologies are slow, we have investigated a linear-scaling single-molecule deposition protocol which generates disordered morphologies in a protocol that emulates vapor deposition of molecular films. Here we have applied this protocol on 5 test systems, with and without post-processing of the individually deposited molecules at every step. For the two simple systems, a noble gas and buckminster fullerenes, we managed to deposit ordered structures. Furthermore we investigated the properties of amorphous structure of films made of Alq3, PCBM and Alpha-NPD molecules, which are widely used in organic electronics, and compared our results to molecular dynamics simulations for each molecule.

HL 92.6 Thu 16:00 Poster A

Texturization and Passivation of Monocrystalline Silicon Wafers for High-Efficiency Solar Cells — •Jan Kegel[1,2], Mathias Mews[2], Heike Angermann[2], Uta Stürzebecher[3], and Bert Stegemann[1] — [1]Hochschule für Technik und Wirtschaft, Berlin, Germany — [2]Helmholtz Zentrum Berlin, Berlin, Germany — [3]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik GmbH, Erfurt, Germany

Wet-chemical treatment of crystalline Si wafers for the preparation of heterojunction solar cells are optimized with respect to low reflection losses, low recombination losses and long carrier lifetimes. It is demonstrated that a joint optimization of both saw damage etch and texture etch is necessary to control the optical and electronic properties of the resulting pyramid morphology. Effective surface passivation is achieved by deposition of intrinsic amorphous Si (a-Si:H(i)) layers. We demonstrate that optimized parameters for deposition of a-Si:H(i) on planar wafers can be transferred to the deposition on textured substrates. Moreover, the influence of the deposition temperature on the optical layer properties is elucidated, and the impact of post-deposition plasma-hydrogenation and annealing on the charge carrier lifetime and the implied open-circuit voltage is revealed.

HL 92.7 Thu 16:00 Poster A

Investigating the infrared conversion efficiency of Black Silicon solar cells by measuring the differential spectral responsivity (DSR) — •Kay-Michael Günther[1], Stefan Winter[2], Thomas Gimpel[3], Wolfgang Schade[1,3], and Stefan Kontermann[3] — [1]Clausthal University of Technology, EFZN, Am Stollen 19B, 38640 Goslar, Germany — [2]PTB Braunschweig, Bundesallee 100, 38116 Braunschweig, Germany — [3]Fraunhofer Heinrich Hertz Institute, Am Stollen 19B, 38640 Goslar, Germany

Exposing a silicon surface to femtosecond-laser pulses under a SF6 atmosphere leads to the incorporation of sulfur, which acts as a donor. After several pulses on the same spot, the surface becomes roughened. Therefore, with a single fabrication step, a pn-junction as well as a low reflecting surface can be created. This material is called Black Silicon. Previous works showed, that Black Silicon has a very high absorptance in the infrared region. It is believed, that high concentrations of sulfur states lead to the formation of an intraband within the bandgap.

To investigate the conversion efficiency of a Black Silicon Solar cell in the infrared, we measure the differential spectral responsivity in the range from 280 to 1200 nm. Compared to a standard high efficiency silicon solar cell, the Black Silicon cell of the same size exhibits a significantly increasing spectral responsivity above 1030 nm and even a higher spectral responsivity above 1150 nm.

HL 92.8 Thu 16:00 Poster A

Investigation of the sulfur doping profile of femtosecond-laserdoped Black Silicon solar cells — •Kay-Michael Günther[1], Alexander Bomm[2], Thomas Gimpel[2], Michal Schulz[1], Holger Fritze[1], Wolfgang Schade[1,2], and Stefan Kontermann[2] — [1]Clausthal University of Technology, EFZN, Am Stollen 19B, 38640 Goslar, Germany — [2]Fraunhofer Heinrich Hertz Institute, Am Stollen 19B, 38640 Goslar, Germany

Irradiating silicon with femtosecond-laser pulses under a SF6 atmosphere leads to the incorporation of sulfur and a structured surface. Very high sulfur concentrations can be achieved and an enhanced absorptance in the infrared spectral region is observed. This material is called Black Silicon and is used to fabricate solar cells and infrared photodetectors.

In this work, we investigate the sulfur doping profile of Black Silicon with 5 pulses per spot with secondary ion mass spectroscopy (SIMS) and capacitance-voltage spectroscopy (CV). Due to the strong surface roughness and the intrinsic pn-junction of the material, we applied a CV technique which uses impedance spectroscopy (IS) to compensate for additional space charges and series resistances. We compare samples with different annealing steps and different process atmospheres and we show that only a part of the incorporated sulfur is electrically active.

HL 92.9 Thu 16:00 Poster A

Optimization of indium tin oxide-free semitransparent polymer-based solar cells — •Verena Wilkens[1], Antonio España Petatań[1], Sebastian Wilken[1], Kambulakwao Chakanga[2], Omid Madani Ghahfarokhi[2], Karsten von Maydell[2], Jürgen Parisi[1], and Holger Borchert[1] — [1]University of Oldenburg, Dept. of Physics, Energy and Semiconductor Research Laboratory, 26111 Oldenburg, Germany — [2]Next Energy, EWE-Forschungszentrum für Energietechnologie e.V., 26129 Oldenburg, Germany

The absorption of conjugated polymers is usually limited to the visible range, which leads to lower photocurrents of polymer-based organic solar cells (OSCs), compared to established technologies based on inorganic semiconductors. On the other hand, such narrow absorption profiles enable the realization of semitransparent devices, which can be utilized in power-generating window applications. The most challenging issue for that purpose is the development of almost transparent contacts with sufficient electrical properties. Here, we present semitransparent OSCs based on poly(3-hexylthiophene) (P3HT) and phenyl-C_{61}-butyric acid methyl ester (PCBM), which are free from the expensive transparent conductor indium tin oxide (ITO). Instead of ITO, we report on the application of aluminum-doped zinc oxide (ZnO:Al), prepared by dc-magnetron sputtering. As hole contact, ultra-thin films (e.g. Ag or Au) with an adequate transparency in

the required wavelength regime were used. We introduced additional interfacial layers like molybdenum oxide (MoO_3) and tungsten oxide (WO_3), in order to improve charge extraction and light incoupling.

HL 92.10 Thu 16:00 Poster A

Application of $CuInS_2$ and ZnO nanoparticles in colloidal quantum dot photovoltaics — •Dorothea Scheunemann, Sebastian Wilken, Katja Frevert, Florian Witt, Holger Borchert, and Jürgen Parisi — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, 26111 Oldenburg

Colloidal quantum dots (CQD) are attractive for photovoltaics because of their solution processability and spectral tunability due to quantum size effects. Rapid advances in CQD photovoltaics in the recent years have led to high power conversion efficiencies. Previous works mainly focused on highly toxic materials containing cadmium or lead which might limit their possible application. One promising alternative material is $CuInS_2$ (CIS) which has shown attractive device performance in thin film solar cells. Here, we present solution processed CIS nanoparticles as absorber layer in nanocrystal based solar cells. In order to achieve efficient charge separation we use a heterojunction based on a bilayer structure of CIS and intrinsically n-doped ZnO nanocrystals. One issue in thin film photovoltaics is the optimization of the absorber thickness, taking into account light absorption as well as charge carrier collection. Therefore, we determined the absorption coefficient and transport properties which can serve as input parameters into an electro-optical simulation in order to determine the optimal absorber thickness.

HL 92.11 Thu 16:00 Poster A

Investigation of stacked elemental layers for Cu(In,Ga)Se_2 thin film preparation by rapid thermal selenization — •Christiane Stroth, Jörg Ohland, Ulf Mikolajczak, Thomas Madena, Jan Keller, Jürgen Parisi, Maria Hammer, and Ingo Riedel — Energy and Semiconductor Research Laboratory, Department of Physics, University of Oldenburg, 26111 Oldenburg, Germany

Rapid thermal selenization of pure metallic (Cu-In-Ga) or selenium-containing (Cu-In-Ga-Se) precursors is a favorable method to fabricate Cu(In,Ga)Se_2 absorber films for application in thin film solar cells. Because of its upscaling potential and the short process time it is a promising approach for the fabrication of CIGSe photovoltaic modules on industrial scale.

As a preliminary work for prospective plasma-enhanced selenization of stacked elemental layers (SEL) the elements copper, indium and gallium were sequentially deposited on molybdenum coated soda-lime glass by thermal evaporation. The stacking order was varied and the precursors were annealed with different heating rates. Morphology, elemental depth distribution and phases of the layers were investigated before and after annealing using scanning electron microscopy, energy-dispersive X-ray spectroscopy and X-ray diffraction. Furthermore the influence of different heating rates on phase transitions during annealing was studied by in-situ X-ray diffraction.

HL 92.12 Thu 16:00 Poster A

Temperature-dependent quantum efficiency measurements on Cu(In,Ga)Se_2 thin film solar cells — •Thorsten Sonnet, Janet Neerken, Dirk Otteken, Jürgen Parisi, Ingo Riedel, and Maria Hammer — Energy and Semiconductor Research Laboratory, Department of Physics, University of Oldenburg, 26111 Oldenburg, Germany

Solar cells based on Cu(In,Ga)Se_2 absorber layers demonstrate high power conversion efficiencies around 20%. However, solar cells obtained from industrial production exhibit lower efficiencies. In order to understand the physical mechanisms, the characterization of internal and external losses of the solar cell is important. While the temperature dependence of the open circuit voltage of the cells is an established tool to characterize recombination processes, the fact of a temperature dependent photocurrent is often overlooked. In order to characterize the collection efficiency, temperature-dependent internal quantum efficiency (IQE(T)) measurements were performed. The spectral response of the sample is measured within a temperature range from 100 K to 300 K. A reference cell and reflectance measurements of the sample at room temperature are used to calculate the internal quantum efficiency. From these measurements the temperature-dependent carrier diffusion length and thus the minority carrier lifetime can be extracted.

HL 92.13 Thu 16:00 Poster A

Evolution of the performance parameters of Cu(In,Ga)Se2 solar cells during light soaking at different temperatures — •Johannes Schoneberg, Jörg Ohland, Janet Neerken, Jan Keller, Jürgen Parisi, Maria Hammer, and Ingo Riedel — Department of Physics, University of Oldenburg, 26111 Oldenburg, Germany

Among all thin film photovoltaic technologies high-efficiency solar cells based on Cu(In,Ga)Se2 (CIGSe) absorber layers demonstrate the highest power conversion efficiencies around 20% . Metastabilities in device performance of CIGSe solar cells might lead to considerable light- or heat-induced variation of the solar cell parameters and therefore the efficiency. The fact that devices from different manufacturers exhibit more or less pronounced metastable behavior with different dynamics makes the topic interesting for a detailed analysis. A systematic study in which CIGSe solar the transient performance is monitored during light soaking, annealing and operation at different voltage bias will promote a more general understanding of the metastable device behavior. In this work CIGSe solar cells were light soaked at different light intensities and activation temperatures, while the performance parameters are monitored in a time series. From the results we intend to derive the activation energy between the relaxed and the light soaked states.

HL 92.14 Thu 16:00 Poster A

Investigation of defect energies of co-evaporated CIGSe solar cells — •Nils Neugebohrn, Maria S. Hammer, Christiane Stroth, Janet Neerken, Jan Keller, Jürgen Parisi, and Ingo Riedel — Energy and Semiconductor Research Laboratory, Department of Physics, University of Oldenburg, 26111 Oldenburg, Germany

$CuInGaSe_2$ thin film solar cells are a promising candidate for the next generation low-cost and high efficiency solar cells. However, the relation between defect energies and the metastable/transient behavior of the performance is still an unsatisfyingly resolved issue. In CIGSe solar cells various anomalies are observed, which can provide insights in present defect dynamics, recombination mechanisms or possible transport barriers. Examples are the so called roll over and cross over effects in temperature dependent current-voltage characteristics (IV(T)) and shifting defect energies in deep level transient (DLTS) and admittance spectroscopy (AS(T)) depending on the conditioning of the solar cell prior to the measurement. In order to accurately investigate the impact of (pre-) conditioning, the defined initial or relaxed state of high efficiency CIGSe solar cells have been characterized by aforementioned methods. The results of this study and first results for cells in metastable conditions are presented.

HL 92.15 Thu 16:00 Poster A

Thin film GaN/Cu2O heterojunction solar cells — •Philipp Hering, Julian Benz, Daniel Reppin, Martin Becker, and Bruno Meyer — 1. phys. Inst., JLU-Giessen, Heinrich-Buff-Ring 16, 35392 Giessen

Due to its high absorption coefficient, non-toxicity, and the abundance of its composing elements, cuprous oxide (Cu2O) is a promising absorber material in photovoltaic devices, even despite of the relatively large band gap (2.17 eV). With increasing success, more attention has recently been paid to Zinc Oxide/Cuprous Oxide heterojunctions. At higher forward voltages, however, the large conduction band offset impedes the minority carrier current across the interface: The theoretically attainable efficiency is decreased by about 50%. As a way out, we chose Gallium Nitride as window layer: It offers a conduction band offset of less than 0.2 eV in relation to Cu2O. Our cells were manufactured at room temperature by radio frequency sputter deposition of cuprous oxide, utilizing a copper target under addition of oxygen on top of Gallium Nitride templates. The templates consisted of a thin layer of GaN:Si, grown on a sapphire substrate by metal organic chemical vapor deposition. The sputtering was followed up by photolithographic structuring. For device characterization Current/voltage curves were obtained under AM1.5g illumination, different light intensities, as well as various temperatures, and the external quantum efficiency measured.

HL 92.16 Thu 16:00 Poster A

Optical and electrical characterization of InP-based InGaAsP/InGaAs low bandgap multijunction solar cells — •Anja Dobrich[1], Klaus Schwarzburg[1], Agnieszka Paszuk[2], and Thomas Hannappel[1,2,3] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin — [2]Technische Universität Ilmenau, Institut für Physik, Fachgebiet Photovoltaik, Ilmenau — [3]CiS Forschungsin-

stitut für Mikrosensorik und Photovoltaik, Erfurt

Since III-V semiconductor concentrator solar cells grown by MOVPE become actually more attractive for terrestrial applications, it is a great issue to increase the efficiency while costs are reduced. III-V triple junction solar cells have demonstrated the highest conversion efficiencies (>41%) of any photovoltaic technology to date. Higher efficiencies can be achieved with a four-junction configuration, which has optimized band gaps. This can be realized with a mechanically stacked GaAs-based GaInP/GaAs top-tandem and an InP based InGaAsP/InGaAs bottom-tandem cell. Based on the latter two absorber materials, a low bandgap tandem solar cell with optimized bandgaps was developed. In the need for a suitable method to analyze our tandem cells, we developed an apparatus that allows for a fast and convenient evaluation of many cell performance parameters for illumination intensities equivalent up to 50 suns. The experimental setup makes it possible to measure all relevant data with the sample mounted on a probe station and to address each subcell of the tandem individually. Since the lifetime of minority carriers is one of the most important properties we analyzed the lifetime with time- and spatially-resolved photoluminescence.

HL 92.17 Thu 16:00 Poster A

Analysis of electronic subgap states in amorphous semiconductor oxides on the example of Zn-Sn-O — Wolfgang Körner[1], •Daniel F. Urban[1], and Christian Elsässer[1,2] — [1]Fraunhofer Institute for Mechanics of Materials IWM, Freiburg — [2]IAM-ZBS, Karlsruhe Institute of Technology

A molecular dynamics and density-functional-theory study of amorphous Zn-Sn-O with focus on the use as transparent conducting oxide material is presented. The amorphous structures generated by MD are subsequently relaxed using the local-density-approximation of DFT. The Zn/Sn ratio, the oxygen content and individual point defects are investigated concerning their thermodynamic and electronic properties and compared to the data for crystalline structures. Defect levels in the electronic band structure of ZnO are analyzed in terms of the density of states, which is calculated within the LDA and with a self-interaction-correction. We relate the electronic sub-gap states, which were recently observed experimentally, to structural features of the amorphous samples. We find the valence band tail, caused by the disordered O 2p orbitals, to be superimposed by deep defect states that can be assigned to under-coordinated O atoms. Doping with H atoms is found to suppress these states and improves the transparency. The deep levels below the conduction band arise mainly from under-coordinated Sn atoms or Zn–Sn pairs. The addition of oxygen can be a possible route to reduce such defect levels.[2]

[1] W. Körner, P. Gumbsch and C. Elsässer, PRB (2012) accepted.
[2] W. Körner and C. Elsässer, Thin Solid Films (2012) submitted.

HL 92.18 Thu 16:00 Poster A

Defect states in amorphous silicon nitrides: a-$Si_3N_xH_y$ — •Leif Eric Hintzsche[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

Amorphous silicon nitrides are commonly deposited as passivation layers on Si based solar cells with their stoichiometries depending mainly on the applied deposition process. By using ab initio molecular dynamics simulations, we investigated important structural and electronic properties, such as atomic coordination and electronic defect states, for different silicon nitride stoichiometries. We found two dominant defect classes in silicon nitrides: (a) under-coordinated Si atoms and (b) states localized on Si-Si bonds. Furthermore, we observed that in sub-stoichiometric silicon nitrides, percolation networks with longer Si chains lead to a considerable number of delocalized defect states in the band gap. While hydrogen can passivate under-coordinated Si atoms, electronic defects related to the latter class are hardly changed. These findings suggest that the dominant defect class also changes depending on the stoichiometry and the concentration of hydrogen.

HL 92.19 Thu 16:00 Poster A

Formation energy of point defects with transition metal (TM = Cr, Mn and Fe) doped barium titanate from first-principles studies — Sanjeev K. Nayak[1], •Waheed A. Adeagbo[1], Hans T. Langhammer[2], and Wolfram Hergert[1] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, Von-Seckendorff-Platz 1, 06120 Halle, Germany — [2]Institute of Chemistry, Martin-Luther-University Halle-Wittenberg, Kurt-Mothes-Str. 2, 06120 Halle, Germany

We study the electronic properties of substitutional doped transition metal (TM = Cr, Mn and Fe) in barium titanate from the first-principles studies. We explore the stability of different valency states for the TM dopants which are probabilistic in experimental conditions. For such a consideration, we have modeled the system by charged supercells and also by possible charge compensation mechanism through the presence of oxygen vacancy (V_O). The analysis on the stability of defects is done by comparing the formation energy of defects. The regular expression of the Zhang-Northrup formulation for the formation energy of charge defects is used in our calculation together with the band gap correction. We use the Vienna *ab initio* simulation package (VASP). The supercell consists of 3×3×1 periodic repetition of hexagonal $BaTiO_3$ unit cell, which is the crystal structure of about 2 mol% TM-doped material at room temperature and normal pressure, and constitute of 54 functional units of $BaTiO_3$ where one Ti ion is substituted by a TM ion. Thus the defect concentration we are dealing with is about 1.85 mol% and this is in the range of experimental limits.

HL 92.20 Thu 16:00 Poster A

Metal organic chemical vapor deposition of GexSbyTez layers grown by using degermane — •Sally Riess[1,2], Daniela Schlösser[1,2], Michael Lübben[1,2], Toma Stoica[1,2], Martina von der Ahe[1,2], Kamil Sladek[1,2], Anna Haab[1,2], and Hilde Hardtdegen[1,2] — [1]Peter Grünberg Institut 9, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology

GexSbyTez (GST) films grown on Si(111) substrates by epitaxy tend to be polycrystalline and therefore rough. Especially the incorporation of Germanium in the films is problematic. Thin and smooth film surfaces are however a prerequisite for memory applications. In the past we demonstrated that the metal organic chemical vapor deposition (MOCVD) growth of highly mismatched III/V materials such as InAs/GaAs can be accomplished conformally, if a low temperature growth process is used. This knowledge is transferred to MOCVD growth of GST. To this end as a Ge precursor digermane was employed which is expected to decompose at low temperatures. Commercial sources for Sb (triethylanthimony) and Te (diethyltellur) were chosen, which are suitable for low temperature deposition. At first the growth of Sb2Te3 layers was optimized. Than digermane was added to the growth process. Growth was evaluated by SEM, XRD and Raman measurements. It was found that GST can be deposited at the same conditions as Sb2Te3. SEM pictures show well coalesced, trigonal crystalline structures and XRD measurements verify the integration of Ge. The influence of growth parameters on layer growth will be presented.

HL 93: Photovoltaics (HL, jointly with CPP, O)

Time: Friday 9:15–13:45 Location: H2

HL 93.1 Fri 9:15 H2

Simulation of TRPL on thin film solar cells — •Matthias Maiberg, Maria Gaudig, and Roland Scheer — Institute of Physics, Martin-Luther-University Halle-Wittenberg, Von-Danckelmann-Platz 3, 06406 Halle, Germany

In the recent years time-resolved photoluminescence (short: TRPL) on semiconductor devices has been established as a non-destructive, non-invasive, contactless characterization method. The decay of the signal has not been fully understood yet. Therefore we studied TRPL on semiconductor layers and thin film solar cells by simulation with Synopsys TCAD. At first we investigated the influence of excitation, diffusion, photon recycling, bulk-defects and defects at the contacts, as well as space charge and potential fluctuations on the PL-decay separately by quasi-onedimensional simulations of absorber layers and thin film solar cells. We also studied the influence of grain boundaries, since

materials like Cu(In,Ga)Se_2 and $Cu_2ZnSnSe_4$ are in general polycrystalline. We show, that the samples can be characterized by excitation dependent measurements in the open circuit case. We can explain some effects found in photoluminescence experiments, like a decrease of the lifetime with an increasing excitation, a maximum lifetime due to saturated bulk-defects, and a lifetime of more than $10\mu s$ in case of charge separation due to the electric field in the space charge region.

HL 93.2 Fri 9:30 H2

3D reciprocal space imaging of individual Cu(In,Ga)Se_2 nanocrystallites inside a thin film solar cell — •Taras Slobodskyy[1], Anatoliy Slobodskyy[2], Boris Landgraff[1], Christian Heyn[1], and Wolfgang Hansen[1] — [1]Institute for Applied Physics, University of Hamburg, Jungiusstraße 11, D-20355 Hamburg, Germany — [2]Karlsruhe Institute of Technology (KIT), Light Technology Institute (LTI), Kaiserstraße 12, 76131 Karlsruhe, Germany

In this contribution we will present results of an investigation of strain distributions inside of individual Cu(In,Ga)Se_2 nanocyrstallites located inside a solar cell absorber layer. The strain is imaged using synchrotron radiation.

We find that the investigated crystallites are non homogeneously strained. The strain is produced by surrounding nanocrystals in the polycrystalline semiconductor film and carries information about the intercrystalline interactions. The measurements are done non destructively and without additional sample preparation or X-ray beam nanofocusing.

The demonstrated technique provides a way for connecting variations in the properties of individual crystallites inside of a working solar cell to the resulting energy conversion efficiency.

HL 93.3 Fri 9:45 H2

Investigations of chemical gradients in Cu(In,Ga)Se_2 thin film solar cells grown on polyimide substrate by high spatially resolved cathodoluminescence microscopy — •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

Optical properties of Cu(In,Ga)S_2(CIGS)-absorber layers for thin film solar cells have been studied by high spatially resolved cathodoluminescence (CL) at low temperature (T = 5K) to investigate lateral und vertical changes of the composition within the quaternary absorber. CIGS layers were grown on flexible polyimide foil by using an ion-beam assisted roll-to-roll process. To ensure high efficiency sodium fluoride was evaporated by an additional source during the process. The substrate temperature was varied above the standard value enabled by using an advanced polyimide substrate resisting higher temperatures. Cross sections of the thin film solar cells were prepared to investigate the vertical distribution of composition and its changes influenced by the substrate temperature. IV measurements showed an increase of the efficiency with higher substrate temperature suggesting less fluctuation of the composition and a smoother vertical gallium gradient. Furthermore a variation of the sodium content was made by variation of the evaporation temperature. Integral luminescence properties were investigated which showed a red shift and a broadening of the main peak with increased sodium content.

HL 93.4 Fri 10:00 H2

Admittance spectroscopy on Cu(In,Ga)Se_2 solar cells with respect to sodium content — •Felix Daume[1,2], Andreas Rahm[1], and Marius Grundmann[2] — [1]Solarion AG, Ostende 5, 04288 Leipzig, Germany — [2]Institut für Experimentelle Physik II, Universität Leipzig, Linnéstraße 5, 04103 Leipzig, Germany

Solar cells based on Cu(In,Ga)Se_2 (CIGSe) absorbers deposited on flexible polyimide substrate enable cheap manufacturing with roll-to-roll equipment and the application in new environments such as low-load rooftops. Among present thin film flexible solar cell technologies, CIGSe achieves the highest efficiencies. The proper incorporation of sodium into the CIGSe absorber is indispensable to achieve these high efficiencies. In this study, sodium fluoride is co-evaporated during CIGSe deposition.

CIGSe solar cells with different sodium contents were investigated by admittance spectroscopy. We calculated activation energies for the N1 signature which, in literature, is widely attributed to defects. Overall concentrations and density profiles across the band gap were derived for this signature. Additionally, we derived the net doping of the CIGSe absorbers from capacitance-voltage measurements. A model based on defects at the CdS(n-type)/CIGSe(p-type) interface is proposed to explain our observations with respect to the sodium content.

HL 93.5 Fri 10:15 H2

High-resolution Spectroscopic Mapping of Polymer Fullerene Blend Films for Organic Solar-Cell Applications — Xiao Wang, Kai Braun, Alfred J. Meixner, and •Dai Zhang — Institute of Physical and Theoretical Chemistry, Uni. Tübingen, Tübingen

Polymers and fullerenes are widely employed in the field of organic solar cells as the electronic donors and acceptors. The morphology and the photo-physical properties of the polymer and fullerenes blends at nanometer scale are critical for achieving a high performance of the solar cells. Employing a home-built parabolic mirror assisted apertureless near-field optical (Raman and photoluminescence) microscope, we demonstrated high resolution near-field spectroscopic mappings of the polymer:fullerene blend films. Our investigation focused on the additive effect for a C-PCPDTBT:PCBM blend film. From the simultaneously recorded morphology and spectroscopic information, the interplay among the blend film morphology, the local donor and acceptor molecular distributions, and the photoluminescence quenching efficiency were discussed. The PL and Raman signals of the electron donor and acceptor have been probed at an optical resolution of approximately 10 nm which allow the direct identification of the chemical nature of the different domains. Moreover, we were able to reveal and quantify the local quenching, which is related to the electron transfer from donor to acceptor.

HL 93.6 Fri 10:30 H2

Investigation of the s-shape caused by the hole selective layer in organic bulk heterojunction solar cells — •Lothar Sims[1,2], Ulrich Hörmann[2], René Kogler[3], Roland Steim[4], Wolfgang Brütting[2], and Pavel Schilinsky[1] — [1]Belectric OPV GmbH, Landgrabenstr. 94, 90443 Nürnberg — [2]University of Augsburg, Institute of Physics, Universitätsstr. 1, 86135 Augsburg — [3]Evonik Industries AG, Kirschenallee, 64293 Darmstadt — [4]STORM Energy GmbH, Rathenauplatz 2, 90489 Nürnberg

During the operation period of an organic solar cell different failure mechanisms can occur which limit the lifetime of the device. Among these failure mechanisms the so called s-shape or second diode, where the current density-voltage (JV) curve bends towards the origin in the 4th quadrant, plays an important role. We investigated the origin of the s-shape caused by the hole selective layer (HSL) using N,N'-bis(3-methylphenyl)-N,N'-bis(phenyl)-benzidine (TPD) coevaporated with different amounts of Dipyrazino[2,3-f:2',3'-h]quinoxaline-2,3,6,7,10,11-hexacarbonitrile (HATCN) as a model system. The low glass transition temperature of TPD allows investigating the impact of WF and mobility of the HSL on device performance and thus s-shape independently of each other. The observed JV-curves were simulated by solving the drift-diffusion, i.e. continuity and Poisson equations numerical via the program PC1D. While WF rather influences the open circuit voltage, mobility seems to be the reason for the s-shape. The results show that an accumulation of holes near the hole selective/semiconductor layer interface might be responsible for the observed s-shape.

HL 93.7 Fri 10:45 H2

The role of defects in nanocrystalline zinc oxide interlayers for polymer-based solar cells — •Sebastian Wilken, Dorothea Scheunemann, Florian Witt, 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 polymer-based bulk heterojunction solar cells, the absorber blend has intrinsically no preferential transport direction for photogenerated charge carriers due to the statistical intermixing of both the donor and acceptor phase. Therefore, additional charge-selective interfacial layers, which are semipermeable membranes for either electrons or holes in an ideal case, are widely used in order to achieve efficient charge extraction at the respective contacts. One well established material for electron collection is zinc oxide (ZnO), which can be processed at moderate temperatures and deposited via solution-based techniques in form of colloidal nanocrystals (NCs). Here, we discuss the influence of defect states in interlayers made of ZnO NCs on the overall solar cell performance. For that purpose, ZnO NCs with different surface-to-volume ratios were wet-chemically synthesized and introduced into indium tin oxide-free polymer solar cells in the inverted device architecture. As indicated by photoluminescence, we show that surface defects

play a more and more dominant role with decreasing NC size and, thus, limit the photovoltaic efficiency. For a more detailed analysis of the involved defect states, photo-induced current transient spectroscopy (PICTS) was performed for devices with varying amount of surface defects.

HL 93.8 Fri 11:00 H2

Solar diode sensor — •Hao Shen[1], Martin Hoffmann[1], Juan Daniel Prades[2], Francisco Hernandez-Ramirez[3], and Andreas Waag[1] — [1]Institute of Semiconductor Technology, TU Braunschweig, D-38105 Braunschweig, Germany — [2]Department of Electronics, Uni. Barcelona, E-08028 Barcelona, Spain — [3]Catalonia Institute for Energy Research (IREC), E-08930 Barcelona, Spain

The nanodevice architecture presented here has been designed to overcome the current issues in gas sensor technologies: reducing power consumption and lowering operating temperature. Conductometric sensors based on semiconductor metal oxides need the continuous supply of the energy in the form of heat or UV light, to activate the chemical interaction between gases and the sensing surface. New concepts for energy harvesting units as an in-built module are demanded to make self-powered gas sensors. Herein we report a solar diode sensor (SDS) based on new designed CdS@n-ZnO/p-Si nanoelements which unifies gas sensing (CdS@n-ZnO) and solar energy harvesting (n-ZnO/p-Si diode) functionalities in a singular material unit and device. The SDS sensing mechanism (change of open circuit voltage), in comparison to the well-known conductometric sensors (change of resistance), is systematically studied and explained in terms of gas-material surface interactions and the subsequent changes in the doping level (ND), which is manifested in the variation of Voc in CdS@n-ZnO/p-Si. The fabricated SDS was capable of quantitatively detecting oxidising and reducing gases with reproducible response at room temperature and without the need of any other energy sources except solar illumination.

HL 93.9 Fri 11:15 H2

Simulation of temperature distribution in ZnO:Al thin films for laser annealing experiments — •Christian Isenberg, Cay-Christian Kalmbach, Daniyal Sattarian, Uwe Stute, and Alexander Horn — Laser Zentrum Hannover e.V., Hollerithallee 8, 30419 Hannover, Germany

Transparent Conducting Oxides (TCOs) have become widespread as transparent electrodes in photovoltaics and transparent electronics. Thermal post deposition treatments by furnace annealing have shown to improve the electrical and optical properties of TCO thin films. Laser annealing of TCOs allows control over the peak temperature as well as the spatial and temporal temperature distributions of TCO thin films and substrates, preserving the substrate by heating only the TCO layer. Therefore, treating TCOs with tailored laser radiation allows larger temperature than furnace annealing even on temperature sensitive substrates. Numerical calculations using Crank-Nicolson method have been conducted to estimate the temperature distribution in ZnO:Al thin films during laser annealing process. In the special case of temperature-independent material parameters, the numerical solution is reduced to an analytical solution, determined by convolution of the heating source term with a Green's function for a geometry of a thin film on a semi-infinite substrate. Numerical results are compared to temperature measurements, done by a thermographic camera during laser annealing process.

Coffee break

HL 93.10 Fri 11:45 H2

Selective laser ablation of Al_2O_3 passivation layers from optically black silicon surfaces — •Martin Otto[1], Katharina Widder[1], Tino Rublack[1], Matthias Zilk[2], Thomas Käsebier[2], Gerhard Seifert[1], and Ralf B. Wehrspohn[3] — [1]Martin-Luther-University Halle-Wittenberg, Institute of Physics -μ MD Group, Heinrich-Damerow-Strasse 4, 06120 Halle, Germany — [2]Friedrich Schiller University Jena, Institute of Applied Physics, Max-Wien-Platz 1, 07743 Jena, Germany — [3]Fraunhofer Institute for Mechanics of Materials Halle, Walter-Hülse-Str. 1, 06120 Halle, Germany

Inductive coupled plasma reactive ion etching (ICP-RIE) of silicon enables excellent broad band and wide angle antireflective surface properties. The stochastically emerging needle like nano-structures let the silicon surface appear optically black due to its high absorption coefficient of over 97% integrated from 300 nm to 1175 nm. Concomitant, highly enhanced surface recombination is introduced. The latter, may be effectively suppressed by a well suited passivation layer of Al_2O_3 deposited by thermal ALD. Laser ablation is commonly used in the PV industry to open local contact areas in dielectric passivation stacks. In this work we show the feasibility to ablate alumina thin films from nano-structured black silicon (b-Si) solar cell front surfaces. Microstructural geometric analysis by focussed ion beam and SEM reveal certain structural changes in the zone of ablation which are believed to be beneficial for contact formation. Simultaneously, neither the deposition of Al_2O_3 layers of varying thickness nor their ablation lead to a very significant degradation of the optical surface properties.

HL 93.11 Fri 12:00 H2

Surface Modification of Nano-Textured Black Silicon for Photovoltaic Applications — •Michael Algasinger[1], Svetoslav Koynov[1], Julie Paye[1], Florian Werner[2], Max Bernt[1], Martin S. Brandt[1], and Martin Stutzmann[1] — [1]Walter Schottky Institut, Technische Universität München, 85748 Garching, Germany — [2]Institute for Solar Energy Research Hamelin, Am Ohrberg 1, 31860 Emmerthal, Germany

The morphology and the electronic properties of nano-textured silicon, obtained by a metal-catalyzed wet etching process and its improvement by an additional chemical treatment are examined with regard to solar cell applications. Photoluminescence and optical reflectivity measurements show evidence for a nano-porous silicon (np-Si) phase in the as-prepared nanostructure. It is found that an additional wet-chemical treatment removes the np-Si fraction and significantly alters the surface of the nanostructure. Cross-sectional scanning electron microscopy images reveal a drastic reduction of the surface area, to values of only 3 - 6 times of that of a planar surface. Electron spin resonance measurements were performed to investigate the type and quantity of defects induced by the nano-texturing process. First results on the passivation of surface defects via atomic layer deposition of Al_2O_3 are presented. Photoconductance decay measurements of passivated nanostructures, which received the additional post-etching treatment, show a significant increase in effective carrier lifetimes.

HL 93.12 Fri 12:15 H2

Surface morphology of black silicon produced by metal-catalyzed wet etching — •Maximilian Bernt, 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), is a material with an optically graded surface, which shows reflectivity as low as 1 - 5 % in the whole range of Si absorption and additional light trapping effects. Due to its unique optical properties, b-Si is an interesting material for photovoltaic applications. However, b-Si produced by Au-catalyzed wet etching of crystalline Si (c-Si) wafers exhibits a nano-porous silicon (np-Si) phase in the as-prepared nano-structure. This np-Si phase leads to an increased surface area which could alter the electrical properties significantly. The formation of the nano-texture was investigated at different stages of the etch process by cross sectional scanning electron microscopy. The evolution of the np-Si phase with increasing etch time was observed by photoluminescence and optical reflectivity measurements. In addition, the influence of the doping level of n- and p-type c-Si substrates on the etch process and the morphology of the resulting nano-texture was studied.

HL 93.13 Fri 12:30 H2

Valence band offsets estimation of Al_2O_3 films on silicon by XPS and UPS measurements — •Johannes Ziegler[1], Volker Naumann[2], Martin Otto[1], Alexander Sprafke[1], and Ralf B. Wehrspohn[1,3] — [1]Martin-Luther-University Halle-Wittenberg, Institute of Physics, Halle, Germany — [2]Fraunhofer Center for Silicon Photovoltaics CSP,Halle, Germany — [3]Fraunhofer Institute for Mechanics of Materials Halle, Halle, Germany

A quantitative measurement of valence band offsets in isolator-silicon junctions might help to realize heterojunction devices such like semiconductor-isolator-semiconductor (SIS) solar cells. We measured XPS and UPS spectra of thin (2–50 nm thick) Al_2O_3 films deposited on silicon by thermal ALD. The valence band offsets of these structures are estimated from the XPS spectra using the method of Kraut et.al. [1] . A slight trend in the valence band offsets 3.3–4.5 eV with increasing film thickness 2–50 nm was calculated from the XPS spectra. To estimate the valence band offsets from the UPS spectra 3.3–3.4 eV of 2–10 nm thick Al_2O_3 on silicon, a simple straight forward approach based on linear regression of the spectra on the band edges is

used. We compare the results of both measurements and discuss possible sources for the measured increase of the valence band offset with increasing Al_2O_3 film thickness.

[1] A. Kraut, R. W. Grant, J. R. Waldrop and S. P. Kowalczyk, Phys. Rev. Lett. 44,p.1620 (1982), http://link.aps.org/doi/10.1103/PhysRevLett.44.1620

HL 93.14 Fri 12:45 H2

Charge trapping in Al2O3 passivation layers for silicon solar cells — •Paul Jordan[1], Frank Benner[1], Ingo Dirnstorfer[1], and Thomas Mikolajick[1,2] — [1]NaMLab gGmbH, Dresden, Germany — [2]Lehrstuhl für Nanoelektronische Materialien, TU Dresden, Dresden, Germany

Novel highly efficient silicon solar cells require an excellent level of surface passivation, to minimize recombination losses of photo-generated carriers. During the last decade, the dielectric Al2O3 became the material of choice for the passivation of p-type silicon. The excellent passivation properties are mainly caused by negative charges located within the dielectric. In this study the origin of the negative charges is investigated using capacitance-voltage and microwave detected photoconductivity measurements. It will be shown that the negative charges are partly caused by electrons, injected from silicon into the dielectric. The trapping dynamics are analyzed by the means of the post program discharge technique, which is commonly applied for memory devices. Furthermore, the trapping and detrapping rates depend on the thickness of the ultra-thin SiO2 interface between Si and Al2O3. For an interface thickness of about 2 nm, the asymmetry of trapping and detrapping rates significantly enhances the negative charge density. As a consequence an optimum interface thickness is essential for the excellent passivation property of Al2O3.

HL 93.15 Fri 13:00 H2

Investigation of carrier traps in pn-junctions of fully-processed silicon photovoltaic cells — •Teimuraz Mchedlidze, Leopold Scheffler, and Jörg Weber — Technische Universität Dresden, 01062 Dresden, Germany

Mesa-diodes with a surface area about 1 mm^2 and a height of 50 μm were fabricated on top of fully-processed Si photovoltaic-cell wafers for detection and investigation of carrier traps in pn-junctions. All fabrication steps were performed at room temperature and fully preserved the initial structure of the cell inside the mesa-diode. Schottky diodes were fabricated on neighbor locations of the wafers after etching off the PV-cell structure to a depth of 50 μm. The DLTS spectra detected for the mesa- and Schottky-diodes show significant difference, namely the deep carrier traps detected in the mesa-structures were below the detection limit in the Schottky-diodes. Profiling of the trap density for the mesa-diodes showed a steep decrease with increasing distance from the pn-junction. Parameters of the detected traps, their possible origin and reasons for the differences between spectra detected for mesa- and Schottky-diodes are presented and discussed.

HL 93.16 Fri 13:15 H2

Iron acceptor association in compensated multicrystalline silicon — •Christian Möller[1,2], Kevin Lauer[1], Fabien Gibaja[3], Til Bartel[3], and Fritz Kirscht[3] — [1]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik GmbH, SolarZentrum Erfurt, Konrad-Zuse-Str. 14, 99099 Erfurt, Germany — [2]TU Ilmenau, Institut für Physik, Weimarer Str. 32, 98693 Ilmenau, Germany — [3]Calisolar GmbH, Magnusstraße 11, 12489 Berlin

Monitoring the acceptor concentration in compensated multicrystalline silicon by a minority-charge carrier lifetime measurement is applicable for production control due to the fast and easy lifetime measurement. The iron acceptor pair association is studied for several acceptors position dependent over the whole height of a compensated multicrystalline ingot. Acceptor pair and height dependent induced differences in the defect kinetics are visible. The calculated position depending doping concentrations of several ingots from charge carrier lifetime measurements are discussed and compared with the expected doping concentration calculated via Scheil equation.

HL 93.17 Fri 13:30 H2

Femtosecond laser processed sulfur-emitter solar cells — •Thomas Gimpel[1], Kay-Michael Günther[2], Anna Lena Baumann[1], Wolfgang Schade[1], and Stefan Kontermann[1] — [1]Fraunhofer Heinrich Hertz Insitute, EnergieCampus, Am Stollen 19B, 38640 Goslar, Germany — [2]Energieforschungszentrum Niedersachsen, EnergieCampus, Am Stollen 19B, 38640 Goslar, Germany

A simple fs-laser process enables structuring and sulfur incorporation simultaneously. This process is applied on a single side to different silicon substrates independent from the crystal structure. Without any advanced solar engineer processes like passivation, dopant source layer deposition, its diffusion and removal, efficiencies of 8.2% are achieved, at present. Due to an incorporated intermediate band this material has the potential to convert infrared light even at wavelengths below the silicon band gap. New applications e.g. in a crystalline silicon tandem solar cell are under development.

HL 94: Quantum wires and nanocrystals: Optical properties

Time: Friday 9:30–11:00 Location: H13

HL 94.1 Fri 9:30 H13

GaN nanowires as opto-chemical sensors — •Jens Wallys[1], Sara Lippert[1], Florian Furtmayr[1,2], Sebastian Koslowski[1], Jörg Schörmann[1], Jörg Teubert[1], and Martin Eickhoff[1] — [1]I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Germany — [2]Walter Schotky Institut, Technische Universität München, Germany

GaN nanowires (NWs) grown by plasma-assisted molecular beam epitaxy (PAMBE) feature a low density of structural defects and a high surface to volume ratio. Their electrochemical stability and strong luminescence at room temperature make them promising candidates for opto-chemical sensor applications.

In this contribution we examine Si-, Ge-, and Mg-doped GaN NW ensembles with different doping concentrations in contact with an electrolyte by photoluminescence (PL) spectroscopy and investigate the PL changes related to variations in the chemical environment. With a three electrode setup the potential at the NW electrode can be precisely controlled to optimize the signal response for specific sensing applications e.g. detection of small pH variations caused by biological systems.

The influences of doping with shallow donors (Si or Ge) or acceptors (Mg) on the response characteristics are discussed in terms of achievable sensitivity, detection energy, and measurement stability. The results will be discussed using a qualitative model for the PL response taking non-radiative surface recombination and charge transfer from the NWs to the electrolyte into account.

HL 94.2 Fri 9:45 H13

Optical properties and gas sensing capabilities of Ge and Si doped GaN nanowires — •Pascal Becker[1], Svenja van Heeswijk[1], Pascal Hille[1], Jörg Schörmann[1], Jörg Teubert[2], Sangam Chatterjee[2], Alexej Chernikov[1], and Martin Eickhoff[1] — [1]I.Physikalisches Institut, Justus-Liebig-Universität Gießen — [2]Philipps-Universität Marburg, Fachbereich Physik

We report on the optical properties and the optical gas response of Si- and Ge-doped self-assembled GaN nanowires (NWs) grown by plasma-assisted molecular beam epitaxy. GaN:Si and GaN:Ge NWs were grown on n-type Si(111) substrates with typical lengths of approx. 1.5 μm.

The NW ensembles were analyzed by temperature dependent and time resolved photoluminescence (PL) spectroscopy and the influence of Ge- and Si-doping was compared to undoped NW samples. Their emission properties are influenced by the doping concentration possibly by variation of the surface band bending (SBB).

Furthermore, the presence of oxidizing gases leads to a significant decrease of the PL-intensity. The doping concentration significantly influences this PL-quenching which will be interpreted in terms of SBB-variations.

HL 94.3 Fri 10:00 H13

Optical characterization of In(Ga)As/In(As)P nanowires with micro photoluminescence and absorption spectroscopy — •Michael M. Bormann, Julian Treu, Mengyu Liang, Simon Hertenberger, Stefanie Morkötter, Christian Grasse, Stephan Sprengel, Max Bichler, Markus-Christian Amann,

Jonathan J. Finley, Gerhard Abstreiter, and Gregor Koblmüller — Walter Schottky Institut and Physik Department, TU München, Garching, Germany

In this work we present the optical properties of high-In content In(Ga)As nanowires (NW) and InAs/InAsP core-shell NWs grown by molecular beam epitaxy (MBE) and hybrid MBE-metal-organic vapor phase epitaxy on Si substrates. The emission characteristics of these NWs are measured either directly in free-standing geometry or after transfer in horizontal geometry by a specific micro photoluminescence (uPL) setup designed for the infrared spectral range. Both temperature and power-dependent measurements are performed highlighting the dynamics of the PL peak energy and intensities. The InGaAs NWs show a characteristic transition in PL peak energy with increasing Ga content and also with dominant wurtzite crystal phase [1]. In addition, we elucidate the effect of the InAsP shell thickness onto the intensity and near-band edge emission of InAs NWs. Furthermore, we present absorption measurements of homogeneous InGaAs NW arrays obtained with a UV/VIS/NIR setup. [1] S. Hertenberger, et al., Appl. Phys. Lett. 101, 043116 (2012).

HL 94.4 Fri 10:15 H13

Single core-shell GaAs/AlGaAs nanowires: a close look by near-field optical spectroscopy — •Alexander Senichev[1], Vadim Talalaev[1,2], Jörg Schilling[2], George Cirlin[3,4,5], and Peter Werner[1] — [1]Max-Planck-Institut, Halle, Germany — [2]Martin-Luther-Universität, ZIK "SiLi-nano", Halle, Germany — [3]A. F. Ioffe Physico-Technical Institute, St. Petersburg, Russia — [4]St. Petersburg Physics and Technology Center for Research and Education, St. Petersburg, Russia — [5]Institute for Analytical Instrumentation, St. Petersburg, Russia

We report on the growth and the study of optical properties of self-catalyzed GaAs/AlGaAs core-shell nanowires (NW). These GaAs/AlGaAs NWs were generated by molecular beam epitaxy. The presence of zincblende (ZB) and wurtzite (WZ) crystal phases in NW is discussed. We investigate a homogeneity of photoluminescence (PL) intensity along a NW and the appearing of features in PL spectra, corresponding to the exciton emission from ZB and WZ structure, with a high spatial resolution (< 200 nm). For this purpose a low-temperature near-field scanning optical microscope operating at a temperature 10 K inside a high vacuum chamber was applied. Selecting of specific NW allow us to get PL and transmission electron microscopy measurements of the same single NW. Preliminary measurements showed inhomogeneous PL intensity distribution along NW and presence of additional spectral line in vicinity of NW apex. For statistical analysis, other NWs from the same growth series are under investigation.

HL 94.5 Fri 10:30 H13

Acousto-electric control of exciton dynamics in GaAs/AlGaAs core-shell nanowires containing a single radial GaAs quantum well — •Matthias Weiss[1], Jörg Kinzel[1], Daniel Rudolph[2], Max Bichler[2], Gregor Koblmüller[2], Gerhard Abstreiter[2], Jonathan Finley[2], Achim Wixforth[1], and Hubert Krenner[1] — [1]Lehrstuhl für Experimentalphysik 1 / Universität Augsburg, 86159 Augsburg,Germany — [2]Walter Schottky Institut / TU München, 85748 Garching, Germany

Radio frequency (RF) surface acoustic waves (SAW) represent a versatile tool to control and manipulate charge and spin excitations in semiconductor quantum structures. Here, we analyze the influence of the dynamic electric field induced by a SAW on the optical emission of single semiconductor nanowires. The investigated NWs consist of a GaAs core and an AlGaAs shell containing a single 5nm wide radial GaAs quantum well (QW). The optical emission is studied by conventional, low-temperature micro-photoluminescence (μ-PL) spectroscopy in combination with a stroboscopic excitation. For both, the GaAs core and the radial QW, at high SAW power, we observe clear signatures of acousto-electric exciton dissociation and conveyance of electrons and holes. However, in an intermediate range of SAW amplitudes, we observe fingerprints of quantum dot (QD)-like emission centers within the narrow QW. These QD manifest themselves by several sharp spectral lines which exhibit dynamic spectral shifts. Moreover, we observe intensity oscillations being connected to the local acoustic phase, which was previously observed by embedded, planar QD structures.

HL 94.6 Fri 10:45 H13

Band structure and photoluminescence on silicon nanocrystals — •Prokop Hapala and Pavel Jelinek — Institute of Physics , Academy of Sciences of the Czech Republic, Cukrovarnická 10, Prague, 16253, Czech Republic

Since the first observation of photoluminescence in silicon nanocrystals (SiNCs) there is a debate whether the band structure theory is appropriate to make any statements about this kind of systems. While translational symmetry - the fundamental assumption of Bloch theorem - is violated, the only rigorous treatment would be considering SiNC as a molecule with molecular orbitals (MOs) instead of bands. On the other hand, in literature it is common practice to use band structure arguments, such as "(in-)direct band gap" to rationalize optical properties of NCs. We analyze band structure of up to 3nm SiNCs using Fourier transform of MOs obtained from DFT calculations. By this method we can rationalize effects of surface passivation (-OH, -CHO, -H, -CH3) and size (1.5-3nm) on optical properties of SiNCs.

HL 95: Spintronics/Quantum information: Vacancies in diamond and SiC (HL, jointly with TT)

Time: Friday 9:30–12:45 Location: H14

HL 95.1 Fri 9:30 H14

Optical detection of coherent electron spin states of vacancy defects in silicon carbide — •Sang-Yun Lee[1], Helmut Fedder[1], Torsten Rendler[1], Matthias Widmann[1], Nguyen Tien Son[2], Erik Janzén[2], and Jörg Wrachtrup[1] — [1]University of Stuttgart, Stuttgart, Germany — [2]Department of Physic, Chemistry and Biology, Linköping University, Linköping, Sweden

The diamond has been known as a hosting material in which an existing single spin system can be addressed optically at room temperature. A recent study has revealed that the individually detectible spin state can also exist in silicon carbide (SiC) [1]. However, the recent experimental finding has been done only on a newly found unknown defect in SiC. Among the other well known defects in SiC, the silicon vacancy (V_{Si}) can be another candidate because its coherent spin state has been successfully observed at room temperature with long life time by electron spin resonance [2], though the single spin detection is yet in question. While the conventional spin resonance method is suffered by the limited sensitivity, the optically detected magnetic resonance has been successfully used for the single spin detection. Thus the first step to elucidate whether this defect can be used as a room temperature solid state spin qubit, is to test the optical detection of its spin state at room temperature. We hereby report the optically detected spin coherence of the V_{Si} spin ensemble at room temperature. Our efforts on single spin detection will be presented too.

[1] W. F. Koehl, *et al.*, Nature 479, 84 (2011)
[2] V. A. Soltamov, *et al.*, Physical Review Letters 108, 226402 (2012)

HL 95.2 Fri 9:45 H14

Resonant addressing and manipulation of silicon vacancy spin qubits in silicon carbide — •Daniel Riedel[1], Franziska Fuchs[1], Hannes Kraus[1], Andreas Sperlich[1], Vladimir Dyakonov[1,2], Alexandra Soltamova[3], Vladimir Ilyin[4], Pavel Baranov[3], and Georgy Astakhov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, D-97074 Würzburg — [2]ZAE Bayern, D-97074 Würzburg — [3]Ioffe Physical-Technical Institute, St. Petersburg, RU-194021 Russia — [4]Saint Petersburg Electrotechnical University, St. Petersburg, RU-194021 Russia

Although several candidates have yielded feasible features for solid-state quantum information processing, there is a search for new systems with even higher potential [1].
We report that silicon vacancy (V_{Si}) defects in silicon carbide comprise the technological advantages of semiconductor quantum dots and the unique spin properties of nitrogen-vacancy defects in diamond.
Similar to atoms, the V_{Si} qubits can be controlled under the double radio-optical resonance conditions, allowing for selective addressing and manipulation [2]. Magnetic resonance techniques are used to clar-

ify the V_{Si} spin multiplicity and reveal a long spin memory.
Our results pave the way for potential applications of the V_{Si} defect in quantum information processing and spintronics.

References:
[1] D. DiVincenzo, Nature Materials 9, 468 (2010).
[2] D. Riedel et al., Physical Review Letters 109, 226402 (2012).

HL 95.3 Fri 10:00 H14

Intrinsic defects in silicon carbide LEDs as a perspective single photon source — •Franziska Fuchs[1], Victor Soltamov[2], Stefan Väth[1], Pavel Baranov[2], Eugeny Mokhov[2], Georgy Astakhov[1], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Ioffe Physical-Technical Institute, St. Petersburg, 194021 Russia — [3]ZAE Bayern, 97074 Würzburg

Single photon sources, reliably emitting on demand, are necessary for optical quantum computer architectures. Several systems seem suitable for this purpose, including atoms, molecules, quantum dots and colour centres in diamond. All these systems are difficult to implement, since they either only work at low temperatures, or do not emit at typical wavelengths used in existing telecommunication infrastructure. We suggest another system - silicon vacancy defects in silicon carbide, emitting photons in the near infrared [1]. We fabricated light emitting diodes based on intrinsic defects in silicon carbide. The room temperature electroluminescence reveals two strong emission bands in visible and NIR, the latter assigned to silicon vacancy defects. Our approach can be used to realize an electrically driven single photon source for quantum telecommunication.

[1]Riedel et al.: Resonant Addressing and Manipulation of Silicon Vacancy Qubits in Silicon Carbide, Phys. Rev. Lett.109,226402(2012)

HL 95.4 Fri 10:15 H14

A novel metastable spin triplet in diamond — •Matthias Widmann[1], Sang-Yun Lee[1], Helmut Fedder[1], Torsten Rendler[1], Moritz Eyer[1], Sen Yang[1], Petr Siyushev[1], Marcus Doherty[2], and Jörg Wrachtrup[1] — [1]3. Physikalisches Institut, University Stuttgart, Germany — [2]Laser Physics Center, National University, Canberra, Australia

In this talk a newly found, photo stable single spin center in a HTHP diamond nano-pillar, will be introduced. This new defect poses many properties, similar to those of the well-known NV-center in diamond. However, optically detected magnetic resonance showed positive contrast at room temperature in contrast to NV-centers. The photo physics and spin physics of this new defect have been studied to understand the enhancement of photon emission (contrast up to 45 %) at three different electron spin resonance frequencies. It will be shown that the defect contains a singlet ground-, and excited state, and a metastable spin 1 triplet state which act as a shelving state. The strong enhancement of photon emission by ESR can be attributed to the huge difference in the deshelving rates of each triplet states. It will be also shown that the coherent spin manipulation of the metastable triplet state is possible at room temperature. Even though the electron spin coherence time is limited by the life time of the triplet state (up to 2.5 μs), these findings suggest that the electron spin in this spin system can be used to read-out the coupled nuclear spin state because the nuclear spin can be protected during the initialization and storage processes thanks to the spin-less electron ground state.

HL 95.5 Fri 10:30 H14

Nuclear spin control with a transient electron spin ancilla — •Helmut Fedder[1], Sang-Yun Lee[1], Matthias Widman[1], Torsten Rendler[1], Moritz Eyer[1], Sen Yang[1], Petr Siyushev[1], Marcus Doherty[2], Neil Manson[2], and Jörg Wrachtrup[1] — [1]3. Physikalisches Institut and Research Center SCoPE, University Stuttgart, Germany — [2]Laser Physics Center, Research School of Physics and Engineering, Australian National University, Canberra, Australia

Electron spins associated with point defects in crystals are promising systems for solid state quantum technology [1-3]. In particular, defects with a spin-less ground state and an excited triplet state have been proposed as universal ancillae for addressing nuclear spins [2]. In here we demonstrate the control of an individual ^{13}C lattice nuclear spin in diamond by exploiting a hitherto unknown electron spin defect that features an excited triplet state. Using optical and microwave control, we demonstrate coherent manipulation of the triplet electron spin and characterize its photo-physics. We then show coherent manipulation of the nuclear spin in the spin-less electronic ground state.

[1] J.J.L. Morton et al. Solid-state quantum memory using the 31P nuclear spin. Nature 455, 1085 (2008).
[2] V. Filidou et al. Ultrafast entangling gates between nuclear spins using photoexcited triplet states. Nature Phys. 8, 596 (2012).
[3] P.C. Maurer et al. Room-Temperature Quantum Bit Memory Exceeding One Second. Science 336, 1283 (2012).

HL 95.6 Fri 10:45 H14

Entanglement by measurement and Bell inequality violation with spins in diamond — •Wolfgang Pfaff[1], Tim H. Taminiau[1], Lucio Robledo[1], Hannes Bernien[1], Matthew Markham[2], Daniel J. Twitchen[2], and Ronald Hanson[1] — [1]Kavli Institute of Nanoscience Delft, Delft University of Technology, Netherlands — [2]Element Six, Ltd., Ascot, UK

Single spins in diamond have emerged as a promising platform for quantum information processing in the solid state. In particular, individual nuclear spins coupled to nitrogen-vacancy (NV) centers have been recognized as excellent candidates for solid state qubits, because they combine outstanding stability, excellent control by spin resonance techniques, and high-fidelity optical initialization and readout provided by the NV center.

Here we report the achievement of a milestone towards quantum computation with spins: The creation of high quality quantum entanglement between two nuclear spins in diamond. Entanglement is an important resource for quantum computation and lies at the heart of many key quantum protocols, such as teleportation and error correction. We show that we can produce entangled states of high fidelity using a projective quantum measurement. Our technique is non-destructive, and thus leaves the quantum information that is required for further computation unharmed. This enables us to demonstrate a violation of Bell's inequality for the first time with spins in the solid state.

Ref: Pfaff et al., Nature Phys., doi:10.1038/nphys2444 (2012).

Coffee break

HL 95.7 Fri 11:15 H14

Spin polarisation mechanism in nitrogen-vacancy and related colour centres of diamond — Lachlan Rogers[1], Neil Manson[2], and •Fedor Jelezko[1] — [1]Institut für Quantenoptik, Universität Ulm, Ulm, Deutschland — [2]Laser Physics Centre, Australian National University, Canberra, Australia

Optically induced spon polarisation of the negatively charged nitrogen vacancy centre in diamond (NV^-) has been known for a considerable time but there has not been a satisfactory account of how it arises. This lack of explanation is of concern because spin polarisation is the key unique property that allows the centre to function as a room temperature qubit. An optical emission band with ZPL at 1042 nm is understood to arise from a transition between spin-singlet levels which lie between the triplet ground and excited states. We report properties of the singlet levels obtained using spectroscopic techniques on the 1042 nm band. Importantly, we resolve the long-standing uncertainty over the order of these singlets. This improved understanding of the singlet system leads to a tentative description of the physical mechanism for spin polarisation in the NV^- centre.

This raises the tantalising possibility of engineering "designer" colour centres for specific applications. For instance, the neutral NV^0 centre is known to have a metastable level between its ground and excited states. Manipulating it to open the intersystem crossing from this level back to the ground state would likely give rise to optically induced spin polarisation, opening a second solid-state optically-controlled qubit in diamond.

HL 95.8 Fri 11:30 H14

Detecting and Polarizing Nuclear Spins in Diamond — •Jochen Scheuer[1], Paz London[2], Jianming Cai[3], Ilai Schwarz[3], Alex Retzker[4], Martin B. Plenio[3], Masayuki Katagiri[5,6], Tokuyuki Teraji[6], Satoshi Koizumi[6], Junichi Isoya[5], Ran Fischer[2], Liam McGuinness[1], Boris Naydenov[1], and Fedor Jelezko[1] — [1]Institut für Quantenoptik, Universität Ulm, Ulm, Germany — [2]Department of Physics, Technion, Israel Institute of Technology, Haifa, Israel — [3]Institut für Theoretische Physik, Universität Ulm, Ulm, Germany — [4]Racah Institute of Physics, The Hebrew University of Jerusalem, Jerusalem, Israel — [5]Graduate School of Library, Information and Media Studies, University of Tsukuba, 1-2 Kasuga,

Tsukuba, Ibaraki, Japan — [6]National Institute for Materials Science, Tsukuba, Ibaraki, Japan

Control and measurement of nuclear spins is essential for medicine, chemistry and physics, but the sensitivity of conventional measurement schemes is limited due to low thermal polarization of nuclei under ambient conditions. We use an electron-nuclear double resonance technique, known as Hartmann-Hahn double resonance, to demonstrate experimentally polarization of single and multiple nuclear spins in a room temperature solid. By transferring polarization from an optically cooled electron spin associated with the nitrogen-vacancy (NV) defect, to carbon nuclei we are able to control spin bath dynamics. This work opens new possibilities for different fields of science, from control over decoherence and use of mesoscopic ensemble of nuclear spins as qubits to enhancement of contrast in magnetic resonance imaging.

HL 95.9 Fri 11:45 H14

Tailoring the Diamond: Microwave structures surrounding nano-fabricated solid immersion lenses registered to single emitters in diamond on demand — •Luca Marseglia[1], Florian Striebel[1], Andreas Häussler[1], Boris Naydenov[1], Jan Meijer[2], and Fedor Jelezko[1] — [1]Institut für Quantenoptik, Universität Ulm, Albert-Einstein-Allee 11, 89081 Ulm - Germany — [2]Ruhr-Universität Bochum, Universitätsstraße 150, 44801, Bochum, Germany.

The negatively charged Nitrogen Vacancy color center (NV) is a spin active defect with a long spin lifetime at room temperature. It is a three level system whose value of the ground state spin can be driven by applying a small microwave field making a NV centre a good candidate as qubit for quantum information purpose. To exploit the splitting of the ground state of the NV the control and the precision of a microwave field applied on a single NV is crucial. So we have successfully coupled the NV to a microwave structures, made of metal, lithographically deposited on the diamond, applying high intensity microwave field improving the addressing of the spin and the driving of the Rabi oscillation of the NV. Besides to directly improve the coupling efficiency from a planar surface we formerly developed a technique to fabricate solid immersion lenses (SILs), using Focus Ion Beam (FIB) system, who geometrically avoid any refraction at the diamond-air interface. Eventually we will create a microwave structure, placed precisely on the nanofabricated SIL coupled to the colour centre. These integrated structures will allow us to handle the spin of the NV centre with very high precision and microwave field intensity.

HL 95.10 Fri 12:00 H14

Coherent Control of a ^{13}C NV$^-$ center — •Burkhard Scharfenberger[1], William J. Munro[2], and Kae Nemoto[1] — [1]National Institute of Informatics, 2-1-2 Hitotsubashi, Chiyoda-ku, Tokyo 101-8430, Japan — [2]NTT Basic Research Laboratories, NTT Corporation, 3-1 Morinosato Wakamiya, Atsugi, Kanagawa 243-0198, Japan

We investigate the theoretically achievable fidelities for coherently controlling an effective three qubit system consisting of a negatively charged NV center in diamond coupling via an hyperfine interaction to one nearby ^{13}C nuclear spin using only micro- and radio wave pulses. With its long coherence times and comparatively simple optical accessibility, already the 'bare' NV$^-$ center has an interesting potential in quantum computing related applications. Although a number of experiments have already been conducted using NV centers with one or more ^{13}C nearby, fidelities achieved are limited not only by experimental inaccuracies but a lack of theoretical understanding of the system dynamics. We seek to redress this by fully modelling the NVC systems behaviour in the ground state manifold, including all hyperfine interactions (between N and V as well as C and V) and dissipation where parameters are taken from previous experimental work as well as theoretical ab-initio studies. We show that for close-by carbons, the strong hyperfine interaction leads to unwanted mixing of levels which ultimately limits fidelities in single-qubit driving and entanglement generation to less than 99% in the experimentally interesting weak magnetic fields regime.

HL 95.11 Fri 12:15 H14

Resolving individual spin defects in diamond beyond the diffraction limit by exploiting their charge state dynamics — •Nabeel Aslam, Matthias Pfender, Gerald Waldherr, Philipp Neumann, and Jörg Wrachtrup — 3. Physikalisches Institut, Universität Stuttgart, Germany

The nitrogen-vacancy center in diamond is an electron and nuclear spin system that shows exceptionally good coherence properties at room temperature. This makes it a promising system for the implementation of quantum information processing. Furthermore the ability to sense magnetic and electric fields on the nanometer scale has been demonstrated for NV defects. Individual spin detection and initialization is performed optically by a confocal microscope which fails in resolving individual defects with a distance smaller than the diffraction limit. Here we demonstrate a novel microscopy method that is able to exploit the stochastically switching between different charge states achieving resolutions of 10 nm, well below the diffraction barrier. Compared with targeted switching based methods like STED this method applies at least five magnitudes lower laser power for a certain resolution. This is in fact a great improvement for the future use of nanodiamonds as biomarkers in cells with nanometer resolution. Even better resolutions can be achieved by combining this method with spin state manipulation.

HL 95.12 Fri 12:30 H14

Investigations on nitrogen-vancancy center creation and its physical properties — •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

The negatively charged nitrogen-vacancy (NV$^-$) center embedded in extended and nanoscale diamond structures is a promising candidate for quantum information processing (QIP), magnetometry and even for biomarkers. A basic requirement for these applications is a precise prediction of the placement and a detailed understanding of the physical properties of the NV$^-$ center. Using a range of simulation techniques we consider the formation of NV$^-$ centers from the statistical standpoint, before performing accurate calculations for the optical properties of individual NV$^-$ centers. In particular, we investigate the channeling effect during shallow implantations in molecular dynamics and Monte Carlo simulations. Furthermore, a combination of a spin-polarized atomic effective pseudopotential and a configuration interaction approache is used to obtain many body effects in the excitonic spectra.

HL 96: GaN: Growth and doping

Time: Friday 9:30–12:15 Location: H15

HL 96.1 Fri 9:30 H15

Dependence of band gap bowing of epitaxial $In_xGa_{1-x}N$ on composition, strain and ordering effects by first-principles calculations — •Ying Cui, Sangheon Lee, Gerard Leyson, Christoph Freysoldt, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40627 Düsseldorf

The band gap of $In_xGa_{1-x}N$ alloys does not only depend on the In composition, but also on the strain state and the ordering of In atoms. We performed a theoretical study to disentangle the different effects. According to our results, the band gaps of $In_xGa_{1-x}N$ alloys show parabolic behavior in compressive regions and linear dependence in the tensile regions. We further find a universal bowing behavior in $In_xGa_{1-x}N$ alloys for the whole In content range under constant relative strain. Inhomogeneous In distributions lead to a narrower band gap, but are energetically unfavorable. Based on the calculated results, an interpolating form for the band bap as a function of ordering, biaxial strain and chemical content for $In_xGa_{1-x}N$ alloys is suggested. Our results provide guidance to determine the band gaps of $In_xGa_{1-x}N$ alloys under real experiment conditions.

HL 96.2 Fri 9:45 H15

Ordering phenomena in $In_xGa_{1-x}N$ grown epitaxially on GaN(0001) — •Sangheon Lee, Christoph Freysoldt, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40627 Düsseldorf

The spatial distribution of In in $In_xGa_{1-x}N$ epitaxial layers attract much attention, as In compositional fluctuations are often invoked to explain the realization of the high-efficiency blue light-emitting diodes ($x \simeq 0.15$) despite the large number of threading dislocations. However, the mechanisms determining the spatial distribution of In in the fully grown $In_xGa_{1-x}N$ epitaxial layers are not well understood. We therefore developed an effective crystal growth modeling technique that combines a semi-grand-canonical Monte Carlo simulation with an *ab-initio* parameterized empirical force field. We elucidate local strain effects on the spatial distribution of In in coherent $In_xGa_{1-x}N$ grown epitaxially on GaN(0001), with particular attention to the effect of the surface. In particular, we observe a strong tendency towards ordering in $In_xGa_{1-x}N$ of $x < 0.33$, resulting in a stack of $\sqrt{3} \times \sqrt{3}$ patterned InGaN monolayers. The effect of temperature on the ordering and thermodynamics is discussed, revealing that the ordering phenomena persists at real growth temperatures. The ordering phenomena are identified as a key factor that determines characteristic In compositional fluctuations in $In_xGa_{1-x}N$ epitaxial layers with varying total indium contents.

HL 96.3 Fri 10:00 H15

Island nucleation during double pulsed growth of InN with RF-MBE — •Andreas Kraus, Uwe Rossow, Heiko Bremers, and Andreas Hangleiter — Institut für Angewandte Physik, Technische Universität Braunschweig

Although InN is predicted to have outstanding material properties the data obtained experimentally are more or less disappointing. In particular the carrier mobility is much lower than predicted. Since the growth of InN is very difficult, this discrepancy is most likely due to the low quality of the investigated material. Recently, the quality of MBE-grown InN has been improved by applying pulsed source fluxes. In our recent work we presented a double-pulsed growth method, where periodically the equivalent of less than one monolayer In is followed by a distinct time of nitridation. With this method a surface morphology made of huge and atomically flat grains (≈ 2 μm in diameter) was achieved.

To get a deeper understanding of this growth behavior a series of samples with various numbers of periods was grown. The growth was monitored in-situ by reflection high energy electron diffraction and by optical reflectometry. Ex-situ the samples were characterized by atomic force microscopy, scanning electron microscopy and high resolution X-ray diffraction.

At small period numbers only little islands with dendritic features at their boundaries are visible. These grains evolve to the huge ones that were observed previously. If the period number is large enough that the grains meet each other, they coalesce to a closed surface.

HL 96.4 Fri 10:15 H15

MBE growth and characterization of AlN and $Al_xGa_{1-x}N$ with various x. — •Christopher Hein[1], Andreas Kraus[1], Heiko Bremers[1], Uwe Rossow[1], Kamran Forghani[2], Ferdinand Scholz[2], and Andreas Hangleiter[1] — [1]Institut für Angewandte Physik, TU-Braunschweig, Germany — [2]Institut für Optoelektronik, Universität Ulm, Germany

Devices based on AlN have gained interest owing to their potential in optoelectronic devices, namely fast detectors, and as a starting material for GaN quantum dot growth. Our experiments include Riber 32P PA-MBE grown AlN layers and $Al_xGa_{1-x}N$/GaN MQW's. The samples were grown on MOVPE AlN and GaN templates. They were characterized in-situ using RHEED and an infrared reflectometry setup for thickness analysis. XRD measurements served as ex-situ determination of the structural quality and the composition of our MQW's. The growth temperature behaviour of $Al_xGa_{1-x}N$ was investigated with a series of samples in the range of 700 to 850°C. The surface morphology was investigated using SEM and AFM. We found that for optimized Al fluxes in the nucleation layer, the epilayer surface morphology could be improved. Two growth modes have been investigated, the continuous mode which can easily lead to droplet formation and a metal pulsed method which further increases the possible Al/N flux ratio before droplet formation. We also discuss XRD analysis and UV-PL studies of our MQW samples.

HL 96.5 Fri 10:30 H15

InGaN quantum wells grown on 2" semipolar GaN — •Tobias Meisch[1], Sabine Schörner[2], Junjun Wang[1], Klaus Thonke[2], and Ferdinand Scholz[1] — [1]Institut für Optoelektronik, Universität Ulm, 89081 Ulm — [2]Institut für Quantenmaterie, Arbeitsgruppe Halbleiterphysik, Universität Ulm, 89081 Ulm

We have grown high quality (10-11) GaN and (11-22) GaN on (11-23) and (10-12) patterned sapphire respectively. The patterning of the substrate was done by reactive ion etching to produce periodic trenches about 1.5 μ m deep and 1.5 μm wide, revealing a c-plane-like facet on one side. All other facets are subsequently covered with SiO2 to inhibit epitaxial growth. In the following MOVPE process, GaN nucleates on this unmasked side facet, grows out of the trench and forms a coalesced semipolar surface. By decreasing the trench depth to 400 nm, we could reduce the RMS of the surface roughness by about a factor of two. First experiments on depositing InGaN quantum wells on the homogeneous GaN surface show much lower indium incorporation on the (11-22) plane as compared to the conventional c-plane. However, by a substantial increase of the indium flux, the QW emission could be shifted to 520 nm. Using comparable growth conditions, QWs on (10-11) GaN show an emission wavelength of 482 nm and a much higher intensity.

Coffee break

HL 96.6 Fri 11:00 H15

Towards identification of the shallow donor oxygen in AlN photoluminescence spectra — •Martin Feneberg[1], Benjamin Neuschl[2], Klaus Thonke[2], Matthias Bickermann[3], and Rüdiger Goldhahn[1] — [1]Abt. Materialphysik, Inst. für Exp. Physik, Otto-von-Guericke-Universität Magdeburg — [2]Gruppe Halbleiterphysik, Inst. für Quantenmaterie, Universität Ulm — [3]Leibniz-Institut für Kristallzüchtung, Berlin

In photoluminescence spectra of wurtzite AlN, several bound exciton emission bands can be observed. Recently, one of them could be identified as being related to substitutional silicon on aluminum site [1]. In this study, we present a correlation of secondary ion mass spectroscopy and photoluminescence at liquid helium temperature of a variety of AlN single crystals. From our analysis we tentatively assign a bound exciton line as being related to substitutional oxygen on nitrogen site. For this defect, DX center formation is expected, what is discussed in light of our experimental findings.

[1] B. Neuschl, et al. Phys. Stat. Sol. B 249, 511 (2012).

HL 96.7 Fri 11:15 H15

Activation of a new europium center in Europium-implanted GaN by both Mg and Si codoping — •Jayanta Kumar Mishra[1], Torsten Langer[1], Uwe Rossow[1], Stepan Shvarkov[2], Andreas Wieck[2], and Andreas Hangleiter[1] — [1]Institut für Angewandte Physik, TU Braunschweig — [2]Angewandte Festkförperphysik,Ruhr-Universitfät Bochum, Germany

Rare earth ions implanted into GaN are promising for optoelectronic applications. They show luminescence in the visible range while the luminescence from this material system is sharper as well as independent of temperature due to intra 4f transition of rare earth ions. To improve the emission efficiency we implanted Europium in GaN codoped with Mg at dose range from $10^9 cm^{-2}$ to $10^{14} cm^{-2}$ with an energy of 100 keV. The red emission from $^5D_0 \rightarrow ^7F_2$ of europium was remarkably enhanced by Mg codoping. It further enhances by both Mg and Si codoping. The typical Eu^{3+} luminescence in GaN at 2.000 eV (620 nm) is not found to be dominant. A new peak which is already present in europium-implanted Mg-doped GaN at 2.0047 eV (618.9 nm) is enhanced about ten times. This peak is found to be more than three times more intense than the typical 620 nm line of Mg-doped GaN:Eu. A new site dominates in the spectrum especially in the $^5D_0 \rightarrow ^7F_2$ transition range which is different from the sites present in undoped GaN:Eu. The excitation process of europium ions is proposed to take place through a donor-acceptor pair related energy transfer mechanism.

HL 96.8 Fri 11:30 H15

Nonradiative recombination due to Ar implantation induced point defects in GaInN/GaN quantum wells — •Torsten Langer[1], Hans-Georg Pietscher[1], Holger Jönen[1], Uwe Rossow[1], Heiko Bremers[1], Dirk Menzel[2], and Andreas Hangleiter[1] — [1]Institut für Angewandte Physik, Technische Universität Braunschweig — [2]Institut für Physik der Kondensierten Materie, Technische Universität Braunschweig

We quantitatively investigate nonradiative recombination at point defects via temperature dependent time-resolved photoluminescence spectroscopy on argon implanted MOVPE-grown GaInN/GaN sin-

gle quantum wells (QW). An implantation dose dependent (doses: 10^{11} cm^{-2} - 10^{13} cm^{-2}) reduction of nonradiative lifetimes from several nanoseconds (unimplanted sample) to less than 100 ps at room temperature is observed. This shortening of nonradiative lifetimes is attributed to nonradiative recombination due to increased implantation induced defect densities. An effective hole capture coefficient can be estimated to about 10^9 cm^3s^{-1} via the measured nonradiative lifetimes and simulated (SRIM) defect densities. The thermal stability of the defects is analyzed using rapid thermal annealing at 800°C in order to recover the crystal from implantation damage. At high temperatures, nonradiative recombination in the barriers becomes dominant: defect density dependent losses with an activation energy equal to half the difference between the GaN band gap and the peak position of the QW luminescence are observed.

HL 96.9 Fri 11:45 H15

Influence of Si- and Ge-doping on the properties of AlGaN layers — •Christoph Berger, Hartmut Witte, Armin Dadgar, Jürgen Bläsing, Peter Veit, Annette Diez, and Alois Krost — Otto-von-Guericke-Universität Magdeburg, Institut für Experimentelle Physik, Magdeburg

We investigate n-doping of $Al_{0.2}Ga_{0.8}$ layers using silane and germane as dopants. For this purpose doped AlGaN films with thicknesses of about 400 nm were grown on an undoped $Al_{0.2}Ga_{0.8}$-buffer. With both dopant sources, it was possible to achieve electron concentrations of nearly 10^{20} cm^{-3} as determined by Hall-effect measurements. However, when doping was applied, an increase in tensile stress was observed by means of in-situ curvature measurements. This effect becomes more pronounced at higher dopant fluxes and higher dislocation densities of the buffer. For Si-doping this effect is similar to GaN, where Si-doping is known to lead to dislocation climb. On the contrary, it can be shown that for Ge-doping the tensile stress is caused by a change in alloy composition as determined by X-ray diffraction. With higher Ge-fluxes, the Al-concentration of the film increases, consequently the Ge-doped film grows tensely strained on the buffer. Interestingly, the influence on the composition also depends on the dislocation density.

HL 96.10 Fri 12:00 H15

Optical properties of highly Ge doped GaN — •Christian Nenstiel[1], Max Bügler[1], Stephanie Fritze[2], Armin Dadgar[2], Hartmut Witte[2], Antje Rohrbeck[2], Jürgen Bläsing[2], Gordon Callsen[1], Alois Krost[2], and Axel Hoffmann[1] — [1]Institut für Festkörperphysik, TU-Berlin, Hardenbergstrasse 35, 10623 Berlin, Germany — [2]Institut für Experimentelle Physik, Fakultät für Naturwissenschaften

In this contribution a systematic study of highly doped GaN:Ge is presented and compared to highly doped GaN:Si. The samples were grown by MOVPE on sapphire substrates. All samples consist of AlN/AlGaN seed followed by an undoped GaN buffer layer. Subsequently, an approximately 700 nm thick doped layer was grown. The doping has been varied resulting in a variation of free carrier concentration from 8 x 10^17 to 1.9 x 10^20 cm^-3 measured by Hall-effect. The X-Ray Diffraction and Raman measurements show a high structural quality and homogeneous incorporation of Ge even at the highest doping concentration. On the Nomarski microscopy images is a smooth surface visible with just a small amount of pits. The Photoluminescence data at 7K shows a strong broadening and blue shift of the luminescence with increasing Ge content, additionally the luminescence decay time increases. The results demonstrate that free carrier concentrations up to 1.9 x 10^20 c^m-3 are achievable with Ge doping maintaining a high crystal quality.

HL 97: ZnO

Time: Friday 9:30–12:30 Location: H16

HL 97.1 Fri 9:30 H16

Controlled Growth of ZnO Nanowires from Thermal CVD - The Role of Carrier Gas Flow and Species Diffusion — •Andreas Menzel[1], Raye Goldberg[2], Guy Bursthetin[2], Victor Lumelsky[2], Kittitat Subannajui[1], Yeshayahu Lifshitz[2], and Margit Zacharias[1] — [1]Laboratory for Nanotechnology, IMTEK - Department of Microsystems Engineering, University of Freiburg, Freiburg, Germany — [2]Faculty of Materials Engineering and Russel Berrie Nanotechnology Institute, Technion Israel Institute of Technology, Haifa 32000, Israel

Nanowires (NWs) are promising materials for future electronics, optics and sensor device applications. Typically, ZnO NWs are grown in a tube furnace which includes that the respective material necessary for the desired NW materials is evaporated and transported toward a substrate. Hence evaporation efficiency, diffusion and gas flow are mandatory for a successful growth. When the transported species approaches the substrate nucleation, diffusion and growths occurs. A huge amount of work reports about growth of NWs by thermal CVD, however, the role and influence of growth parameters still remains unclear. Different parameters, geometries (diameters, inner and outer tube configurations etc.) as well as growth parameters (temperature, carrier gas and pressure) are reported, but cannot really be compared. We systematically studied and simulated the distribution of the growth species in such tube processes combined with growth experiments and evaluate their effects on the NW growth. Diffusion and convection can be tuned in a controlled way to achieve balanced steady growth conditions.

HL 97.2 Fri 9:45 H16

Growth of ZnO nanowires for sensor applications — •Manfred Madel, Felix Senf, Teresa Baur, Martin Dickel, Simon Berke, Sebastian Bauer, Ingo Tischer, Benjamin Neuschl, Uwe Röder, and Klaus Thonke — Institut für Quantenmaterie / Gruppe Halbleiterphysik, Universität Ulm

ZnO nanowires with average diameter of 50 nm and length up to 10 μm were grown by chemical vapour deposition and reveal suitability for sensor applications due to a large surface to volume ratio. Good crystal quality and excellent structural definition is shown by scanning electron microscopy, X-ray diffraction as well as by photo- and cathodoluminescence measurements. Photoconductivity measurements were performend either by direct contacting single pillars via a conductive atomic force microscope tip, or using interdigital structures, on which the wires were aligned by a dielectrophoresis method. The wires show a high sensitivity to light with a threshold for persistent photoconductivity of around 2.8 eV. Optical readout with a micro-PL setup shows a clear change of the signal intensity in different gas ambient atmospheres.

HL 97.3 Fri 10:00 H16

Atomistic simulations of organic/ZnO hybrid nanowires — •Adriel Domínguez, Svea grosse Holthaus, Andreia da Rosa, and Thomas Frauenheim — Bremen Center for Computational Materials Science, University of Bremen, Am Fallturm 1, 28359, Bremen, Germany

The understanding of the interaction of organic species with inorganic surfaces and nanostructures constitutes an important step in the development of semiconductor hybrid devices such as solar cells and biosensors. Density functional theory has been employed to investigate the atomic and electronic structure of ZnO nanowires modified with glycine and substituted methane molecules. We have identified -COOH, -NH2, -PO(OH)2 and -SH as suitable anchoring groups for binding to the ZnO nanowires[1-3]. We have found three relevant mechanisms acting on the interface stabilisation: passivation of surface oxygen lone-pairs via dissociative chemisorption processes, electrostatic adsorbate-interaction involving Zn surface sites and hydrogen bonding involving adsorbates and oxygen surface sites. We will further discuss the role of water and hydroxyl groups on the adsorption mode and stabilisation of these functional groups[4].

References: [1] N. H. Moreira, A. L. da Rosa, Th. Frauenheim, Appl. Phys. Lett. 94, 193109 (2009). [2] N. H. Moreira, A. Dominguez, Th. Frauenheim, and A. L. da Rosa, Phys. Chem. Chem. Phys. 14, 15445 (2012). [3] X. Q. Shi, H. Xu, M. A. van Hove, N. H. Moreira, A. L. da Rosa and Th. Frauenheim, Surf. Sci. 606,289 (2012). [4] A. Dominguez, S. grosse Holthaus, A. L da Rosa and Th. Frauenheim, to be submitted.

HL 97.4 Fri 10:15 H16

Electrical and optical properties of room temperature deposited zinc tin oxide thin films and utilisation in all oxide amorphous heterodiodes — •Peter Schlupp, Friedrich Leonard Schein, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Germany

To provide cost-efficient and homogeneous oxide thin films it is desirable to use amorphous materials which can be deposited at room temperature (RT). Zinc tin oxide (ZTO) is a promising n-type channel material and is in contrast to the well explored amorphous transparent semiconducting oxide GaInZnO indium-free and with that less expensive. We present electrical and optical properties of RT-deposited ZTO thin films. The films were fabricated via pulsed laser deposition on glass substrates from an 1:2 $ZnO : SnO_2$ target. The background gas (O_2, N_2 or Ar) pressure was varied systematically from $3 * 10^{-4}$mbar to 0.1mbar. The resistivity can be tuned over several orders of magnitude, from insulating for high and low pressures down to $1.7 * 10^{-4}\Omega$m for intermediate pressure. All films investigated are X-ray amorphous. In the visible spectral range (400-800nm wavelength) the optical transmission is about $T_{vis} = 40 - 85\%$, depending on the fabrication partial pressure. Optimized ZTO layers were used to fabricate an all amorphous pin heterodiode consiting of $ZnCo_2O_4$ and ZTO. The rectification of the device is about $6 * 10^3$ at $U = \pm 1$V at RT. Further, temperature-dependent I-U characteristics will be discussed.

HL 97.5 Fri 10:30 H16

The role of the surface in resonance Raman scattering in ZnO and other wurtzites — •Christian Kranert, Rüdiger Schmidt-Grund, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Semiconductor Physics Group, Leipzig, Germany

We apply the double resonance model of R. M. Martin [1] to the resonance Raman scattering by longitudinal optical (LO) phonons in ZnO, excited well above the band gap ($\lambda = 325\,\mathrm{nm}$). By extending this model with an elastic scattering process at the surface, we provide an improved understanding of the physical background and the spectral properties of the 1LO line. The consideration of the surface-related process, additionally to the well-established elastic scattering by point defects, is essential to conclusively explain several experimental findings. Particularly, the dependence of the peak position on the orientation of the excited surface cannot be understood otherwise. It was previously attributed to the varying wave vectors of the incident and scattered light in the literature which we will disprove theoretically and experimentally. We will present similar experimental results for other wurtzites (GaN, InN, CdS) which show the general validity of this extended model.

[1] R. M. Martin, Phys. Rev. B **10**, 2620 (1974)

Coffee break

HL 97.6 Fri 11:00 H16

Raman scattering of H_2 in ZnO — •Sandro G. Koch, Edward V. Lavrov, and Jörg Weber — Technische Universität Dresden, 01062 Dresden, Germany

ZnO single crystals thermally treated in a H_2, D_2, or $H_2 + D_2$ ambient at 800–1000 °C are studied by Raman scattering. Directly after the treatment most hydrogen forms shallow donors at the bond-centered site. Subsequently, interstitial hydrogen migrates through the lattice and forms electrically inactive H_2. The formation process, thermal stability, interaction with the phonon spectrum, position of the molecule in the host lattice, as well as the ortho-para conversion rate are addressed in this study. It is shown that H_2 in ZnO is almost a free rotator, which is stable in the temperature range 300–600 °C. Arguments are presented that the molecule occupies an interstitial lattice site. It is also shown that at elevated temperatures the para species is absent in Raman spectra, which is explained by thermally activated excitation of the molecule from the $J = 0$ to the $J = 2$ rotational state and phonon broadening of the spectral line associated with $J = 2$.

HL 97.7 Fri 11:15 H16

PLE of ZnO/(Zn,Mg)O quantum well structures on sapphire — •Axel Römer, Markus Wagner, Christian Nenstiel, Gordon Callsen, Max Bügler, and Axel Hoffmann — Technische Universität, Berlin, Germany

In this work ZnO/(Zn,Mn)O multiquantum-well structures are investigated. Through optical characterisation methods we examined the recombination dynamics and luminescence of different samples. Variation of crystal orientation and quantum well thickness in different samples leads to investigation of the dependence of the recombination behaviour of the material system on the quantum well structure and as well of the orientation of the crystal of the samples. Through the measurements it was cleared out which processes take part in the luminescence, whereas the main luminescence of the quantum well was focused on. Further more the samples were investigated with photoluminescence excitation spectroscopy (PLE). Not only the different processes could be observed, it was also possible to examine the excitation channels of those processes. With additional variation of polarisation and temperature through the PLE measurements it is possible to see more interesting details in the recombination dynamics until up to 4eV and get further information about those processes.

HL 97.8 Fri 11:30 H16

Ion-induced luminescence of radiation defects in ZnO — •Ronald Stübner[1], Jörg Weber[1], Daniel Severin[2], and Markus Bender[2] — [1]Technische Universität Dresden, Germany — [2]Gesellschaft für Schwerionenforschung, Darmstadt, Germany

A study of ion-induced luminescence of ZnO at low temperatures is presented. Based on the distinct difference between photo- and ion-induced luminescence spectra, it is concluded that the ion-induced luminescence results from excitonic recombinations at irradiation induced native defects. By comparison of the properties of the observed luminescence features with the data known from the literature, these features are assigned to the so far unidentified I_{10} defect (3.353 eV). The zinc interstitial is suggested as the possible origin of the I_{10} line.

HL 97.9 Fri 11:45 H16

Irradiation studies on differently orientated ZnO thin films — •Florian Schmidt[1], Holger von Wenckstern[1], Stefan Müller[1], Daniel Spemann[2], and Marius Grundmann[1] — [1]Universität Leipzig, Institut für Experimentelle Physik II, Abteilung Halbleiterphysik, Linnéstraße 5, 04103 Leipzig — [2]Universität Leipzig, Institut für Experimentelle Physik II, Abteilung Nukleare Festkörperphysik, Linnéstraße 5, 04103 Leipzig

Zinc oxide (ZnO) is a wide-bandgap semiconductor which is known for its high radiation hardness. The influence of proton bombardment on the incorporation of defects in $\pm c$-oriented ZnO bulk crystals [1] and thin films [2] has been reported previously, no data are available regarding the exposure of differently orientated ZnO to protons. The orientation of the thin films is predetermined by the orientation of the sapphire substrates. We grew *c*-, *a*-, and *m*-plane ZnO thin films on *a*-, *r*-, *m*-plane sapphire, respectively, by pulsed laser deposition. To study the effect of radiation, the films were irradiated by 2.25 MeV protons with fluences ranging from $1 \times 10^{13}\,\mathrm{cm}^{-2}$ to $2 \times 10^{14}\,\mathrm{cm}^{-2}$ and characterized by means of *C-V* measurements, deep level transient spectroscopy (DLTS) and Laplace DLTS.

Proton irradiation generates a deep-level, labelled E4 in the literature [3], which was tentatively assigned to the oxygen vacancy. The generation rate of this defect in the ZnO thin films was determined.

[1] F. D. Auret *et al.*, Appl. Phys. Lett., **79**(19), 3074 (2001).
[2] F. Schmidt *et al.*, Appl. Phys. Lett. **101**, 012103 (2012).
[3] T. Frank *et al.*, Appl. Phys. A **88**, 141 (2007).

HL 97.10 Fri 12:00 H16

Iron-induced gap states in ZnO thin films — •Rainer Pickenhain[1], Florian Schmidt[1], Sebastian Geburt[2], Carsten Ronning[2], Holger von Wenckstern[1], and Marius Grundmann[1] — [1]Universität Leipzig, Institut für Experimentelle Physik II, Abteilung Halbleiterphysik, Linnéstraße 5, 04103 Leipzig — [2]Institute for Solid State Physics, University of Jena, Helmholtzweg 3, D-07743 Jena

States of the transition metal iron within the bandgap of ZnO are not satisfyingly understood yet. Experimental evidence concerning internal transitions at about 1.8 eV [1] and 0.4 eV [2], respectively, of iron in Fe^{3+} and Fe^{2+} configuration exist. A concise experimental determination of the energetic position of these states within the bandgap was, however, not accomplished. In this study we present results on a ZnO thin film that was iron-implanted with a total fluence of 2×10^{11} ions/cm^2. Due to the implantation/annealing process the net doping density decreased from $8 \times 10^{16}\,\mathrm{cm}^{-3}$ to $1 \times 10^{16}\,\mathrm{cm}^{-3}$. By employing low-rate optical deep level transient spectroscopy (LR-ODLTS) we were able to detect two formerly not discovered states in the ZnO bandgap which we attribute to the incorporation of iron on zinc lattice site. These states lie at room temperature about 150 meV over the ZnO valenceband and 2200 meV below the ZnO conduction band minimum.

Temperature-dependent measurements reveal that transition energies of these states increase similar to the ZnO bandgap down to 4 K.

[1] R. Heitz *et al.*, Phys. Rev. B, **45**, 8977 (1992).
[2] E. Malguth *et al.*, Phys. Stat. Sol. (b) **245**, 455 (2008).

HL 97.11 Fri 12:15 H16

Synchrotron based spectroscopic ellipsometry of MgZnO — •Maciej D. Neumann[1], Christoph Cobet[2], Martin Feneberg[3], Rüdiger Goldhahn[3], Jean-Michel Chauveau[4], and Norbert Esser[1] — [1]Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., 12489 Berlin, Germany — [2]Johannes Kepler Universität Linz, 4040 Linz, Austria — [3]Otto-von-Guericke-Universität Magdeburg, 39106 Magdeburg, Germany — [4]Centre de Recherche sur l'Hétéro-Epitaxie et ses Applications, 06565 Sophia Antipolis, France

Using a newly developed synchrotron VUV ellipsometer allowing variable angle of incidence studies, non-polar MBE grown MgZnO samples with Mg contents up to 45% were investigated in the photon energy range from 2 to 25 eV. For the first time, both the parallel and perpendicular components of the complex dielectric tensor are presented. The strength of optical anisotropy above 10 eV decreases continuously with increasing Mg content. It suggests that the optical transitions in this range are strongly related to the Zn-3d levels. The results are in remarkable agreement to novel ab-initio calculations.

HL 98: Topological insulators (TT, jointly with DS, HL, MA, O)

Time: Friday 9:30–13:00 Location: H18

HL 98.1 Fri 9:30 H18

Structure factor of a weakly interacting helical liquid — •Suhas Gangadharaiah[1,2], Thomas L. Schmidt[2], and Daniel Loss[2] — [1]Indian Institute of Science Education and Research, Bhopal, India — [2]Department of Physics, University of Basel, CH-4056 Basel, Switzerland

We calculate the density structure factor $S(q,\omega)$ of a weakly interacting helical liquid in the presence of a magnetic field B. The latter opens a gap of width $2B$ in the single-particle spectrum $\epsilon_\pm(k)$, and leads to a strongly nonlinear spectrum near $k = 0$. For chemical potentials $\mu > B$, the system then behaves as a nonlinear helical Luttinger liquid, and a mobile-impurity analysis reveals interaction-dependent power-law singularities in $S(q,\omega)$. For $\mu < B$, the low-energy excitations are gapped, and we determine $S(q,\omega)$ by using an analogy to exciton physics. We discuss the implications of the magnetic field induced non-linear spectrum on the Coulomb drag between the helical liquids.

HL 98.2 Fri 9:45 H18

Strongly interacting Majorana modes in an array of Josephson junctions — Fabian Hassler[1] and •Dirk Schuricht[2] — [1]Institute for Quantum Information, RWTH Aachen University — [2]Institute for Theory of Statistical Physics, RWTH Aachen University

An array of superconducting islands with semiconducting nanowires in the right regime provides a macroscopic implementation of Kitaev's toy model for Majorana wires. We show that a capacitive coupling between adjacent islands leads to an effective interaction between the Majorana modes. We demonstrate that even though strong repulsive interaction eventually drive the system into a Mott insulating state the competition between the (trivial) band-insulator and the (trivial) Mott insulator leads to an interjacent topological insulating state for arbitrary strong interactions.

HL 98.3 Fri 10:00 H18

All-electrical measurement of crossed Andreev reflection in topological insulators — •Rolf W. Reinthaler[1], Patrik Recher[2], and Ewelina M. Hankiewicz[1] — [1]Faculty of Physics and Astrophysics, University of Würzburg, Würzburg, Germany — [2]Institute for Mathematical Physics, Technical University Braunschweig, Braunschweig, Germany

Using a generalized wave matching method we solve the full scattering problem for quantum spin Hall insulator (QSHI) - superconductor (SC) - QSHI junctions. We find that for systems narrow enough so that the bulk states in the SC part couple both edges, the crossed Andreev reflection (CAR) is significant and the electron cotunneling (T) and CAR become spatially separated. We study the effectiveness of this separation as a function of the system geometry and the level of doping in the SC. Moreover, we show that the spatial separation of both effects allows for an all-electrical measurement of CAR and T separately in a 5-terminal setup or by using the spin selection of the quantum spin Hall effect in an H-bar structure [1].

We acknowledge financial support by the DFG grant HA 5893/3-1.

[1] R. W. Reinthaler, P. Recher, and E. M. Hankiewicz, arXiv:1209.5700 (2012)

HL 98.4 Fri 10:15 H18

Zero-voltage conductance peak from weak antilocalization in a Majorana nanowire — •Michael Wimmer[1], Dimitri Pikulin[1], Jan Dahlhaus[1], Henning Schomerus[2], and Carlo Beenakker[1] — [1]Instituut-Lorentz, Universiteit Leiden, The Netherlands — [2]Department of Physics, Lancaster University, United Kingdom

We show that weak antilocalization by disorder competes with resonant Andreev reflection from a Majorana zero-mode to produce a zero-voltage conductance peak of order e^2/h in a superconducting nanowire. The phase conjugation needed for quantum interference to survive a disorder average is provided by particle-hole symmetry - in the absence of time-reversal symmetry and without requiring a topologically nontrivial phase. We identify methods to distinguish the Majorana resonance from the weak antilocalization effect.

HL 98.5 Fri 10:30 H18

Spectral properties of disordered multi-channel Majorana wires — •Patrick Neven, Dmitry Bagrets, and Alexander Altland — Institut für Theoretische Physik, Universität zu Köln, Köln, Germany

Proximity coupled multi-channel spin-orbit quantum wires may support midgap Majorana states at the ends. We study the fate of these Majorana fermions in the presence of disorder in such wires. Inspired by the widely established theoretical methods of mesoscopic superconductivity, we develop a quasiclassical approach which is valid in the limit of strong spin-orbit coupling. A numerical solution of the Eilenberger equation reveals that disordered topological wires are prone to the formation of a zero-energy anomaly (class D impurity spectral peak) in the local density of states which shares the key features of a Majorana peak. We also find that the $\mathbb{Z}_2$ topological invariant distinguishing between the state with and without Majorana fermions (symmetry class B and D, resp.) is related to the Pfaffians of quasiclassical Green's functions.

HL 98.6 Fri 10:45 H18

Topological invariants and interacting one-dimensional fermionic systems — •Salvatore R. Manmana[1,2,3], Andrew M. Essin[3], Reinhard M. Noack[4], and Victor Gurarie[3] — [1]Institut für Theoretische Physik, Universität Göttingen, Germany — [2]JILA, University of Colorado and NIST, Boulder (CO), USA — [3]Department of Physics, University of Colorado at Boulder, USA — [4]Fachbereich Physik, Philipps-Universität Marburg, Germany

We study one-dimensional, interacting, gapped fermionic systems described by variants of the Peierls-Hubbard model, and we characterize their phases via a topological invariant constructed out of their Green's functions. We demonstrate that the existence of topologically protected, zero-energy states at the boundaries of these systems can be tied to the value of the topological invariant, just like when working with the conventional, non-interacting topological insulators. We use a combination of analytical methods and the numerical density matrix renormalization group method to calculate the values of the topological invariant throughout the phase diagrams of these systems, thus deducing when topologically protected boundary states are present. We are also able to study topological states in spin systems because, deep in the Mott insulating regime, these fermionic systems reduce to spin chains. In this way, we associate the zero-energy states at the end of an antiferromagnetic spin-1 Heisenberg chain with a topological invariant equal to 2.

HL 98.7 Fri 11:00 H18

Fluctuation driven topological Hund insulator — •Jan Carl Budich[1], Bjoern Trauzettel[2], and Giorgio Sangiovanni[2] — [1]Department of Physics, Stockholm University, Se-106 91 Stockholm, Sweden — [2]Institute for theoretical physics and astrophysics, 97074 Würzburg, Germany

We investigate in the framework of dynamical mean field theory a two-band Hubbard model based on the Bernevig-Hughes-Zhang Hamiltonian describing the quantum spin Hall (QSH) effect in HgTe quantum wells. In the presence of interaction, we find that a system with topologically trivial non-interacting parameters can be driven into a QSH phase at finite interaction strength by virtue of local dynamical fluctuations. For very strong interaction, the system reenters a trivial insulating phase by going through a Mott transition. We obtain the phase diagram of our model by direct calculation of the bulk topological invariant of the interacting system in terms of its single particle Green's function.

15 min. break

HL 98.8 Fri 11:30 H18

Floquet Topological Quantum Phase Transitions in the Wen-Plaquette Model — •Victor Manuel Bastidas Valencia, Clive Emary, Gernot Schaller, and Tobias Brandes — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Our aim in this talk is to describe the nonequilibrium behavior of the topological quantum phase transition in the Ac-driven Wen-plaquette model. We show that under the effect of a nonadiabatic driving the system exhibits a novel topological phase. We define generalized topological order parameters by considering cycle-averaged expectation values of string operators in a Floquet state.

HL 98.9 Fri 11:45 H18

Fermion-parity anomaly of the critical supercurrent in the quantum spin-Hall effect — •Jan Dahlhaus[1], Dmitry Pikulin[1], Timo Hyart[1], Henning Schomerus[2], and Carlo Beenakker[1] — [1]Instituut-Lorentz, Universiteit Leiden, Niederlande — [2]Department of Physics, Lancaster University, United Kingdom

The helical edge state of a quantum spin-Hall insulator can carry a supercurrent in equilibrium between two superconducting electrodes (separation L, coherence length ξ). We calculate the maximum (critical) current I_c that can flow without dissipation along a single edge, going beyond the short-junction restriction $L \ll \xi$ of earlier work, and find a dependence on the fermion parity of the ground state when L becomes larger than ξ. Fermion-parity conservation doubles the critical current in the low-temperature, long-junction limit, while for a short junction I_c is the same with or without parity constraints. This provides a phase-insensitive, dc signature of the 4π-periodic Josephson effect.

HL 98.10 Fri 12:00 H18

Topological kicked rotators — •Jan Dahlhaus[1], Jonathan Edge[1], Jakub Tworzydlo[2], and Carlo Beenakker[1] — [1]Instituut-Lorentz, Universiteit Leiden, Niederlande — [2]Institute of Theoretical Physics, University of Warsaw, Poland

Topology is a nice mathematical concept that can have profound consequences on condensed matter systems. Maybe the most prominent examples are the quantum Hall effect, the quantum spin Hall effect and the 3D topological insulator. I will present a way to realize the ideas of band topology in a well-known and intensively-studied model - the quantum kicked rotator. This allows to study the Anderson localization properties of topological phase transitions numerically in a very efficient way, especially in higher dimensions. Furthermore it may open a way for experimental measurements of this transition behaviour with cold atomic gases in optical lattices.

HL 98.11 Fri 12:15 H18

Theory of correlated topological insulators with broken axial spin symmetry — •Stephan Rachel — TU Dresden, 01069 Dresden, Germany

The two-dimensional Hubbard model defined for topological band structures exhibiting a quantum spin Hall effect poses fundamental challenges in terms of phenomenological characterization and microscopic classification. We consider weak, moderate, and strong interactions and argue that the resulting phase diagrams depend on the microscopic details of the spin orbit interactions which give rise to the non-trivial topology. In particular, it turns out that there is a crucial difference between models with broken and with conserved axial spin symmetry. These results suggest that there is a general framework for correlated 2D topological insulators with broken axial spin symmetry.

[1] Rachel, LeHur, PRB 82, 075106 (2010)
[2] Schmidt, Rachel, von Oppen, Glazman, PRL 108, 156402 (2012)
[3] Cocks, Orth, Rachel *et al.*, PRL 108, 205303 (2012)
[4] Reuther, Thomale, Rachel, PRB 86, 155127 (2012)

HL 98.12 Fri 12:30 H18

Interaction effects on almost flat surface bands in topological insulators — •Matthias Sitte, Lars Fritz, and Achim Rosch — Universität zu Köln, Institut für Theoretische Physik, Zülpicher Str. 77, 50937 Köln, Deutschland

We investigate ferromagnetic instabilities of the two-dimensional helical Dirac fermions hosted on the surface of three-dimensional topological insulators. We concentrate on ways to increase the role of interactions by means of modifying the bulk properties which in turn changes the surface Dirac theory characteristics. We discuss both long-ranged Coulomb interactions controlled by the dimensionless coupling constant $\alpha = e^2/(\hbar\epsilon v_F^{\mathrm{surf}})$ as well as short-ranged Hubbard-like interactions of strength U which can induce spontaneous surface ferromagnetism, thereby gapping the surface Dirac metal. In both cases, we find that a prerequisite for observing this effect is to reduce the Fermi velocity v_F^{surf}, and we consider different mechanisms to achieve this. While for long-ranged Coulomb interactions we find that screening hinders ferromagnetism, for short-ranged interactions screening is not that vital and the instability can prevail.

HL 98.13 Fri 12:45 H18

Local spin susceptibility and surface states in doped three-dimensional topological insulators with odd-parity superconducting pairing symmetry — •Björn Zocher[1,2] and Bernd Rosenow[1] — [1]Institut für Theoretische Physik, Universität Leipzig, D-04103 Leipzig, Germany — [2]Max Planck Institut für Mathematik in den Naturwissenschaften, D-04103 Leipzig, Germany

We investigate characteristic features in the spin response of doped three-dimensional topological insulators with odd-parity unequal-spin superconducting pairing. To get insight into the nature of the superconducting pairing symmetry, we show that the odd-parity unequal-spin pairing can be mapped onto p-wave pairing and that these systems have gapless Majorana surface modes. The Majorana modes contribute to the local spin susceptibility, giving rise to a characteristic temperature behavior of the Knight shift and the spin-lattice relaxation time in magnetic resonance experiments. Because of their different decay lengths, the Majorana modes can be observed and clearly distinguished from the Dirac modes of the topological insulator by local probes which allow for a depth-controlled study of the electron spins on the nanometer length scale.

HL 99: Transport: Spintronics and magnetotransport 2 (TT, jointly with HL, MA)

Time: Friday 9:30–10:30 Location: H20

HL 99.1 Fri 9:30 H20

Bulk sensitive photoelectron spectroscopy on CrO_2 thin films — •Jonas Weinen[1], Stefano Agrestini[1], Martin Rotter[1], Simone G. Altendorf[1], Zhiwei Hu[1], Chun-Fu Chang[1], Arun Gupta[2], Yen Fa Liao[3], Ku-Ding Tsuei[3], and Liu Hao Tjeng[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden — [2]The University of Alabama, Tuscaloosa, USA — [3]National Synchrotron Radiation Research Centre, Hsinchu, Taiwan

For transition metal compounds with a high oxidation state the so-called charge transfer energy can become negative, with the result that a spontaneous electron redistribution could occur in which oxygen holes are formed. Such seems to be the case for the ferromagnet

CrO_2. Using the LDA+U method, Korotin et al. [PRL **80**, 4305 (1998)] calculated that the material is a metal and remains a metal even for very large values of U. This suggests that it is not so much the Cr 3*d* states that determine whether the system is metallic or insulating, but rather that it is the O 2*p* states which straddle the chemical potential.—Several photoelectron spectroscopy (PES) studies have been reported in the literature, but the results are not consistent, supposedly related to the fact that the surface of CrO_2 tends to decompose to Cr_2O_3 under vacuum conditions, so that surface sensitive PES may not have probed the true bulk spectrum of CrO_2.—We set out to perform bulk sensitive photoemission experiments below and above T_C on CrO_2 thin films using our HAXPES system at SPring-8. Our results suggest that CrO_2 may be considered more like a bad metal rather than a normal metal.

This work is also supported by DFG through FOR1346.

HL 99.2 Fri 9:45 H20

Initial stages of epitaxial growth of Fe_3O_4/MgO (001) thin films: atomic reconstruction at the polar interface — •Chun-Fu Chang[1], Zhiwei Hu[1], Stefan Klein[2], Ronny Sutarto[2], Philipp Hansmann[2], Arata Tanaka[3], Julio Criginski Cesar[4], Nicholas Brookes[4], Hong-Ji Lin[5], Hui-Huang Hsieh[6], Chien-Te Chen[5], A. Diana Rata[1], and Liu Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]II. Physikalisches Institut, Universität zu Köln, Köln, Germany — [3]Department of Quantum Matter, ADSM, Hiroshima University, Hiroshima, Japan — [4]ESRF, Grenoble Cédex, France — [5]NSRRC, Hsinchu, Taiwan — [6]Chung Cheng Institute of Technology, National Defense University, Taoyuan, Taiwan

By means of reflection high energy electron diffraction and Fe $L_{2,3}$ x-ray absorption spectroscopy we find evidence for an atomic structural reconstruction at the interface of polar Fe_3O_4/MgO (001) thin films. This reconstruction takes place over several monolayers, while each monolayer still preserves the Fe_3O_4 stoichiometery. Our findings for such a transition interface layer may have important implications especially in the field of spintronics, where ultrathin Fe_3O_4 films are widely used for various sensitive devices.

HL 99.3 Fri 10:00 H20

Investigation of the Verwey transition in Fe_3O_4 thin films — •Xionghua Liu, Akfiny Hasdi Aimon, A. Diana Rata, Chun-Fu Chang, and Liu Hao Tjeng — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

Magnetite Fe_3O_4 is one of the most investigated materials from the class of transition metal oxides. It shows a first-order anomaly in the temperature dependence of the electrical conductivity at T_V= 120 K, the famous Verwey transition. However, thin films of Fe_3O_4 show always a lower T_V compared to the bulk material. In order to find out the reason for the decreased T_V in magnetite thin films we have performed a systematic investigation of the transport properties in dependence of the oxygen pressure and thickness. Epitaxial Fe_3O_4 films were grown by Molecular Beam Epitaxy on MgO(100) and $MgAl_2O_4$ (100) substrates and the structural and spectroscopic characteristics were in-situ determined by RHEED and XPS, respectively. Resistivity measurements have been performed ex-situ by PPMS. Results of this study and ongoing work will be presented.

HL 99.4 Fri 10:15 H20

Electronic Structure and Magnetic Properties of Sc doped EuO Thin Films — •Andreas Reisner[1], Simone Altendorf[1], Chun-Fu Chang[1], Hong-Ji Lin[2], Chien-Te Chen[2], and Liu Hao Tjeng[1] — [1]Max-Planck-Institute for Chemical Physics of Solids, Nöthnitzer Str.40, 01187 Dresden, Germany — [2]National Synchrotron Radiation Research Center, Hsin-Ann Road, 30076 Hsinchu, Taiwan, R.O.C.

Europium monoxide is a ferromagnetic semiconductor with a Curie temperature T_C of 69 K. Upon doping the material can show an increase of the Curie temperature, a metal-to-insulator transition and a high spin polarization of the charge carriers. Applying pressure can also enhance T_C. Mostly other trivalent rare earth metals are used as dopant. Here we set out to explore the possibility of using transition metals as dopants. As a start we focus on the non magnetic Sc ions. We are able to achieve excellent crystalline growth of Sc-doped EuO thin films on YSZ (001) substrates using molecular beam epitaxy. We will report our results on the crystal structure as characterized by RHEED and LEED, the electronic structure as determined by XPS and ARPES, and on the magnetic propertes as measured by SQUID.

HL 100: Resistive switching (DS, jointly with DF, HL, KR)

Time: Friday 9:30–12:45 Location: H32

HL 100.1 Fri 9:30 H32

***Ab initio* study of defects in $SrTiO_3$ bulk and (100) surfaces** — •Ali Al-Zubi, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut (PGI) & Institute for Advanced Simulation (IAS), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Oxygen vacancies are believed to play a major role in the conduction mechanisms that enable resistive switching in oxide materials. Employing density functional theory (DFT) and the DFT+U model,we use the full-potential linearized augmented plane wave method as implemented in the `FLEUR` code to study the formation of point defects in the perovskite $SrTiO_3$ with varying coordination. We calculated the formation energy of an O-vacancy in both bulk supercells and (100) surface including different, c(2×2) and p(2×2), in-plane unit cells and different terminations. After performing full relaxation, we found that the bulk and SrO-terminated surface have a nonmagnetic, while TiO_2-terminated surface has a ferromagnetic solution. Using the c(2×2) unit cell, the vacancy formation energy was smaller for the bulk than for the SrO- and even TiO_2-terminated surface. On the other hand, the p(2×2) unit cell shows that TiO_2-terminated surface has the lowest formation energy, more than 1 eV lower than the bulk value. Similar comparisons will be presented when including the the DFT+U model that is used to correct the bulk bandgap and improve the localization of the defect states.

We gratefully acknowledge financial support of the DFG, SFB 917 Nanoswitches–A4 project.

HL 100.2 Fri 9:45 H32

Resistive switching properties in ion beam modified $SrTiO_3$ — •Jura Rensberg, Benjamin Roessler, Christian Katzer, Frank Schmidl, and Carsten Ronning — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Germany

Resistive switching phenomena, which are for instance observed in perovskite-type transition metal oxides, attract intensive attention for their potential application in future nonvolatile memory. Strontium titanate ($SrTiO_3$) exhibits bipolar resistive switching between a high- and a low-resistance state when applying an appropriate electric field. It is often proposed that the underlying mechanism for bipolar resistive switching in $SrTiO_3$ originates from oxygen-vacancy migration along filaments based on extended defects such as dislocations or grain boundaries.

Here we report on well-defined damage formation due to ion irradiation which allows a better control of the lateral and vertical defect arrangements and concentrations. Therefore, we deposited 100 nm single crystalline $SrTiO_3$ thin films with low intrinsic defect concentration on niobium doped $SrTiO_3$ substrates by pulsed laser deposition and implanted these samples with swift heavy gold ions. After irradiation the films were characterized using transmission electron microscopy and Rutherford backscattering spectrometry. Under ion irradiation, the as-deposited crystalline films undergo amorphisation due to the formation and overlap of amorphous tracks. The electrical properties of $SrTiO_3$, i.e. the resistive switching properties are discussed in terms of damage concentration.

HL 100.3 Fri 10:00 H32

Cation defect engineering in SrTiO3 thin films by PLD with Verification and implication on memristive properties — Sebastian Wicklein[1], •Chencheng Xu[1], Alessia Sambri[2], Salvatore Amoruso[2], David Keeble[3], Annemarie Köhl[1], Werner Egger[4], and Regina Dittmann[1] — [1]Peter Grünberg Institut 7, Forschungszentrum Jülich GmbH, Germany — [2]Università degli Studi di Napoli Federico II, Dipartimento di Scienze Fisiche & CNR-SPIN, I-80126 Napoli, Italy — [3]University of Dundee, School of Engineering,

Physics and Mathematics, Dundee DD1 4HN, Scotland — [4]University Bundeswehr, D-85577 Munich, Germany

The origin of the c-axis expansion in homoepitaxial STO thin films is investigated by positron annihilation lifetime spectroscopy (PALS): Low laser fluence results in Ti vacancy rich sample while high laser fluence for the Sr vacancy rich sample.

XPS measurement on the ablated spot on the targets shows that increased laser fluence ablates more Ti. The ToF (Time of Flight) data from OES (optical emission spectrometry) indicate a preferred scattering of Ti because of background gas. The two effects together lead to tunable stoichiometry of the film.

In the MIM (metal insulator metal) structure Sr-rich films exhibit the most stable switching behavior and highest on/off ratio, while in the LC AFM (local conducting atomic force microscopy) switching the on/off ratio of Ti is the higest.

HL 100.4 Fri 10:15 H32

Resistive Switching in thermally oxidized Titanium — •Daniel Blaschke[1], Ilona Skorupa[1], Bernd Scheumann[1], Andrea Scholz[1], Peter Zahn[1], Sibylle Gemming[1], Kay Potzger[1], Agnieszka Bogusz[2], and Heidemarie Schmidt[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, P.O. Box 510119, 01314 Dresden - Germany — [2]Dept. Electr. Eng. & Inf. Techn., TU Chemnitz, 09107 Chemnitz

In recent years the resistive switching of binary transition metal oxides like NiO, Nb2O5 and TiO2 has attracted considerable attention for application in nonvolatile memory storage systems.

For our investigations we used a thin rutile TiO2 film, which was prepared by the thermal oxidation of a 100nm thick e-beam evaporated Ti film. The oxidation temperatures were varied from 500°C to 800°C at an oxygen partial pressure of 1 atmosphere. We will present the dependence of the crystal structure and the switching behavior on the oxidation temperature as well as an interesting feature on the time-dependent evolution of the resistance during the Reset process.

The project is funded by the Initiative and Networking Fund of the Helmholtz Association (VH-VI-422).

HL 100.5 Fri 10:30 H32

Non-volatile resistive switching in multiferroic YMnO3 thin films — •Agnieszka Bogusz[1,2], Ilona Skorupa[1], Andrea Scholz[1], Oliver G. Schmidt[2,3], and Heidemarie Schmidt[2] — [1]Institute of Ion Beam Physics and Materials Research, Helmholz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]Faculty of Electrical Engineering and Information technology, Chemnitz University of Technology, 09107 Chemnitz, Germany — [3]Institute for Integrative Nanosciences, IFW-Dresden, 01069 Dresden, Germany

Intensive research on multiferroic materials [1] is driven by the possibility of creating novel, miniaturized tunable multifunctional devices [2]. This work investigates resistive switching behavior of YMnO3 thin films, which can be utilized in new generation memory devices. Series of YMnO3 films were grown by pulsed laser deposition on Si substrates with Pt bottom electrode at temperatures varying between 500°C and 850°C. Characterization of as-grown samples by X-ray diffraction and scanning electron microscopy was followed by determination of electrical properties of films in metal-insulator-metal (MIM) configuration. Results showed that the YMnO3 films grown at 800°C exhibit the best resistive switching properties with high resistance ratio (>10000) of high over low resistance state. Switching mechanism is ascribed to the structural transitions within the film upon applied current.

[1] A. Bogusz et al., Defect Diffus. Forum 323-325, 115 (2012)

[2] Y. Shuai, H. Schmidt et al., J. Appl. Phys. 109, 124117 (2011); J. Appl. Phys. 111, 07D906 (2012)

HL 100.6 Fri 10:45 H32

Practical guide for validated memristance measurements — •Nan Du[1,2], Yao Shuai[3], Wenbo Luo[3], Christian Mayr[4], Rene Schüffny[4], Oliver G. Schmidt[1,2], and Heidemarie Schmidt[1] — [1]TU Chemnitz, Faculty of Electrical Engineering and Information Technology, 09107 Chemnitz, Germany — [2]Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [3]Helmholtz Research Center Dresden-Rossendorf, 01328 Dresden, Germany — [4]TU Dresden, Department of Electrical Engineering and Information Technology, 01062 Dresden, Germany

L.O. Chua predicted rather simple charge-flux curves for active and passive memristors and presented active memristor circuit realizations already in the 70s. However, despite the fact that memristors give rise to complicated hysteretic current-voltage curves, memristors are traced in current-voltage curves. Here we give a practical guide how to use normalized charge-flux curves for the prediction of current-voltage characteristics of memristors with stable electrical characteristics in dependence on the shape and amplitude of the input voltage or input current signals. In the case of memristive BiFeO3 thin film capacitor structures [1] the normalized charge-flux curves superimpose for different numbers of measurement points and a different measurement time per measurement point. Such normalized charge-flux curve can be used for the prediction of current-voltage characteristics of plastic synapses in neuromorphic systems [2]. [1] Y. Shuai et al., J. of Appl. Phys. 109, 124117-124117-4 (2011). [2] C. Mayr et al., NIPS 2012, in press.

Coffee break (15 min)

HL 100.7 Fri 11:15 H32

Creating an Oxygen Gradient in Nb_2O_5 by Argon Irradiation for Resistive Switching Memory — •Helge Wylezich[1], Hannes Mähne[1], Daniel Blaschke[2], Stefan Slesazeck[1], and Thomas Mikolajick[1] — [1]NamLab gGmbH, Nöthnitzer Str. 64, D-01187 Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden

It is common knowledge that an oxygen gradient is mandatory for bipolar resistive switching [1]. We confirmed this by investigations of thin films with Nb_2O_5 as switching layer. Samples with two inert Pt electrodes are nearly symmetric and do not show bipolar resistive switching behavior. Replacing one Pt electrode with a reactive one – for example Al or Nb – results in an unsymmetrical device. These samples could be switched reproducible. It is also possible to create an oxygen gradient by depositing a stack of two different niobium oxide layers. While the first layer consists of stoichiometric Nb_2O_5 the second layer is sputtered substoichiometric [2].

A new approach is to get an oxygen gradient by irradiating the oxide layer with argon. Two effects appear: The argon sputters the surface of the Nb_2O_5 layer and so the oxide thickness decreases. Because the Nb-atoms are heavier than the O-atoms, the oxygen sputter rate is higher and the surface becomes niobium rich. The investigated samples consist of a Pt-Nb_2O_5-Pt stack. The oxide layer was irradiated by different Ar-doses before top electrode deposition. At the highest dose Φ = 3e16 cm^{-2} the resulting oxygen gradient enables resistive switching.

[1] Bertaud et al. (TSF 520, 2012)

[2] Mähne et al. (MEMCOM Workshop 2012)

HL 100.8 Fri 11:30 H32

Multilevel resistive switching in Ar+ irradiated BiFeO3 thin films — •Yao Shuai[1], Xin Ou[2], Wenbo Luo[2], Nan Du[3], Danilo Bürger[2,3], Oliver G. Schmidt[3,4], and Heidemarie Schmidt[3] — [1]State Key Laboratory of Electronic Thin Films and Integrated Devices, UESTC, China — [2]Helmholtz-Zentrum Dresden-Rossendorf e.V., Institute of Ion Beam Physics and Materials Research, Germany — [3]University of Technology Chemnitz, Faculty of Electrical Engineering and Information Technology, 09107 Chemnitz, Germany — [4]Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany

Low energy Ar+ ion irradiation has been applied to an Au/BiFeO3/Pt capacitor structures before deposition of the Au top electrode. The irradiated thin films exhibit multilevel resistive switching without detrimental resistance degradation, which makes the intermediate resistance states more distinguishable as compared to the non-irradiated thin film [1]. The stabilization of resistance states after irradiation is discussed based on the analysis of conduction mechanism during the resistive switching in BiFeO3 with a rectifying Au top electrode and a nonrectifying Pt bottom electrode [2]. Furthermore, it is shown how the conduction mechanisms change from room temperature to 423 K. [1] Y. Shuai, X. Ou et al., IEEE Device Letters, 2012, in press. [2] Y. Shuai, S. Zhou, D. Bürger, M. Helm, H. Schmidt, J. Appl. Phys. 109 (2011), 124117-4.

HL 100.9 Fri 11:45 H32

Influence of thickness ratio on resistive switching in BiFeO3:Ti/BiFeO3 bilayer structures — •Tiangui You[1], Wenbo Luo[2], Yao Shuai[1,2], Nan Du[1], Danilo Bürger[1,3], Ilona Skorupa[3], Oliver G. Schmidt[1,4], and Heidemarie Schmidt[1] — [1]Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]University of Electronic Science and Technology of China, 610054

Chengdu, China — [3]Helmholtz-Zentrum Dresden-Rossendorf, P.O. Box 510119, 01314 Dresden, Germany — [4]IFW-Dresden, 01069 Dresden, Germany

Nonvolatile resistive switching in BiFeO3 (BFO) [1] has attracted increasing attention; however, the underlying resistive switching mechanism is still controversial which restricts its application in nonvolatile memory devices. BFO:Ti/BFO bilayer structures with a 540 nm thick BFO layer and different thickness of BFO:Ti layer were grown on Pt/Sapphire substrates by pulsed laser deposition using the same growth conditions. Circular Au top electrodes were prepared with magnetron sputtering. Au/BFO/Pt single layer structures show a symmetric I-V curve without hysteresis due to the formation of Schottky contacts at both the top and bottom interface. However, Au/BFO/BFO:Ti/Pt bilayer structures exhibit an obvious resistive switching behavior under both voltage polarities. The influence of the thickness of BFO:Ti on the conduction mechanisms in Au/BFO/BFO:Ti/Pt bilayer structures is discussed to reveal similarities and differences between single and bilayer structures.

Reference [1] Y. Shuai et al., J. Appl. Phys., 109, 124117(2011)

HL 100.10 Fri 12:00 H32

Nanoscale resistive switching in epitaxial and polycrystalline BiFeO3 thin films — •Yao Shuai[1], Wenbo Luo[1], Chuangui Wu[1], Wanli Zhang[1], Oliver G. Schmidt[2,3], and Heidemarie Schmidt[2] — [1]State Key Laboratory of Electronic Thin Films and Integrated Devices, UESTC, China — [2]University of Technology Chemnitz, Faculty of Electrical Engineering and Information Technology, 09107 Chemnitz, Germany — [3]Institute for Integrative Nanosciences, IFW Dresden, 01069 Dresden, Germany

Nonvolatile [1], bipolar, and multilevel [2] resistive switching has been observed in ca. 500 nm thick polycrystalline BiFeO3 thin films with rectifying, circular Au top electrodes and a nonrectifying Pt bottom electrode. The diameter of the Au top electrodes amounts to ca. 0.5 mm. By scanning a positionable top contact with a diameter of only 10 nm over polycrystalline BiFeO3 thin films under a constant applied dc voltage, the high and low resistance state can be locally written and afterwards read. It has been observed that for thinner polycrystalline BiFeO3 films with a thickness below 300 nm, no resistive switching can be observed either with large or with small scale top contacts. Bipolar resistive switching can also be realized in ca. 50 nm thick epitaxial BiFeO3 films on SrRuO3/SrTiO3 with a positionable top contact. This resistance is mainly determined by the ferroelectric polarization and the barrier height of the top and bottom contact. For thicker epitaxial BiFeO3 films the unique relation between ferroelectric polarization and resistance state is diminished. [1] Y. Shuai et al., J. Appl. Phys. 109 (2011). [2] Y. Shuai et al., IEEE Device Letters (2012) in press.

HL 100.11 Fri 12:15 H32

An electronic implementation of amoeba anticipation — •Mirko Hansen[1], Karlheinz Ochs[2], Martin Ziegler[1], and Hermann Kohlstedt[1] — [1]Faculty of Engineering, Christian-Albrechts-Universität zu Kiel, 24143 Kiel, Germany — [2]Ruhr-Universität Bochum, 44780 Bochum, Germany

In nature, the capability to memorize environmental changes can already be observed in unicellular organisms like amoebas[1]. An amoeba changes its locomotive speed when it is exposed to unfavorable conditions. If a series of unfavorable conditions is applied, the amoeba later on behaves similarly on a single incident. Pershin et al.[2] are able to emulate this behavior using a simple resistive switching circuit model consisting of an inductor, a capacitor and a resistive switching device. We experimentally implement this model using a resistive switching device. A theoretical analysis of the circuit is presented to gain further insight into the functionality of this model and to give advice for the implementation of resistive switching devices in LC-circuits.

[1] T. Saigusa, A. Tero, T. Nakagaki, Y. Kuramoto, Phys. Rev. Lett. **100**, (2008) 018101

[2] Y. V. Pershin, S. La Fontaine, M. Di Ventra, Phys. Rev. E **80**, (2009) 021926

HL 100.12 Fri 12:30 H32

Lattice dynamics in Sb- and Te-based phase-change materials — •Ronnie Ernst Simon[1,2], Ilya Sergueev[3], and Raphaël Pierre Hermann[1,2] — [1]Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, Jara-FIT Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany — [2]Faculté des Sciences, Univer- sité de Liège, B-4000 Liège, Belgium — [3]Deutsches Elektronen- Syn- chrotron, D-22607 Hamburg, Germany

Phase-change materials exhibit a significant change of the optical reflectivity and electrical resistivity upon crystallization which renders these materials applicable for optical storage devices and non-volatile electronic memories. In order to understand the switching kinetics between the amorphous and the metastable crystalline states a detailed knowledge of the lattice dynamics of the different phases is crucial. A suitable technique for the investigation of lattice dynamics is nuclear inelastic scattering (NIS) which gives access to the element specific density of phonon states (DPS). We performed NIS measurements in Sb- and Te-based phase-change materials in the amorphous and crystalline phases. We have recently extended the experimental possibilities by demonstrating the feasibility of high pressure NIS measurements, up to 75 GPa, in Sb_2Te_3 . The ESRF is acknowledged for the provision of synchrotron radiation beamtime at ID18.

HL 101: Graphene: Preparation and characterization II (O, jointly with HL, TT)

Time: Friday 10:30–13:00 Location: H17

HL 101.1 Fri 10:30 H17

Engineering of 2D-Nanomaterials by Swift Heavy Ion Irradiation — •Oliver Ochedowski, Hanna Bukowska, Sevilay Akcöltekin, and Marika Schleberger — Universität Duisburg-Essen, Lotharstrasse 1, 47057 Duisburg

Two dimensional (2D) nanomaterials prepared from layered crystal materials have attracted a great amount of interest in multiple fields of science. These nanomaterials can be metallic (e.g. graphene), semiconducting (MoS2) or insulating (Mica) with properties often different from their bulk counterparts. Here, we will demonstrate how the morphology of several 2D-nanomaterials can be modified by swift heavy ion (SHI) irradiation in the MeV regime under glancing incidence angle. The induced modifications are investigated by means of atomic force microscopy. In the case of graphene we will show by Kelvin probe force microscopy how SHIs can be used to alter the electronic structure and induce doping of the graphene.

HL 101.2 Fri 10:45 H17

Fabrication of laterally structured graphene/carbon nanomembrane hybrids — •Andreas Winter[1], Stefan Wundrack[2], Rainer Stosch[2], and Andrey Turchanin[1] — [1]Universität Bielefeld, 33615 Bielefeld — [2]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig

Laterally structured free-standing micro- and nanostructures of single-layer graphene (SLG) embedded into dielectric sheets with a thickness comparable to graphene are of great interest for applications in electronic or optoelectronic devices. However, their fabrication is not a trivial task at present. Here, we demonstrate how such hybrids can be engineered using electron-irradiation-induced crosslinking of graphene micro-/nanostructures with carbon nanomembranes (CNMs). CNMs are a dielectric 2D carbon material with the thickness of about 1 nm consisting of cross-linked randomly oriented benzene rings. We show scalable production of well-defined laterally patterned CNM-SLG hybrids of various architectures and characterize their structural, chemical and electronic quality by complementary spectroscopic and microscopic techniques including helium ion microscopy and Raman spectroscopy. Application areas of the generated hybrids will be discussed.

HL 101.3 Fri 11:00 H17

Non-destructive chemical functionalization of single-layer graphene for electronic applications — Mirosław Woszczyna[1], Miriam Grothe[1], Andreas Winter[2], Annika Willunat[1], Stefan Wundrack[1], Rainer Srosch[1], Franz Ahlers[1], Thomas Weimann[1], and •Andrey Turchanin[2] — [1]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany — [2]Faculty of Physics, University of Bielefeld, 33615 Bielefeld, Germany

Chemical functionalization of single-layer graphene (SLG) is of key importance for implementations of this material in functional electronic devices such as, e.g., field effect transistor (FET) based nanosensors. However, the electronic quality of graphene typically degrades after the functionalization with presently employed methods, significantly restricting the application areas. Here, we present a route to non-destructive chemical functionalization of graphene via engineering of carbon nanomembrane (CNM)/SLG hybrids. We employ SLG, grown by methane CVD on Cu foils, and amino-terminated 1 nm thick CNMs, generated by electron-beam-induced crosslinking of aromatic self-assembled monolayers, to fabricate hybrid CNM/SLG FETs on oxidized silicon wafers. Structural, chemical and electronic properties of these devices are characterized by Raman spectroscopy, X-ray photoelectron spectroscopy and electrical transport measurements. We unambiguously show that the intrinsically high electronic quality of pristine SLG is preserved in the amino-functionalized hybrids opening broad avenues for their use in graphene-based FETs.

HL 101.4 Fri 11:15 H17

Etching Nanoscale tunnels into graphite- a new route to produce suspended graphene — •Maya Lukas[1], Velimir Meded[1], Aravind Vijayaraghavan[1,2], Li Song[3,4], Pulickel M. Ajayan[4], Karin Fink[1], Wolfgang Wenzel[1], and Ralph Krupke[1,5] — [1]Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology, D-76021 Karlsruhe — [2]School of Computer Science, The University of Manchester, UK — [3]Research Center for Exotic Nanocarbons, Shinshu University, Nagano, Japan — [4]Department of Mechanical Engineering & Materials Science, Rice University, Houston, TX , USA — [5]Department of Materials and Earth Sciences, Technische Universität Darmstadt, D-64287 Darmstadt

Catalytic hydrogenation of graphite, although known since the 1970s, has recently attracted renewed attention, as a route for nanopatterning of graphene and to produce graphene nano-ribbons. These reports show that metallic nanoparticles etch surface layers of graphite or graphene anisotropically along the crystallographic zigzag <11-20> or armchair <1010> directions.

We report the sub-surface etching of highly oriented pyrolytic graphite (HOPG) by Ni nanoparticles, to form a network of tunnels, as seen by SEM and STM. The layers on top of tunnels which are only a few layers below the surface bend inward, while their local density of states remains fundamentally unchanged. Our work opens a new route to produce suspended graphene for the study of fundamental mechanical and electronic properties. M. Lukas, V. Meded *et al., Nat. Commun.* accepted for publication

HL 101.5 Fri 11:30 H17

Direct e-beam writing of single-layer graphene nanostructures — •Nils-Eike Weber[1], Henning Vieker[1], Stefan Wundrack[2], Rainer Stosch[2], and Andrey Turchanin[1] — [1]Fakultät für Physik, Universität Bielefeld — [2]Physikalisch-Technische Bundesanstalt, Braunschweig

We demonstrate direct writing of single-layer graphene nanostructures employing electron irradiation of aromatic self-assembled monolayers (SAM) and subsequent annealing. The process consists of the following technological steps: (i) formation of an aromatic SAM on a Cu substrate; (ii) electron-beam-irradiation of the SAM resulting in locally cross-linked SAM areas; (iii) conversion of these areas into single-layer graphene via annealing. In this way graphene nanostructures of various architectures are directly defined in the SAM by electron beam lithography reducing several manufacturing steps, which are typically applied for the patterning of two-dimensional sheets including graphene (baking and developing electron-beam resist, plasma etching, resist striping). The formed nanostructures were characterized by Raman spectroscopy, scanning electron and helium ion microscopy. We demonstrate their successful transfer from the original copper foils onto oxidized silicon wafers, where they can directly be integrated into electronic devices.

HL 101.6 Fri 11:45 H17

Understanding of the imaging contrast in STM/NC-AFM of graphene on metals — •Elena Voloshina[1], Edoardo Fertitta[1], Andreas Garhofer[2], Florian Mittendorfer[2], Mikhail Fonin[3], Torben Haenke[4], Oliver Schaff[4], Thorsten Kampen[4], Andreas Thissen[4], and Yuriy Dedkov[4] — [1]Physikalische und Theoretische Chemie, Freie Universität Berlin, 14195 Berlin, Germany — [2]Institute of Applied Physics, Vienna University of Technology, Gusshausstr. 25/134, 1040 Vienna, Austria — [3]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [4]SPECS Surface Nano Analysis GmbH, Voltastraße 5, 13355 Berlin, Germany

Realization of graphene moiré superstructures on the surfaces of 4d and 5d transition metals offers templates with periodically modulated electron density, which is responsible for a number of fascinating effects, including the formation of quantum dots and the site selective adsorption of organic molecules or metal clusters on graphene. Here, applying the combination of scanning probe microscopy/spectroscopy and the density functional theory calculations, we gain a profound insight into the electronic and topographic contributions to the imaging contrast of the epitaxial graphene/Ir(111) system. We show directly that in STM imaging the electronic contribution is prevailing compared to the topographic one. In the force microscopy and spectroscopy experiments we observe a variation of the interaction strength between the tip and high-symmetry places within the graphene moiré supercell, which determine the adsorption sites for molecules or metal clusters on graphene/Ir(111).

HL 101.7 Fri 12:00 H17

Precise imaging of graphene — •Thomas Hofmann, Alfred J. Weymouth, Joachim Welker, and Franz J. Giessibl — Institut für Experimentelle und Angewandte Physik, Universität Regensburg

Atomic imaging of graphene with a scanning probe microscope is challenging due to its small atomic lattice. We show that metallic tips, which have been characterized prior to the measurement, cannot truthfully image the graphene surface due to their large, non-spherical electron density [1]. Calculations predict that the metal tip atom strongly interacts with the graphene surface [2]. Carbon oxide front atom identification (COFI) [2] shows that contact of a clean metal tip with graphene can lead to graphene flakes attaching to the tip apex. This results in blurred images and multi-valley force versus distance curves. As a solution we use a metal tip, functionalized with an inert carbon monoxide molecule as suggested by Gross et al. [3]. The closed-shell nature of the CO drastically reduces the attraction between tip and graphene. Additionally, the small size of the CO allows truthful imaging of the graphene surface.

[1] *J. Welker, and F. J. Giessibl, Science 336, 6080 (2012)

[2]*M. Ondráček, P. Pou, V. Rozsíval, C. González, P. Jelínek, and R. Pérez, PRL 106, 176101 (2011)

[3]*L. Gross, F. Mohn, N. Moll, P. Liljeroth, and G. Meyer, Science 325, 5944 (2009)

HL 101.8 Fri 12:15 H17

Role of substrate-molecular interactions in arrangement and collective motion of fullerene islands on graphene — •Martin Švec[1], Pablo Merino[2], Yannick Dappe[3], Cesar Gonzalez[1], Enrique Abad[4], Pavel Jelinek[1], and Jose-Angel Martin-Gago[5] — [1]Institute of Physics, ASCR, Prague, CZ — [2]CAB INTA-CSIC, Madrid, ES — [3]CEA, IRAMIS, SPCSI, FR — [4]UAM, Madrid, ES — [5]ICMM-CSIC, Madrid, ES

Fullerenes interacting with graphene are a model system, that should be entirely driven by van der Waals (vdW) interactions. We concentrate on the interactions occurring between fullerenes and the single-layer graphene grown on SiC(0001) [1]. By using a VT-STM at 40K, regular islands of fullerenes were found. The particular orientation of the fullerenes in the islands, which occupy 4x4 graphene unit cells each, is critically evaluated by a comparison of STM measurements to extensive STM simulations with realistic fullerene-terminated tips. The determined orientation of fullerenes is independently confirmed by complex theoretical calculations of several adsorption configurations, taking into account the vdW interaction between the constituents of this system. Furthermore, islands of fullerenes were found collectively moving on the graphene. Surprisingly, according to the theory, the cohesion among the fullerenes is weaker than adhesion to the surface. Nevertheless, cohesion is a decisive factor in the collective motion, thanks to a low diffusion barrier of fullerenes on graphene.

[1] M. Švec et al., Phys. Rev. B 86 121407(R)(2012)

HL 101.9 Fri 12:30 H17

XPS Analysis of Wet-Chemically Prepared Graphene Oxide — •Ole Lytken, Michael Röckert, Jie Xiao, Christian Papp, Hans-Peter Steinrück, Siegfried Eigler, Michael Enzelberger, Stefan Grimm, Philipp Hofmann, Wolfgang Kroener, Christoph Dotzer, Paul Müller, and Andreas Hirsch — Universität Erlangen-Nürnberg

Graphene is one of the most studied materials of the last few years,

but large scale production of high-quality graphene remains a challenge. One approach to a large scale production of graphene is the oxidation of graphite to graphite oxide, which can be exfoliated to graphene oxide and subsequently reduced to graphene. The challenge of this method is to keep the carbon structure intact during oxidation. We report on the XPS analysis of graphene oxide produced by a mild synthesis method that keeps the carbon structure intact and allows the reduction back to high-quality graphene. Only carbon with a single bond to one neighboring oxygen atom is observed (e.g. alcohols, expoxides or ethers), but no carbonyl (C=O) or carboxyl (-COOH) groups are found. Some common problems related to the interpretation of graphene oxide XPS spectra in the presence of charging and sulfur impurities will be touched upon.

Support by the SFB 953 and the Alexander-von-Humboldt Foundation is gratefully acknowledged.

HL 101.10 Fri 12:45 H17

Morphological and Electronic Study of Moirè Patterns due to Dislocated Graphene on HOPG — •Dilek Yildiz[1], Şener Şen[2], Oğuz Gülseren[2], and Oğuzhan Gürlü[1] — [1]Istanbul Technical University, Istanbul, Turkey — [2]Bilkent University, Ankara, Turkey

Highly oriented pyrolytic graphite (HOPG) is widely used as a calibration sample for scanning tunneling microscopy (STM) studies. It is also used as a substrate in surface science because of its smooth surface. HOPG is composed of stacked two dimensional hexagonal lattices formed by carbon atoms, popularly named as graphene layers. Because of the weak van der Waals bonding between the graphene layers, the topmost layer may be shifted or rotated on HOPG. Due to the rotation of the top layer, super-periodic structures called as Moiré patterns form on HOPG. These formations were investigated in numerous studies; however, they are rediscovered in graphene research and their origin is still not understood. In this study we used different solvents to see their effects on HOPG samples and the formation of super-periodic structures on these surfaces. We investigate the morphological and electronic properties by using scanning tunneling microscopy and spectroscopy (STM and STS) under ambient conditions. We compared electronic properties of Moiré patterns due to their periodicities. In order to shed light onto the observed electronic structures we also performed ab initio calculations on these super periodic structures. (Supported by TUBITAK 109T687 and ITU-BAP 33263).

HL 102: Quantum dots and wires: Transport

Time: Friday 11:15–13:15 Location: H13

HL 102.1 Fri 11:15 H13

Momentum matching in magnetotunneling spectrocopy on quantum dots coupled to a two-dimensional electron gas — •D. Zhou[1], A. Beckel[1], B. Marquardt[1], A. D. Wieck[2], D. Reuter[2], M. Geller[1], and A. Lorke[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [2]Chair for Applied Solid State Physics, Ruhr-Universität Bochum, Germany

We present results from magnetotunneling spectroscopy of self-assembled InAs QDs, weakly coupled to a 2DEG by a GaAs/AlGaAs tunneling barrier. The QDs are embedded in a heterostructure field-effect-transistor using the 2DEG as reservoir as well as detector. A magnetic field applied in the plane of the 2DEG is used to shift the alignment of the wave functions of the two systems in momentum-space. A time-resolved measurement technique is employed to directly determine the tunneling rates as a function of the magnetic field [1].

We find a strong suppression of the tunneling current by almost two orders of magnitude for fields up to 12 T. However, we find an enhancement in tunneling rates for small magnetic fields (<4 T). Comparison between the calculated and measured tunneling probabilities allows us to obtain detailed information on the QD states, such as size and anisotropy of the wave functions. We conclude that resonant tunneling between the dots and the 2DEG is affected by a nonvanishing momentum component perpendicular to the tunneling current even without an applied magnetic field, i. e. a momentum mismatch that significantly affects the tunneling probability.

[1] A. Beckel et al., Appl. Phys. Lett. **100**, 232110 (2012).

HL 102.2 Fri 11:30 H13

Magnetotransport in nanostructured InAs-based High Electron Mobility Transistors — •Olivio Chiatti[1], Sven S. Buchholz[1], Wolfgang Hansen[2], 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

The controlled creation, manipulation and detection of spin-polarized currents entirely by electrical means is the holy grail of spintronics. A possible tool to this end is the spin-orbit coupling in narrow-gap semiconductors, which couples the momentum (orbital motion) of an electron to its spin. Using nanostructures to filter specific momentum modes using electric fields, it should be possible to create and detect spin-polarized currents. [1] Recently, quantum point contacts (QPCs) fabricated 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 QPCs with in-plane gates in InAs quantum well structures, and performed magnetotransport measurements at temperatures down to 300 mK and in magnetic fields up to 10 T. 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 102.3 Fri 11:45 H13

Magnetically induced quantized electron transport through localized magnetic fields in a quantum point contact — •Bernd Schüler, Mihai Cerchez, Hengyi Xu, and Thomas Heinzel — Heinrich Heine University Düsseldorf, Condensed Matter Laboratory, Universitätsstr. 1, 40225 Düsseldorf, Germany

Quantum Dots (QD) in two-dimensional electron gases are typically defined by nano-patterned gate electrodes [1]. While magnetically confined QDs have been proposed theoretically to show some specific phenomena [2], their experimental implementation is still at an early stage [3]. We have designed a ferromagnet/semiconductor hybrid structure device which allows us to form a QD by combining electrostatic potentials with localized magnetic fields in the form of two magnetic spikes at sub-micron distances. While numerical simulations of this system predict Coulomb blockade in the closed regime and Fano type resonances in the open system [4], we observe experimentally transmission resonances in the open system which can be interpreted as signatures of zero-dimensional states weakly bound by the magnetic field profile.

[1] see, e.g., L. P. Kouwenhoven et al., in Mesoscopic Electron Transport, Series E: Applied Sciences (Eds. L. L. Sohn, L. P. Kouwenhoven and G. Schon (Kluwer, 1997). [2] S.J. Lee et al., Phys. Rep. 394, 1, 2004 [3] A. Tarasov et al., Phys. Rev. Lett. 104, 186801, 2010 [4] H. Xu et al. Phys. Rev. B 84, 035319, 2011

HL 102.4 Fri 12:00 H13

Magnetization of modulation-doped quantum dots prepared from InP/InGaAs heterostructures — •Florian Herzog[1], Benedikt Rupprecht[1], Susanne Goerke[1], Marc Wilde[1], Thomas Schäpers[2], Hilde Hardtdegen[2], Sebastian Heedt[2], Christian Heyn[3], and Dirk Grundler[1] — [1]Physik.-Dep. E10, TU München, D-85748 Garching — [2]Peter Grünberg Institute (PGI-9), FZ Jülich, D-52425 Jülich — [3]Institute of Applied Physics, University of Hamburg, D-20355 Hamburg

High-mobility 2D electron systems (2DESs) formed in modulation-doped InP/InGaAs heterostructures exhibit strong spin-orbit coupling due to both Rashba and Dresselhaus effects. We etched arrays of mesoscopic (diameter $d = 3$ μm) and nanoscopic dots ($d = 400$ nm) out of 2DESs to study the effect of lateral confinement on spin-orbit coupling. On such samples, we performed highly sensitive torque magnetometry at a few 100 mK. We report de Haas-van Alphen oscillations in the magnetization for both mesoscopic and nanoscopic dots observed up to a filling factor of $\nu = 28$. Electron densities are found to be as large as for the unpatterned 2DESs, but oscillation amplitudes are drastically smaller. We attribute this to a depletion region at the dot borders. Financial support by the DFG via the priority program “SPP 1285 -

semiconductor spintronics" and NIM is gratefully acknowledged.

HL 102.5 Fri 12:15 H13

Investigation of Spin-Orbit Coupling in Differently Doped InAs Nanowires — •Sebastian Heedt[1], Thomas Gerster[1], Isabel Wehrmann[1,2], Kamil Sladek[1], Hilde Hardtdegen[1], Detlev Grützmacher[1], and Thomas Schäpers[1,3] — [1]Peter Grünberg Institut (PGI-9) and JARA-Fundamentals of Future Information Technology, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]OSRAM Opto Semiconductors GmbH, 93055 Regensburg, Germany — [3]II. Physikalisches Institut, RWTH Aachen University, 52056 Aachen, Germany

Low-temperature quantum transport is presented for top-gated InAs nanowires prepared by selective area metalorganic vapor phase epitaxy. The carrier concentration and the band profile can be controlled by means of doping or the application of a gate voltage. Phase-coherent transport is investigated for temperatures down to 30 mK and magnetic fields up to 10 T. Utilizing an analytical model for the low-field quantum conductivity correction, we are able to extract the phase coherence length l_ϕ and the spin relaxation length l_{so}. The model applies for diffusive wires with diameters falling short of l_ϕ. It accounts for spin relaxation under linear Rashba and linear and cubic Dresselhaus spin-orbit coupling. To investigate these effects, superimposed universal conductance fluctuations have to be eliminated by averaging magnetic field dependent measurements across a wide gate voltage range. Thus, individual nanowires with different doping concentrations are investigated to gain information on how the doping of the highly spin-orbit coupled InAs nanowires impacts the spin-lifetime.

HL 102.6 Fri 12:30 H13

Electrical characterization of free-standing GaAs nanowires by multitip STM — •Stefan Korte[1], Vasily Cherepanov[1], Bert Voigtländer[1], Matthias Steidl[2,3], Weihong Zhao[2,3], Peter Kleinschmidt[2,3], Thomas Hannappel[2,3,4], and Werner Prost[5] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and JARA-Fundamentals of Future Information Technology — [2]TU Ilmenau, Institut für Physik, Fachgebiet Photovoltaik, D-98684 Ilmenau — [3]Helmholtz-Zentrum Berlin, Institut Solare Brennstoffe und Energiespeichermaterialien, D-14109 Berlin — [4]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, D-99099 Erfurt — [5]Center for Semiconductor Technology and Optoelectronics (ZHO), University of Duisburg-Essen, Germany

III-V semiconductor nanowires are promising candidates for future solar cell designs. p-doped GaAs nanowires are grown on an n-doped GaP(111)B substrate by Au-assisted metal-organic vapor-phase epitaxy (MOVPE). For electrical characterization these free-standing nanowires were contacted using a multitip STM. Four point probe measurements reveal their electrical transport properties. The conductance profile along the nanowires and the diode characteristics of the pn-junction to the substrate were measured. Also the elastic mechanical deformation of nanowires and the influence of bending on their resistance has been studied.

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Ultrafast photocurrents and THz generation in single InAs-nanowires — •Nadine Erhard[1], Paul Seifert[1], Leonhard Prechtel[1], Simon Hertenberger[1], Helmut Karl[2], Gerhard Abstreiter[1], Gregor Koblmüller[1], and Alexander W. Holleitner[1] — [1]Walter Schottky Institut, TU München, 85748 Garching, Germany — [2]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

We apply a recently developed pump-probe photocurrent spectroscopy to clarify the ultrafast temporal interplay of the different photocurrent mechanisms occurring in single InAs-nanowire-based circuits with a picosecond time-resolution [1]. The data are interpreted in terms of a photo-thermoelectric current and the transport of photogenerated holes to the electrodes as the dominating ultrafast photocurrent contributions. Moreover, THz radiation is generated in the optically excited InAs-nanowires, which is interpreted in terms of a dominating photo-Dember effect [2]. The results are relevant for nanowire-based optoelectronic and photovoltaic applications as well as for the design of nanowire-based THz sources. Financial support by the ERC-grant NanoREAL is acknowledged.

[1] L. Prechtel, M. Padilla, N. Erhard, H. Karl, G. Abstreiter, A. Fontcuberta i Morral, and A. W. Holleitner, Nano Lett. 12, 2337 (2012).

[2] Nadine Erhard et al., Annalen der Physik (2013).

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Optoelectronic properties of individually positioned InAs nanowires — •Jan Overbeck, Andreas Brenneis, Julian Treu, Simon Hertenberger, Gerhard Abstreiter, Gregor Koblmüller, and Alexander Holleitner — Walter Schottky Institut and Physik-Department, TU München, 85748 Garching, Germany

Small bandgap semiconducting nanowires offer a promising approach to fabricating nanoscale light-sensitive devices like broadband solar cells or mid-infrared photodetectors. We discuss the optoelectronic properties of individually positioned InAs nanowires on p-Si(111) substrates. The substrates exhibit a top layer of SiO_2 which is structured via e-beam lithography creating holes in the oxide with a diameter of ~ 80 nm. The nanowires are then grown vertically on the patterned substrates by solid-source molecular beam epitaxy. To fabricate optoelectronic devices, the nanowires are subsequently contacted via a thin, semitransparent metal film evaporated on top of an insulating layer (BCB). The p-Si substrate forms the second contact of the optoelectronic two-terminal devices. We discuss spatially resolved photocurrent measurements which give insights into the interplay of optoelectronic dynamics in single nanowires and in the Si-substrates.