Semiconductor Physics Division
Fachverband Halbleiterphysik (HL)

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Overview of Invited Talks and Sessions

(Lecture halls POT 51, 81, 112, 151, 251, and HSZ 403; Poster P1A, P2/2-4OG, and P3)

Invited Talks

HL 6.6	Mon	11:15–11:45	POT 151	**Exciton-Polariton Topological Insulator** — •Sebastian Klembt
HL 7.1	Mon	9:30–10:00	POT 251	**Anharmonic semiconductors - Lessons Learned from Halide perovskites** — •Omer Yaffe
HL 7.2	Mon	10:00–10:30	POT 251	**Lattice Screening of Excitons in Lead Halide Perovskites from First Principles** — •Marina R. Filip, Jonah B. Haber, Jeffrey B. Neaton
HL 7.3	Mon	10:45–11:15	POT 251	**Structural dynamics and disorder in halide perovskites** — •David Egger
HL 18.1	Mon	15:00–15:30	POT 151	**Highly efficient sources of single indistinguishable photons** — •Niels Gregersen
HL 19.1	Mon	15:00–15:30	POT 251	**Double perovskite electronic structures: A chemical perspective** — •Adam Slavney, Hemamala Karunadasa, Linn Leppert, Bridget Connor
HL 19.2	Mon	15:30–16:00	POT 251	**Solid state ionics of hybrid halide perovskites: equilibrium situation and light effects** — •Alessandro Senocrate, Gee Yeong Kim, Tae Youl Yang, Giuliano Gregori, Michael Graetzel, Joachim Maier
HL 20.1	Mon	15:00–15:30	POT 81	**Resonantly hybridized excitons in moiré superlattices in van der Waals heterostructures** — •Alexander Tartakovskii
HL 24.1	Tue	9:30–10:00	POT 151	**Ionic Defects in Hybrid Perovskite Solar Cells** — •Carsten Deibel, Sebastian Reichert, Qingzhi An, Yana Vaynzof
HL 26.1	Tue	9:30–10:00	POT 51	**Nanophotonic quantum technology on silicon chips** — •Carsten Schuck
HL 26.2	Tue	10:00–10:30	POT 51	**Resonant excitation and coherent manipulation of quantum dots for quantum information experiments** — •Ana Predojevic
HL 26.5	Tue	11:15–11:45	POT 51	**Fully on-chip single-photon Hanbury-Brown and Twiss experiment integrating semiconductors and superconductors** — •Simone Luca Portalupi, Mario Schwartz, Ekkehart Schmidt, Ulrich Rengstl, Florian Hornung, Stefan Hepp, Konstantin Ilin, Michael Jetter, Michael Siegel, Peter Michler
HL 27.1	Tue	9:30–10:00	POT 81	**Radiative Lifetime and Fine Structure of Excitons in Transition Metal Dichalcogenide Monolayers** — •Xavier Marie
HL 36.1	Tue	14:00–14:30	POT 51	**Towards One-way Quantum Repeaters with Spin Qubits in Nanophotonic Interfaces** — •Tim Schröder
HL 36.5	Tue	15:15–15:45	POT 51	**Classical computing with quantum states of light** — •Stefanie Barz
HL 39.1	Wed	9:30–10:00	POT 112	**Quantum communication with entangled photons from quantum dots** — •Rinaldo Trotta
HL 48.1	Wed	15:00–15:30	POT 112	**Ultrafast nonadiabatic dynamics and intermolecular conical intersections in organic photovoltaic materials** — •Antonietta De Sio
HL 52.1	Wed	15:00–15:30	POT 81	**Modulation Doping in High-Mobility Alkaline-Earth Stannates** — •Bharat Jalan
HL 52.5	Wed	16:45–17:15	POT 81	**Engineering of LiNbO3 films for next generation acoustic and energy harvesting applications** — •Ausrine Bartasyte, Samuel Margueron, Vincent Astié, Giacomo Clementi, Mihaea Ivan, Merieme Oubahaz

HL 52.6	Wed	17:15–17:45	POT 81	**Oxide Memristors for unified data storage and data processing** — •Heidemarie Schmidt
HL 61.1	Thu	9:30–10:00	POT 51	**Supercontinuum second-harmonic generation spectroscopy of 2D semiconductors** — •Steffen Michaelis de Vasconcellos
HL 61.2	Thu	10:00–10:30	POT 51	**Quasi-instantaneous switch-off of deep-strong light-matter coupling** — •Christoph Lange, Maike Halbhuber, Joshua Mornhinweg, Viola Zeller, Cristiano Ciuti, Dominique Bougeard, Rupert Huber
HL 61.5	Thu	11:30–12:00	POT 51	**Watching plasmonic skyrmions spin using ultrafast two-photon photoelectron spectroscopy** — •Harald Giessen, Tim Davis, Bettina Frank, Pascal Dreher, David Janoschka, Frank Meyer zu Heringdorf
HL 62.1	Thu	9:30–10:00	POT 81	**Basics of Gas Sensing with Semiconducting Metal Oxides** — •Nicolae Barsan
HL 62.6	Thu	11:30–12:00	POT 81	**Ultra-thin oxides on InGaN nanowires: Passivation layers for nanostructured photoelectrodes and optical analysis of chemical processes** — Paula Neuderth, Mariona Coll, Jörg Schörmann, Christian Reitz, Jordi Arbiol, Roland Marschall, •Martin Eickhoff
HL 69.1	Thu	15:00–15:30	POT 151	**Scaling networks of compound semiconductor nanowires** — •Anna Fontcuberta i Morral
HL 71.1	Thu	15:00–15:30	POT 51	**Quadratic nanomaterials for nonlinear integrated photonic devices** — •Rachel Grange
HL 71.2	Thu	15:30–16:00	POT 51	**Resonant nanostructured surfaces for parametric frequency conversion** — •Frank Setzpfandt
HL 81.1	Fri	9:30–10:00	POT 81	**Ultrafast Spin-Lasers** — Markus Lindemann, Natalie Jung, Tobias Pusch, Gaofeng Xu, Pascal Stadler, Igor Zutic, Rainer Michalzik, Martin R. Hofmann, •Nils C. Gerhardt

Invited talks of the joint symposium SYNC

See SYNC for the full program of the symposium.

SYNC 1.1	Mon	9:30–10:00	HSZ 01	**Photonic Reservoir Computing and its Application to Optical Communication** — •Ingo Fischer, Apostolos Argyris
SYNC 1.2	Mon	10:00–10:30	HSZ 01	**Metal-oxide resistance switching memory devices as artificial synapses for brain-inspired computing** — •Sabina Spiga
SYNC 1.3	Mon	10:30–11:00	HSZ 01	**Towards brain-inspired photonic computing** — •Wolfram Pernice
SYNC 1.4	Mon	11:15–11:45	HSZ 01	**Photonic Recurrent Ising Sampler** — •Charles Roques-Carmes, Yichen Shen, Cristian Zanoci, Mihika Prabhu, Fadi Atieh, Li Jing, Tena Dubček, Chenkai Mao, Miles Johnson, Vladimir Čeperić, John Joannopoulos, Dirk Englund, Marin Soljačić
SYNC 1.5	Mon	11:45–12:15	HSZ 01	**Beyond von Neumann systems: Computational memory for efficient AI** — •Irem Boybat

Invited talks of the joint symposium SYSD

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30– 9:55	HSZ 02	**Disentangling transport in topological insulator thin films down to the nanoscale** — •Felix Lüpke
SYSD 1.2	Mon	9:55–10:20	HSZ 02	**Spintronics with Terahertz Radiation: Probing and driving spins at highest frequencies** — •Tom Sebastian Seifert, Tobias Kampfrath
SYSD 1.3	Mon	10:20–10:45	HSZ 02	**Non-radiative voltage losses in organic solar cells** — •Johannes Benduhn
SYSD 1.4	Mon	10:45–11:10	HSZ 02	**Multivalent ions for tuning the phase behaviour of protein solutions** — •Olga Matsarskaia
SYSD 1.5	Mon	11:10–11:35	HSZ 02	**Network Dynamics under Constraints** — •Malte Schröder
SYSD 1.6	Mon	11:35–12:00	HSZ 02	**Exciton spectroscopy of van der Waals heterostructures** — •Philipp Nagler

Invited talks of the joint symposium SYAS

See SYAS for the full program of the symposium.

SYAS 1.1	Mon	15:00–15:30	HSZ 02	**Ultrafast Coherent Spin-Lattice Interactions in Ferromagnets** — •Steven L. Johnson
SYAS 1.2	Mon	15:30–16:00	HSZ 02	**Ab-initio treatment of ultrafast spin-dynamics** — •Sangeeta Sharma, J. K. Dewhurst
SYAS 1.3	Mon	16:00–16:30	HSZ 02	**Light-wave driven Spin Dynamics** — •Martin Schultze, Sangeeta Sharma, Markus Münzenberg
SYAS 1.4	Mon	16:45–17:15	HSZ 02	**All-coherent subcycle switching of spins by THz near fields** — •Christoph Lange
SYAS 1.5	Mon	17:15–17:45	HSZ 02	**Ultrafast optically-induced spin transfer in ferromagnetic alloys** — •Stefan Mathias

Invited talks of the joint symposium SYWH

See SYWH for the full program of the symposium.

SYWH 1.1	Wed	15:00–15:30	HSZ 02	**Engineering 2D materials with a twist** — •Cory Dean
SYWH 1.2	Wed	15:30–16:00	HSZ 02	**Flat Bands and Correlated Electronic States in Two Dimensional Atomic Crystals** — •Eva Y. Andrei
SYWH 1.3	Wed	16:00–16:30	HSZ 02	**Lightwave electronics and valleytronics in van der Waals layered materials** — •Rupert Huber
SYWH 1.4	Wed	16:30–17:00	HSZ 02	**Interaction and Topological Effects in Atomically Thin Two-dimensional Materials** — •Steven G. Louie
SYWH 1.5	Wed	17:00–17:30	HSZ 02	**Excitons in 2D Semiconductors and Heterostructures** — •Alexander Högele

Invited talks of the joint symposium SYED

See SYED for the full program of the symposium.

SYED 1.1	Thu	9:30–10:00	HSZ 01	**Ultrafast electron dynamics at laser-irradiated surfaces** — •Baerbel Rethfeld
SYED 1.2	Thu	10:00–10:30	HSZ 01	**Unraveling Momentum-Dependent Electron-Phonon Coupling and its Role in the Origin of Charge Density Wave Phases** — •Bradley Siwick, Martin Otto, Jan-Hendrik Pohls, Laurent Rene de Cotret, Mark Sutton
SYED 1.3	Thu	10:30–11:00	HSZ 01	**Light MATTERs!!!** — •Hrvoje Petek, Andi Li, Zehua Wang, Marcel Reutzel
SYED 1.4	Thu	11:15–11:45	HSZ 01	**Quantum localization and delocalization of charge carriers in molecular organic crystals** — •Jochen Blumberger
SYED 1.5	Thu	11:45–12:15	HSZ 01	**Single-Atom Catalysis (SAC): How Structure Influences Reactivity** — •Gareth Parkinson

Invited talks of the joint symposium SYES

See SYES for the full program of the symposium.

SYES 1.1	Thu	9:30–10:00	HSZ 02	**Understanding the physical variables driving mechanosensing** — •Pere Roca-Cusachs
SYES 1.2	Thu	10:00–10:30	HSZ 02	**Mechanics of life: Cellular forces and mechanics far from thermodynamic equilibrium** — •Timo Betz
SYES 1.3	Thu	10:30–11:00	HSZ 02	**A hydrodynamic approach to collective cell migration in epithelial tissues** — •Jaume Casademunt
SYES 1.4	Thu	11:15–11:45	HSZ 02	**The spindle is a composite of two permeating polar gels** — David Oriola, Benjamin Dalton, Franziska Decker, Frank Julicher, •Jan Brugues
SYES 1.5	Thu	11:45–12:15	HSZ 02	**Adding magnetic properties to epitaxial graphene** — •Rodolfo Miranda
SYES 2.1	Thu	15:00–15:30	HSZ 01	**Interactions in assemblies of surface-mounted magnetic molecules** — •Wolfgang Kuch

SYES 2.2	Thu	15:30–16:00	HSZ 01	**Towards phononic circuits based o optomechanics** — •Clivia M. Sotomayor-Torres
SYES 2.3	Thu	16:00–16:30	HSZ 01	**Optical properties of 2D materials and heterostructures** — •Janina Maultzsch
SYES 2.4	Thu	16:45–17:15	HSZ 01	**Bringing nanophotonics to the atomic scale** — •Javier Aizpurua
SYES 2.5	Thu	17:15–17:45	HSZ 01	**Infrared signatures of the coupling between vibrational and plasmonic excitations** — •Annemarie Pucci

Invited talks of the joint symposium SYCL

See SYCL for the full program of the symposium.

SYCL 1.1	Fri	9:30–10:00	HSZ 02	**Topology and transport in nanostructures with curved geometries** — •Carmine Ortix
SYCL 1.2	Fri	10:00–10:30	HSZ 02	**Properties of domain walls and skyrmions in curved ferromagnets.** — •Volodymyr Kravchuk
SYCL 1.3	Fri	10:30–11:00	HSZ 02	**3D Mesoscopic Magnetic Architectures: Fabrication, Actuation & Imaging** — •Laura Heyderman
SYCL 1.4	Fri	11:15–11:45	HSZ 02	**3D nanostructures for superconductivity and magnetism** — •Oleksandr Dobrovolskiy
SYCL 1.5	Fri	11:45–12:15	HSZ 02	**Effect of Curvature on Topological Defects in Chiral Condensed and Soft Matter** — •Avadh Saxena

Sessions

HL 1.1–1.4	Sun	16:00–18:40	HSZ 403	**Tutorial: Frontiers of Semiconductor Lasers (joint session HL/TUT)**
HL 2.1–2.12	Mon	9:30–12:45	HSZ 03	**Topological Insulators 1 (jointly with DS, MA, HL, O) (joint session TT/HL)**
HL 3.1–3.4	Mon	9:30–11:40	HSZ 105	**Focus: Diamond Technology and Electronics (joint session KFM/DS/HL)**
HL 4.1–4.13	Mon	9:30–13:00	HSZ 201	**Complex Oxides: Bulk Properties (jointly with DS, HL, KFM, MA, O) (joint session TT/MA/HL)**
HL 5.1–5.10	Mon	9:30–12:30	POT 112	**Organic semiconductors I (joint session HL/CPP)**
HL 6.1–6.11	Mon	9:30–13:00	POT 151	**Heterostructures, interfaces and surfaces (joint session HL/O)**
HL 7.1–7.6	Mon	9:30–12:00	POT 251	**Focus Session: When theory meets experiment: Hybrid halide perovskites for applications beyond solar I (joint session HL/CPP)**
HL 8.1–8.8	Mon	9:30–11:30	POT 51	**Nitrides: Devices**
HL 9.1–9.12	Mon	9:30–13:00	POT 81	**2D semiconductors and van der Waals heterostructures I (joint session HL/DS/O)**
HL 10.1–10.8	Mon	9:30–12:50	TOE 317	**Focus: High-resolution Lithography and 3D Patterning (Part I) (joint session KFM/HL/CPP)**
HL 11.1–11.8	Mon	10:30–12:45	GER 38	**Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions I (joint session O/HL/CPP/DS)**
HL 12.1–12.12	Mon	10:30–13:45	WIL C107	**2D Materials I: Electronic Structure, Excitations, etc. (joint session O/CPP/HL)**
HL 13.1–13.6	Mon	15:00–18:15	HSZ 04	**Focus Session: Spin-Charge Interconversion (joint session MA/HL)**
HL 14.1–14.7	Mon	15:00–16:45	HSZ 103	**Topological Insulators 2 (jointly with DS, MA, HL, O) (joint session TT/HL)**
HL 15.1–15.13	Mon	15:00–18:30	HSZ 201	**Graphene (jointly with DY, MA, HL, DS, O) (joint session TT/DY/HL)**
HL 16.1–16.10	Mon	15:00–17:30	GER 38	**Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions II (joint session O/HL/CPP/DS)**
HL 17.1–17.9	Mon	15:00–17:45	POT 112	**Materials and devices for quantum technology I**
HL 18.1–18.10	Mon	15:00–18:15	POT 151	**Quantum dots and wires I**

HL 19.1–19.6	Mon	15:00–17:00	POT 251	**Focus Session: When theory meets experiment: Hybrid halide perovskites for applications beyond solar II (joint session HL/CPP)**
HL 20.1–20.11	Mon	15:00–18:30	POT 81	**2D semiconductors and van der Waals heterostructures II (joint session HL/DS)**
HL 21.1–21.12	Mon	15:00–18:15	WIL C107	**2D Materials II: Electronic Structure, Excitations, etc. (joint session O/CPP/HL)**
HL 22.1–22.8	Tue	9:30–11:30	CHE 89	**2D Materials and their Heterostructures I (joint session DS/O/HL)**
HL 23.1–23.10	Tue	9:30–12:30	POT 112	**Ultra-fast phenomena**
HL 24.1–24.7	Tue	9:30–12:00	POT 151	**Functional semiconductors for renewable energy solutions I (joint session HL/CPP)**
HL 25.1–25.10	Tue	9:30–12:30	POT 251	**Perovskite and photovoltaics I (joint session HL/CPP)**
HL 26.1–26.5	Tue	9:30–11:45	POT 51	**Focus Session: Integrated Quantum Photonics I**
HL 27.1–27.11	Tue	9:30–13:00	POT 81	**2D semiconductors and van der Waals heterostructures III (joint session HL/DS)**
HL 28.1–28.7	Tue	10:00–12:30	ZEU 222	**Focus: Exploitation of Anisotropy in Organic Semiconductors I (joint session CPP/HL)**
HL 29.1–29.13	Tue	10:30–13:45	GER 38	**2D Materials III: Growth and Heterostructures (joint session O/HL)**
HL 30.1–30.43	Tue	13:30–15:45	P3	**Poster I**
HL 31.1–31.7	Tue	14:00–15:45	HSZ 02	**Complex Oxides: Surfaces and Interfaces (jointly with DS, HL, KFM, MA, O) (joint session TT/MA/HL)**
HL 32.1–32.7	Tue	14:00–15:45	HSZ 201	**Twisted Bilayer Graphene (jointly with DY, MA, HL, DS, O) (joint session TT/HL)**
HL 33.1–33.8	Tue	14:00–16:00	POT 112	**Optical properties**
HL 34.1–34.6	Tue	14:00–15:30	POT 151	**Functional semiconductors for renewable energy solutions II (joint session HL/CPP)**
HL 35.1–35.8	Tue	14:00–16:00	POT 251	**Perovskite and photovoltaics II (joint session HL/CPP)**
HL 36.1–36.5	Tue	14:00–15:45	POT 51	**Focus Session: Integrated Quantum Photonics II**
HL 37.1–37.8	Tue	14:00–16:00	POT 81	**2D semiconductors and van der Waals heterostructures IV (joint session HL/DS/O)**
HL 38.1–38.8	Wed	9:30–13:00	HSZ 04	**Focus Session: Magnon Polarons – Magnon-Phonon Coupling and Spin Transport (joint session MA/HL)**
HL 39.1–39.10	Wed	9:30–12:45	POT 112	**Materials and devices for quantum technology II**
HL 40.1–40.10	Wed	9:30–12:30	POT 151	**Thermal, acoustic and transport properties**
HL 41.1–41.10	Wed	9:30–12:30	POT 251	**Perovskite and photovoltaics III (joint session HL/CPP)**
HL 42.1–42.9	Wed	9:30–12:15	POT 51	**Oxide semiconductors**
HL 43.1–43.12	Wed	9:30–13:00	POT 81	**2D semiconductors and van der Waals heterostructures V (joint session HL/DS/O)**
HL 44.1–44.6	Wed	9:30–11:15	ZEU 222	**Focus: Exploitation of Anisotropy in Organic Semiconductors II (joint session CPP/HL)**
HL 45.1–45.12	Wed	9:30–12:45	ZEU 260	**Hybrid Perovskite and Photovoltaics I (joint session CPP/HL)**
HL 46.1–46.11	Wed	10:30–13:30	GER 38	**Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions III (joint session O/HL/CPP/DS)**
HL 47.1–47.13	Wed	10:30–13:45	WIL B321	**2D Materials IV: Interfacial Interactions (joint session O/HL/CPP)**
HL 48.1–48.7	Wed	15:00–17:30	POT 112	**Organic semiconductors II (joint session HL/CPP)**
HL 49.1–49.11	Wed	15:00–18:15	POT 151	**Quantum dots and wires II**
HL 50.1–50.8	Wed	15:00–17:30	POT 251	**Perovskite and photovoltaics IV (joint session HL/CPP)**
HL 51.1–51.10	Wed	15:00–18:00	POT 51	**Semiconductor lasers I**
HL 52.1–52.8	Wed	15:00–18:15	POT 81	**Focus Session: Functional Metal Oxides for Novel Applications and Devices I (joint session HL/DS)**
HL 53.1–53.5	Wed	15:00–16:15	ZEU 260	**Hybrid Perovskite and Photovoltaics II (joint session CPP/HL)**
HL 54.1–54.9	Wed	15:00–17:30	GER 38	**Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions IV (joint session O/CPP/DS/HL)**

HL 55.1–55.11	Thu	9:30–12:30	HSZ 03	**Superconducting Electronics: SQUIDs, Qubits, Circuit QED, Quantum Coherence and Quantum Information Systems 2 (jointly with MA, HL) (joint session TT/HL)**
HL 56.1–56.5	Thu	9:30–10:45	CHE 89	**2D Materials and their Heterostructures II (joint session DS/O/HL)**
HL 57.1–57.5	Thu	9:30–10:45	CHE 91	**Thin Oxides and Oxide Layers I (joint session DS/HL/O)**
HL 58.1–58.10	Thu	9:30–12:30	POT 112	**Nitrides: Preparation and characterization I**
HL 59.1–59.10	Thu	9:30–12:30	POT 151	**THz and MIR physics in semiconductors**
HL 60.1–60.8	Thu	9:30–12:00	POT 251	**Perovskite and photovoltaics V (joint session HL/CPP)**
HL 61.1–61.9	Thu	9:30–13:00	POT 51	**Focus Session: Tailored Nonlinear Photonics I**
HL 62.1–62.10	Thu	9:30–13:00	POT 81	**Focus Session: Functional Metal Oxides for Novel Applications and Devices II (joint session HL/DS)**
HL 63.1–63.7	Thu	9:30–12:20	TOE 317	**Focus: High-resolution Lithography and 3D Patterning (Part II) (joint session KFM/HL/CPP)**
HL 64.1–64.51	Thu	10:00–13:00	P1A	**Poster II**
HL 65.1–65.6	Thu	11:00–12:30	CHE 89	**2D Materials and their Heterostructures III (joint session DS/HL)**
HL 66.1–66.5	Thu	11:00–12:15	CHE 91	**Thin Oxides and Oxide Layers II (joint session DS/HL)**
HL 67.1–67.9	Thu	15:00–17:30	GER 38	**Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions V (joint session O/HL/DS/CPP)**
HL 68.1–68.7	Thu	15:00–16:45	POT 112	**Nitrides: Preparation and characterization II**
HL 69.1–69.9	Thu	15:00–18:00	POT 151	**Quantum dots and wires III**
HL 70.1–70.7	Thu	15:00–16:45	POT 251	**Spin phenomena in semiconductors**
HL 71.1–71.7	Thu	15:00–17:15	POT 51	**Focus Session: Tailored Nonlinear Photonics II**
HL 72.1–72.6	Thu	15:00–16:30	POT 81	**Focus Session: Functional Metal Oxides for Novel Applications and Devices III (joint session HL/DS)**
HL 73.1–73.9	Thu	15:00–17:30	REC C 213	**Semiconductor Surfaces (joint session O/HL)**
HL 74.1–74.24	Thu	15:00–17:30	P2/2OG	**Poster IIIA**
HL 75.1–75.29	Thu	15:00–17:30	P2/3OG	**Poster IIIB**
HL 76.1–76.26	Thu	15:00–17:30	P2/4OG	**Poster IIIC**
HL 77	Thu	18:00–19:00	POT 81	**Annual General Meeting of the Semiconductor Physics Division**
HL 78.1–78.3	Fri	9:30–10:30	HSZ 03	**Nano- and Optomechanics (jointly with CPP, DS, DY, BP) (joint session TT/HL/CPP)**
HL 79.1–79.9	Fri	9:30–12:00	POT 151	**Quantum dots and wires IV**
HL 80.1–80.8	Fri	9:30–12:00	POT 51	**Quantum transport and quantum Hall effects**
HL 81.1–81.7	Fri	9:30–11:45	POT 81	**Semiconductor lasers II**

Annual General Meeting of the Semiconductor Physics Division

Thursday 18:00–19:00 POT 81

HL 1: Tutorial: Frontiers of Semiconductor Lasers (joint session HL/TUT)

The development of semiconductor lasers has been an unprecedented success story and enabled multiple applications which influence many aspects of our modern society. Most important is world-wide optical data communication which relies crucially on semiconductor lasers. Additionally, medical diagnostics and many optical sensing applications are enabled by such optoelectronic devices. In this tutorial, we will highlight the state-of-the-art of semiconductor laser in high-speed data communication and terrestrial and extraterrestrial gas sensing applications. Moreover, we will present recent progress towards the realization and in-depth understanding of thresholdless nanolasers and topological nanolasers as well as cavity-enhanced lasers based on novel quantum materials as active medium.

Organiser: Stephan Reitzenstein (TU Berlin)

Time: Sunday 16:00–18:40 Location: HSZ 403

Tutorial HL 1.1 Sun 16:00 HSZ 403

Interbandkaskaden und weit abstimmbare Laser las Lichtquellen für Sensorik — •Johannes Koeth, Robert Weih, Nicolas Koslowski und Tim Koslowski — nanoplus GmbH, Gerbrunn, Germany

ICLs zeichnen sich unter anderem dadurch aus, dass die Emissionswellenlänge in einem weiten Bereich des mittleren Infrarot durch die Variation der Quantenfilmdicke weitestgehend unabhängig von der Bandlücke des Halbleiters eingestellt werden kann. Da eine Vielzahl von Gasen ihre stärksten Absorptionslinien im Wellenlängenbereich zwischen 3 und 6 μm zeigen, eignen sich ICL basierte DFB-Laser hervorragend für die hochsensitive Absorptionsspektroskopie. Infolge kontinuierlicher Optimierungen des Schichtaufbaus können mittlerweile selbst Laser mit einer Wellenlänge $\lambda > 5\,\mu m$ im Dauerstrichbetrieb bei Raumtemperatur betrieben werden. Sie benötigen dabei kaum mehr als $200\,mW$ Eingangsleistung und erreichen Ausgangsleistungen von bis zu $10\,mW$. DFB Laser sind sehr gut dazu geeignet Absorptionslinien in einem engen Spektralbereicheben auszumessen. Daneben können auch weit abstimmbare, nach dem Vernier-Prinzip betriebene, Laser für Spektroskopie im nahen und mittleren Infrarot verwendet werden.

Tutorial HL 1.2 Sun 16:40 HSZ 403

Advanced semiconductor lasers for high-speed data communication — •Johann Peter Reithmaier — Institute for Nanostructure Technologies and Analytics (INA), CINSaT, University of Kassel, Germany

An overview will be given on advanced semiconductor lasers and related optoelectronic devices, which are mainly utilizing specific properties of low-dimensional electronic systems, such as quantum dots (QDs) or mixed multi-dimensional systems. The special focus will be on laser properties, which are of highly interest for high-speed optical data communication. In particular, examples will be discussed for high-speed direct modulation, ultra-narrow linewidth lasers for coherent communication and high-speed high-temperature operation of semiconductor optical amplifiers. The tutorial will also give some background for the understanding of the more recent obtained record values of QD lasers in temperature stability, nearly-zero linewidth-enhancement factors and emission linewidths below 30 kHz at room temperature.

Tutorial HL 1.3 Sun 17:20 HSZ 403

Theory of Nanolasers — •Christopher Gies — Institut für Theoretische Physik, Universität Bremen, Otto-Hahn-Allee 1, 28334 Bremen

The tutorial will give an introduction to the colorful physics and the modeling of nanolasers. The origin of rate equation will be discussed, focussing on their merits and shortcomings when describing nanolasers. Especially in the high-β regime, spontaneous emission plays an important role even above the laser threshold, emphasizing the impact of fluctuations on the emission characteristics.

The lecture will cover the quantized light field, open-systems approaches for including dissipation, and photon statistics and its relation to photon-correlation fuctions. A strong emphasis will be on how to relate the theoretical approaches to modeling real experiments.

Tutorial HL 1.4 Sun 18:00 HSZ 403

Lasers for emulating topological and spin systems — •Mercedeh Khajavikhan — University of Southern California, Los Angeles, United States of America

In recent years, there has been a growing interest in using micro- and nano-scale lasers for implementing topological and spin systems. Spin models arise in the microscopic description of magnetic materials, where the macroscopic characteristics are governed by exchange interactions among the constituent magnetic moments. On the other hand, topological features are characterized as properties that remain invariant during continuous deformations of the system. The additional degrees of freedom afforded by gain and loss in active elements provide excellent opportunities to emulate these systems in a versatile photonic platform. In this tutorial, we describe some of the activities by our group and others in utilizing nanolasers and microcavities for implementing topological and spin systems. These studies could pave the way towards a new scalable nanophotonic platform to study spin exchange interactions or topological insulators, that can in turn be potentially exploited to design high power laser arrays, investigate more large-scale networks, emulate some magnetic materials, or to address a variety of optimization problems.

HL 2: Topological Insulators 1 (jointly with DS, MA, HL, O) (joint session TT/HL)

Time: Monday 9:30–12:45 Location: HSZ 03

HL 2.1 Mon 9:30 HSZ 03

2D to 3D crossover in topological insulators — Corentin Morice, •Thilo Kopp, and Arno P. Kampf — University of Augsburg, Augsburg, Germany

At the heart of the study of topological insulators lies a fundamental dichotomy: topological invariants are defined in infinite systems, but their main footprint, surface states, only exists in finite systems. In systems in the slab geometry, namely infinite in two dimensions and finite in one, the 2D topological invariant was shown to display three different types of behaviours. In the limit of zero Dirac velocity along z, these behaviours extrapolate to the three 3D topological phases: trivial, weak and strong topological insulators. We show analytically that the boundaries of these regions are topological phase transitions of particular significance, and allow one to fully predict the 3D topological invariants from finite-thickness information. Away from this limit, we show that a new phase arises, which displays surface states but no band inversion at any finite thickness, disentangling these two concepts closely linked in 3D.

HL 2.2 Mon 9:45 HSZ 03

Correlated Ground States in Maximally Symmetric Flat Bands of 2D Topological Insulators — •Nikolaos Stefanidis and Inti Sodemann — Max-Planck-Institut für Physik komplexer Systeme,Nöthnitzer Str. 38, 01187 Dresden

We study the many body-problem in partially filled topological flat bands that are maximally symmetric realisations of two dimensional time-reversal invariant insulators. These bands can be viewed as two flat bands with opposite Chern numbers that are forced to be degenerate by time-reversal-symmetry. For half-filled bands we develop a mean field description of states that spontaneously break time reversal

symmetry and their competition with translationally broken symmetry states and superconductors. At general fillings we prove a rigorous theorem dictating the absence of exact topological degeneracy for any translational and time reversal invariant two-body Hamiltonian. We also solve exactly the two body problem, which turns out to display a remarkable correlation between the center-of-mass and relative-coordinate degrees of freedom of the two particles.

HL 2.3 Mon 10:00 HSZ 03

Dynamic impurities in two-dimensional topological insulator edge states — •Simon Wozny[1], Martin Leijnse[1], Karel Vyborny[4], Wolfgang Belzig[3], and Sigurdur I. Erlingsson[2] — [1]Division of Solid State Physics and NanoLund, Lund University, Box 118, S-22100 Lund, Sweden — [2]School of Science and Engineering, Reykjavik University, Menntavegi 1, IS-101 Reykjavik, Iceland — [3]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [4]Institute of Physics, Academy of Science of the Czech Republic, Cukrovarnická 10, Praha 6, Czech Republic

Two-dimensional topological insulators give host one-dimensional helical states at the edges. These are characterized by spin-momentum locking and time-reversal symmetry protects the states from backscattering by potential impurities. Magnetic impurities break time-reversal symmetry and allow for backscattering. In an earlier work we investigated the effects of random, static, aligned magnetic impurities [1] on the spectrum and found that for fixed magnetic impurity strength the gap in the density of states closes with rising potential strength. We are now moving on to investigate the effect of random, aligned but harmonically rotating magnetic impurities. This is done by calculating the density of states via the time dependent Green's function for the system.

[1] S. Wozny, K. Vyborny, W. Belzig, and S. I. Erlingsson, Phys. Rev. B 98, 165423 (2018)

HL 2.4 Mon 10:15 HSZ 03

Topology and boundary physics in one dimensionional insulators — •Herbert Schoeller, Niclas Müller, Dante Kennes, and Mikhail Pletyukhov — RWTH Aachen University, Germany

Alternative to the characterization of topological insulators in terms of mathematical invariants we present a practical version via the explicit solution of the Schrödinger equation for a generic half-infinite system in one dimension. We show how the boundary condition can be fulfilled by taking appropriate linear combinations of Bloch eigenstates for the infinite system with complex quasimomentum [1]. Via this scheme all edge and bulk states can be explicitly constructed. In the presence of chiral or particle-hole symmetry the existence and stability of zero-energy edge states together with the bulk-boundary correspondence is established, proving the consistency with the standard classification scheme. Without symmetry constraints, we find generically edge states at finite energy in the gap and show that many bulk states are superpositions of Boch waves and exponentially decaying parts, implying interesting boundary physics at finite energy [2].

[1] D.M. Kennes et al., Phys. Rev. B 100, 041103 (2019).
[2] N. Müller et al., arXiv:1911.02295.

HL 2.5 Mon 10:30 HSZ 03

Topological invariants to characterize universality of boundary charge in one-dimensional insulators beyond symmetry constraints — •Mikhail Pletyukhov[1], Dante Kennes[1], Jelena Klinovaja[2], Daniel Loss[2], and Herbert Schoeller[1] — [1]RWTH Aachen University, Germany — [2]University of Basel, Switzerland

We address universal properties of the boundary charge Q_B for a wide class of tight-binding models with non-degenerate bands in one dimension [1]. We provide a precise formulation of the bulk-boundary correspondence by splitting Q_B via a gauge invariant decomposition in a Friedel, polarisation, and edge part. We reveal the topological nature of Q_B by proving the quantization of a topological index $I = \Delta Q_B - \bar{\rho}$, where ΔQ_B is the change of Q_B when shifting the lattice by one site towards a boundary and $\bar{\rho}$ is the average charge per site. For a single band we find this index to be given by the winding number of the fundamental phase difference of the Bloch wave function between two adjacent sites. For a given chemical potential we establish a central topological constraint $I \in \{-1, 0\}$ related to charge conservation and particle-hole duality.

[1] M. Pletyukhov et al, arXiv: 1911.06886, 1911.06890

HL 2.6 Mon 10:45 HSZ 03

Interaction effects in band insulators with topological properties — •Yen-Ting Lin, Volker Meden, Herbert Schoeller, and Dante M. Kennes — Institute for Theory of Statistical Physics, RWTH Aachen, and JARA- Fundamentals of Future Information Technology

One-dimensional models for band insulators such as the Su-Schrieffer-Heeger model or the Rice-Mele model currently regain attention as they show topological properties. We investigate the spinless versions of these models complemented by a two-particle interaction. To study the bulk as well as boundary and topological properties we use the functional renormalization group. The bulk gap shows the interaction dependent scaling predicted by an effective field theory. The density oscillations of an open boundary are modified by the interaction. The decay length of the exponential part is reduced and the inverse square root behavior of the pre-exponential function is altered. In addition, we present results for the boundary charge and the local single-particle spectral function.

HL 2.7 Mon 11:00 HSZ 03

Magnetoconductance, Quantum Hall Effect, and Coulomb Blockade in Topological Insulator Nanowires — •Raphael Kozlovsky, Ansgar Graf, Denis Kochan, Klaus Richter, and Cosimo Gorini — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

Three-dimensional topological insulator (3DTI) nanowires host topologically non-trivial surface states wrapped around an insulating bulk. We investigate the transport properties of such wires subject to external electric and magnetic fields using effective surface Dirac Hamiltonians. By considering shaped (tapered, curved) 3DTI nanowires, we go beyond the well-studied cylindrical geometry [1] and thereby access intriguing mesoscopic transport phenomena: While the conductance of a wire in perpendicular magnetic field is in general quantized due to higher-order topological hinge states, the conductance in longitudinal magnetic field depends on the precise wire geometry. For rotationally symmetric nanowires with varying radius, a coaxial magnetic field leads to a spatial variation of the enclosed magnetic flux giving rise to a non-trivial mass potential along the wire direction. Depending on the radial profile of the wire, this mass potential leads, for instance, to a conductance governed by the transmission through Dirac Landau levels, or to Coulomb blockade.

[1] arxiv:1909.13124 (2019)

15 min. break.

HL 2.8 Mon 11:30 HSZ 03

Electronic structure and properties of the surface of $TlBiSe_2$ in dependence on the coverage by Fe — •Svitlana Polesya[1], Sergiy Mankovsky[1], Alexander Liebig[2], Franz Giessibl[2], and Hubert Ebert[1] — [1]Dept. Chemistry, LMU Munich, Butenandtstrasse 11, D-81377 Munich, Germany — [2]Inst. Expt. and Appl. Physics, University Regensburg, Regensburg, Germany

We will present the results of investigations on the electronic structure of the surface of of the topological insulator $TlBiSe_2$ with different terminations by means of the tight binding KKR band structure method (TB KKR). The appearance of the topologically protected surface states at the Γ point is found in agreement with ARPES experiment. The modification of these states due to Fe adatoms deposited on top of the surface having different terminations, was investigated as a function of the degree of surface coverage by Fe. This study was performed via the CPA (Coherent Potential Approximation) alloy theory, assuming random occupation of the surface positions by Fe. The exchange coupling parameters have been calculated for different amount of Fe atoms covering the surface in order to determine the magnetic structure of the Fe overlayer, that can be probed by STM experiments.

HL 2.9 Mon 11:45 HSZ 03

MBE-grown Sb_2Te_3/Bi_2Te_3 heterostructures - Tuning of the topological surface states — Vanda M. Pereira, Chi-Nan Wu, Liu Hao Tjeng, and •Simone G. Altendorf — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Topological insulators (TIs) are bulk insulators with the bulk band gap only intersected by conducting, Dirac-cone like surface states that are topologically protected. For many materials, the Dirac point of these surface states lays buried in the bulk bands which hinders an experimental observation of the various theoretically predicted topological quantum effects, like the quantum anomalous Hall effect.

In our study, we combine two TIs, namely Sb_2Te_3 and Bi_2Te_3, in a

heterostructure which allows for a tuning of the position of the Dirac point to the Fermi level by varying the layer thicknesses. Using the optimized layer structure, we investigate the changes of the TI properties when interfaced with a magnetic substrate. We will present a characterization of the MBE-grown Sb_2Te_3/Bi_2Te_3 heterostructures on non-magnetic and magnetic substrates by RHEED, XPS, ARPES, XMCD, and transport measurements.

HL 2.10 Mon 12:00 HSZ 03

Topological insulator interfaced with ferromagnetic insulators: Bi_2Te_3 thin films on magnetite and iron garnets — V. M. Pereira[1], S. G. Altendorf[1], C. E. Liu[1], S. C. Liao[1], A. C. Komarek[1], M. Guo[2], H. -J. Lin[3], C. T. Chen[3], M. Hong[4], J. Kwo[2], L. H. Tjeng[1], and •C. N. Wu[1,2] — [1]MPI CPfS, Dresden, Germany — [2]Dept. of Phys., NTHU, Hsinchu, Taiwan — [3]NSRRC, Hsinchu, Taiwan — [4]Dept. of Phys., NTU, Taipei, Taiwan

We report on our study about the growth and characterization of Bi_2Te_3 thin films on top of $Y_3Fe_5O_{12}(111)$, $Tm_3Fe_5O_{12}(111)$, $Fe_3O_4(111)$, and $Fe_3O_4(100)$ single crystal substrates. Using molecular beam epitaxy, we were able to prepare the topological insulator / ferromagnetic insulator heterostructures with no or minimal chemical reaction at the interface. We observed the anomalous Hall effect on these heterostructures and also a suppression of the weak antilocalization in the magnetoresistance, indicating a topological surface state gap opening induced by the magnetic proximity effect. However, we did not observe any obvious x-ray magnetic circular dichroism (XMCD) on the Te M_{45} edges. The results suggest that the ferromagnetism induced by the magnetic proximity effect via Van der Waals bonding in Bi_2Te_3 is too weak to be detected by XMCD, but still can be observed by electrical transport measurements. This is in fact not inconsistent with reported density-functional calculations on the size of the gap opening.

HL 2.11 Mon 12:15 HSZ 03

Time dependent Rashba coupling at the helical edge — •Lorenzo Privitera[1], Niccolò Traverso Ziani[2], Simone Barbarino[3], Jan Carl Budich[3], and Björn Trauzettel[1] — [1]Institute for Theoretical Physics, University of Würzburg, 97074 Würzburg, Germany — [2]Dipartimento di Fisica, Università di Genova, and SPIN-CNR, Via Dodecaneso 33, 16146 Genova, Italy — [3]Institute of Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany

Time-dependent effects in the edges of quantum spin Hall insulators (QSHI) have been the subject of intense research in the last years. In particular, it was recently pointed out that the interplay of electromagnetic temporal noise with Rashba impurities might play a prominent role in the observed breaking of perfect conductance quantization. In this work we study the conductance of a QSHI edge subjected to the time-periodic oscillations of the strength of a single Rashba impurity. We investigate the perturbative regime of the impurity and examine the effects of repulsive interactions through bosonization. The resulting backscattering current is the sum of three different power laws in driving frequency and voltage, marking a clear distinction from non-helical Luttinger liquids. Furthermore, we find that backscattering can become stronger for weak interactions upon tuning the frequency of the driving. Our results provide a further step in the understanding of time-dependent perturbations in 1d electronic liquids and are of particular interest in view of the technological applications arising from the time-dependent manipulation of topological edge states.

HL 2.12 Mon 12:30 HSZ 03

Thermoelectric effects in a helical edge coupled to a quantum magnet — •Peter Silvestrov[1], Piet Brouwer[2], and Patrik Recher[1,3] — [1]Institute for Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany — [2]Physics Department and Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [3]Laboratory for Emerging Nanometrology Braunschweig, 38106 Braunschweig, Germany

We explore the analogy between a helical edge current interacting with a microscopic magnet and the adiabatic quantum motor[1-3], with special emphasis on thermal effects. These include a thermal engine, in which the thermal gradient is converted directly into mechanical work, a device producing an AC current from the temperature gradient, and an electron refrigerator.

[1] Q. Meng, S. Vishveshwara, and T. L. Hughes, Phys. Rev. B **90**, 205403 (2014).
[2] L. Arrachea and F. von Oppen, Physica E **74**, 596 (2015).
[3] P. G. Silvestrov, P. Recher, and P. W. Brouwer, Phys. Rev. B **93**, 205130 (2016).

HL 3: Focus: Diamond Technology and Electronics (joint session KFM/DS/HL)

Time: Monday 9:30–11:40 Location: HSZ 105

Invited Talk HL 3.1 Mon 9:30 HSZ 105

Doped CVD diamond layers for electronic device applications: Experimental and theoretical study — •Ken Haenen — Institute for Materials Research (IMO), Hasselt University, Diepenbeek, Belgium — IMOMEC, IMEC vzw, Diepenbeek, Belgium

While diamond is considered to be the ultimate wide band gap semiconductor due to its combination of superlative properties, the full understanding of the connection between growth conditions and subsequent layer properties is still lacking. In this presentation, focus is first devoted to the deposition of heavily and lightly B-doped CVD diamond films. Employing microwave plasma enhanced CVD in combination with Ib (100)-oriented high pressure high temperature (HPHT) substrates, the influence of the [C]/[H] ratio on key material properties is presented. This includes the surface morphology, crystal quality, and electrical transport properties by employing a wide range of characterization techniques, i.e.. Hall effect in a wide temperature range, FTIR spectroscopy, Raman spectroscopy, X-ray absorption spectroscopy, XPS, AFM, optical microscopy, and transmission electron microscopy. First principles density functional calculations (DFT) were performed to model the interaction of B with the H-terminated diamond surface, corroborating the observed increase of B-doping incorporation with used methane concentration. The insight offered by the combination of experiment and theory clearly provides a pathway to more efficient doping and enhanced crystal quality. Finally, the use of said layers in Schottky barrier diodes is presented.

Invited Talk HL 3.2 Mon 10:00 HSZ 105

Research and development for fabrication of diamond wafers for industrial use — •Hideaki Yamada — AIST, Osaka, Japan

Figure of merits of diamond as a candidate material in power electronics are superior to those of other materials, such as Si, SiC, and GaN. Especially, recent increase of the power density in power devices for high-frequency use require extremely high thermal conductivity of diamond. On the other hand, because of its stable quantum state under the standard condition, variety of sensors with wide dynamic-range and quantum computing have been studied. Therefore, in addition to its mechanical and optical applications, use of diamond in spintronics as well as electronics have been attracted researchers for variety of future applications in industry. One of the bottle necks for realization of them is in technique to fabricate diamond wafers with large area and sufficient quality under acceptable cost. We have developed techniques to enlarge seed substrates, and process them to wafers. To understand mechanism of the crystal growth, we simulated the growth environment numerically and compared them with experimental results. Our recent trials, achievement and future prospective to solve above issues aiming at realization of the industrial use of diamond will be presented with the related current state-of-the-art.

20 min. break

Invited Talk HL 3.3 Mon 10:50 HSZ 105

Diamond: Material of the future for high power, high frequency devices and quantum applications — •Shannon Nicley — Department of Materials, University of Oxford, Oxford, UK

Diamond is an exceptional material in many ways, not only for its well known hardness and highest room temperature conductivity, but also electronic properties like high electron and hole mobilities and a high electronic breakdown field strength. These properties predict that diamond electronic devices should have superior high power and high

frequency performance over other semiconductor materials. Diamond is also a promising solid-state host for atomic scale defects for quantum applications. The realisation of diamond electronic devices and the full implementation of diamond quantum applications have both been limited in part by our ability to reliably grow high quality single crystal diamond. Control over the incorporation of dopant atoms such as boron and phosphorus is key for high power applications, and the ability to grow high purity, low-strain diamond as well as precisely place quantum defects remain areas of active investigation. I will give an overview of the growth of synthetic diamond and review recent progress in the control of boron and phosphorus doping. I will also present a very recently developed method for the deterministic and accurate placement of optically coherent NV centres using a laser writing technique. I will discuss the challenges in this field and give an outlook for both extreme electronic device and quantum applications.

HL 3.4 Mon 11:20 HSZ 105

Preliminary study of diamond based Kinetic Inductance Detectors — •Francesco Mazzocchi, Dirk Strauss, and Theo Andreas Scherer — Karlsruhe Institute of Technology (IAM-AWP), Hermann Von Helmholtz Platz 1, 76344 Eggenstein-Leopoldshafen

Kinetic Inductance Detectors (KIDs) have proven themselves as a very versatile cryogenic detector technology capable of applications in various fields due to their flexibility of design, sensibility and ease of production. We have recently proposed a polarization sensitive Lumped Elements KID as sensor for an innovative polarimetric diagnostics based on quantum cascade lasers (QCL) for application in the nuclear fusion. Each detector unit is composed by 4 pixels arranged at the vertices of a square, each pixels being sensible to only one polarization direction. The current system is based on niobium nitride (NbN) superconductor over High Resistivity Silicon (HRSi) substrate. Such material delivers good performances but its relatively high dielectric constant and loss tangent lead to increased substrate losses. Using a transparent substrate may improve this aspect and also the radiation resistance of such devices. Diamond is the substrate of choice, being a material already widely studied and used in the fusion environment as high power microwave window, due its outstanding optical and mechanical performances. In this work we present the preliminary design study and simulations for a diamond based Kinetic Inductance Detector with both single and poly-crystalline diamond (SCD/PCD) substrates taken into account.

HL 4: Complex Oxides: Bulk Properties (jointly with DS, HL, KFM, MA, O) (joint session TT/MA/HL)

Time: Monday 9:30–13:00 Location: HSZ 201

HL 4.1 Mon 9:30 HSZ 201

Single-crystal growth and magnetic phase diagram of $TbFeO_3$ — •Alexander Engelhardt[1], Georg Benka[1], Christian Oberleitner[1], Andreas Bauer[1], Andreas Erb[2], and Christian Pfleiderer[1] — [1]Physik Department E51, Technische Universität München, 85748 Garching, Germany — [2]Walther-Meißner-Institut, Walther-Meißner-Str. 8, 85748 Garching, Germany

Single crystals of the multiferroic rare earth orthoferrite $TbFeO_3$ were synthesized by means of optical float-zoning. The magnetization, the longitudinal and the transverse ac susceptibility, as well as the specific heat were measured at low temperatures under large applied magnetic fields to determine the complex, anisotropic magnetic phase diagram of $TbFeO_3$ along the three major crystallographic axes. Taken together, our data are consistent with previous studies reported in the literature. As a new result we identify clear evidence in the bulk properties of the formation of a soliton lattice in a small temperature range, so far observed by means of neutron scattering only.

HL 4.2 Mon 9:45 HSZ 201

Melting of excitonic dispersion in $LaCoO_3$: theory and experiment — Atsushi Hariki[1], Ru-Pan Wang[2], Andrii Sotnikov[1,3], Keisuke Tomiyasu[4], Davide Betto[5], Nicholas B. Brookes[5], Yohei Uemura[2], Mahnaz Ghiasi[2], Frank M. F. de Groot[2], and •Jan Kuneš[1,6] — [1]Institute of Solid State Physics, TU Wien — [2]Debye Institute for Nanomaterials Science, Utrecht University — [3]Akhiezer Institute for Theoretical Physic, Kharkiv — [4]Department of Physics, Tohoku University — [5]European Synchrotron Radiation Facility, Grenoble — [6]Institute of Physics, Czech Academy of Sciences

We present Co L_3-edge resonant inelastic x-ray scattering (RIXS) on bulk $LaCoO_3$ across the thermally-induced spin-state crossover around 100 K. Owing to a high energy resolution of 20 meV, we observe unambiguously the dispersion of the intermediate-spin (IS) excitations in the low temperature regime. Approaching the intermediate temperature regime, the IS excitations are damped and the bandwidth reduced. The observed behavior can be well described by a model of mobile IS excitons with strong attractive interaction, which we solve using dynamical mean-field theory for hard-core bosons. Our results provide a detailed mechanism of how HS and IS excitations interact to establish the physical properties of cobaltite perovskites.

HL 4.3 Mon 10:00 HSZ 201

Spin Selective Quasi-Particle Interference in $PdCoO_2$ — •Dibyashree Chakraborti[1,2], Chi Ming Yim[1], Luke Rhodes[1], Seunghyun Khim[2], Andrew Mackenzie[1,2], and Peter Wahl[1] — [1]School of Physics and Astronomy, St. Andrews, Scotland, United Kingdom, KY169SS — [2]Max Planck Institute of Chemical Physics of Solids, Noethnitzer Strasse, Dresden -01187

The metallic delafossite $PdCoO_2$, which is among the most conductive oxides currently known (at 295 K) [1], has risen to prominence due to interesting physical effects, such as unusually long mean free paths, leading to hydrodynamic effects being observed in electron flow [2]. Further, recent Angle Resolved Photoemission Spectroscopy (ARPES) studies have reported exciting surface-physics on the CoO_2-terminated surface. The CoO_2 surface shows evidence of large Rashba spin-splitting, arising from the interplay of energy scales due to strong spin orbit coupling and inversion symmetry breaking at the surface. [3]. In this study, we have identified and investigated the CoO_2 termination of $PdCoO_2$ with low temperature Scanning Tunneling Microscopy (STM). We present and discuss the quasi-particle interference imaging of the Rashba spin-split surface state, and the implications for possible spintronics applications.

[1] C.W. Hicks et al., Phys. Rev. Lett. 109, 116401 (2012)
[2] P.J.W. Moll et al., Science 351, 1061 (2016)
[3] V. Sunko et al., Nature 549, 492 (2017)

HL 4.4 Mon 10:15 HSZ 201

Interplay of Electronic and Spin Degrees in Ferromagnetic $SrRuO_3$: Anomalous Softening of the Magnon Gap and Stiffness — •Kevin Jenni[1], Stefan Kunkemöller[1], Daniel Brüning[1], Thomas Lorenz[1], Yvan Sidis[2], Astrid Schneidewind[3], Augustinus Agung Nugroho[4], Achim Rosch[5], Daniil Iljitsch Khomskii[1], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln, Deutschland — [2]Laboratoire Leon Brillouin, Grenoble, Frankreich — [3]JCNS, Forschungszentrum Jülich, Garching, Deutschland — [4]Institut Teknologi Bandung, Indonesien — [5]Institut für Theoretische Physik, Universität zu Köln, Deutschland

We succeeded to grow large single crystals of $SrRuO_3$ using the floating-zone technique [1,2]. The first inelastic neutron scattering study of the spin dynamics on single crystals yields the expected quadratic spin wave dispersion of a ferromagnet. However the magnon gap and stiffness considerably deviate from an earlier inelastic neutron scattering study on powders [3]. In addition we find a non-monotonous temperature dependence of the anisotropy gap and a softening of the magnon stiffness upon cooling. We discuss how Weyl points caused by SOC in $SrRuO_3$ couple electronic and spin degrees of freedom and how this interplay leads to the characteristic behavior in the spin dynamics [4].

[1] S. Kunkemöller et al., Chrys. Res Tec. 51, 299 (2016)
[2] S. Kunkemöller et al., PRB 96, 220406(R) (2017)
[3] S. Itoh et al., Nat. Commun. 7, 11788 (2016)
[4] K. Jenni et al., Phys. Rev. Lett. 123, 017202 (2019)

HL 4.5 Mon 10:30 HSZ 201

Ca_2RuO_4: DFT + DMFT study of the magnetic order and dynamical susceptibility — •Dominique Geffroy[1,2], Kyo-Hoon

Ahn[1], Hoshin Gong[4], and Jan Kuneš[1,3] — [1]TU Wien, Vienna, Austria — [2]Masaryk University, Brno, Czech Republic — [3]Czech Academy of Science, Prague, Czech Republic — [4]Max Planck POSTECH/Korea Research Initiative, Pohang, Korea

Relativistic Mott insulators are complex compounds in which spin and orbital degrees of freedom become entangled due to a large spin-orbit coupling. Previous studies, both experimental and theoretical[1, 2], have shown that they are good candidates for novel forms of order, including excitonic magnetism[3]. We report results on the theoretical study of the prototypical relativistic Mott insulator Ca_2RuO_4. We use a realistic ab initio DFT + DMFT approach including SU(2) Coulomb interaction and spin-orbit coupling. The emergence of antiferromagnetic order at low temperature is correctly described. We present and discuss the spectra of the the collective modes in the ordered phase within the DMFT approximation.

[1] Jain et al., Nat. Physics 13, 633 (2017)
[2] G. Zhang and E. Pavarini, Phys. Rev. B 95, 075145 (2017)
[3] A. Akbari and G. Khaliullin, Phys. Rev. B 90, 035137 (2014)

HL 4.6 Mon 10:45 HSZ 201

LDA+DMFT Approach to Resonant Inelastic X-Ray Scattering in Rare-Earth Nickelates — •Mathias Winder[1], Atsushi Hariki[1], and Jan Kuneš[1,2] — [1]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria — [2]Institute of Physics, Czech Academy of Sciences, Na Slovance 2, 182 21 Praha 8, Czechia

We present a computational study of L-edge resonant inelastic x-ray scattering (RIXS) across the metal-insulator transition (MIT) of $LuNiO_3$. We apply exact diagonalization to a material specific Anderson impurity model with a by DMFT obtained hybridization function. In contrast to other available methods, this approach enables us to describe simultaneously localized (d-d) and delocalized (unbound electron-hole pair) excitations in the RIXS spectra. We reproduce the experimentally observed behaviour of fluorescence-like and Raman-like features across the MIT and provide its material specific interpretation.

HL 4.7 Mon 11:00 HSZ 201

Interplay of electronic correlations, charge disproportionation and lattice in $RNiO_3$ nickelates with R = Lu, Y, and Bi — •Ivan Leonov — M. N. Mikheev Inst. of Metal Physics, Yekaterinburg, Russia — NUST 'MISiS', Moscow, Russia

In recent years, increasing attention has been drawn to the understanding of the rare-earth-element nickelate perovskites $RNiO_3$, which exhibit a sharp metal-insulator transition (MIT). The MIT is accompanied by a structural phase transformation, complicated by the appearance of unusual charge order and non-collinear magnetic phases in the Mott insulating regime. Here, I will focus on this particular problem and will discuss an application of the DFT+DMFT method to explore the electronic structure, magnetic and lattice properties of a series of $RNiO_3$ nickelates with R = Lu, Y, and Bi. I will discuss our results for the pressure-induced Mott MIT in $RNiO_3$, which is found to be accompanied by a structural transformation. While the rare-earth and Bi $RNiO_3$ are closely related in their electronic state and crystal structure, these materials exhibit sufficiently different electronic properties. Our results for $BiNiO_3$ suggest the important role of the Bi 4s charge ordering (charge difference of ∼0.52 electrons), with a charge transfer between the Bi 4s and O 2p states and a stable Ni^{2+} configuration, for understanding of the MIT in $BiNiO_3$ [1]. We find that electronic correlations are important to explain the electronic structure, magnetic state, and lattice stability of $RNiO_3$ (R = Lu, Y, and Bi).

[1] I. Leonov et al., Phys. Rev. B **100**, 161112(R) (2019).

15 min. break.

HL 4.8 Mon 11:30 HSZ 201

Origin of orbital ordering in $LaTiO_3$ and $YTiO_3$ — •Xuejing Zhang and Eva Pavarini — Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany

The origin of orbital ordering (OO) in correlated oxides is strongly debated. Two main mechanisms have been proposed as possible explanation for OO phenomena. The first is the classical Jahn-Teller effect and the second is the electronic super-exchange, introduced by Kugel-Khomskii. In the case of the paradigmatic e_g systems $KCuF_3$ and $LaMnO_3$ it has been shown that the electronic Kugel-Khomskii mechanism is not sufficient to drive the OO transition alone, at the temperatures at which orbitally order is typically observed by the co-operative Jahn-Teller distortion.[1,2] In the case of t_{2g} compounds, however, the problem remains open. In these systems both the electron-lattice coupling and the hopping integrals are typically smaller than those for e_g compounds; on the other hand, orbital degeneracy is larger, which enhances the effects of super-exchange. Here we investigate representative t^1_{2g} systems in which OO is observed, the Mott insulators $LaTiO_3$ and $YTiO_3$. We show that the Kugel-Khomskii transition temperature is about 390 K, comparable to the one of $KCuF_3$. This shows that static distortions are needed to explain the presence of OO at high temperature.

[1] E. Pavarini, E. Koch and A. I. Lichtenstein, Phys. Rev. Lett. 101, 266405 (2008).
[2] E. Pavarini and E. Koch, Phys. Rev. Lett. 104, 086402 (2010).

HL 4.9 Mon 11:45 HSZ 201

Charge transport in oxygen-deficient $EuTiO_3$: The emerging picture of dilute metallicity in quantum-paraelectric perovskite oxides — •Johannes Engelmayer[1], Xiao Lin[1], Christoph Grams[1], Raphael German[1], Tobias Fröhlich[1], Joachim Hemberger[1], Kamran Behnia[2], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Laboratoire Physique et Etude de Matériaux, PSL Research University, 75005 Paris, France

Quantum paraelectric $SrTiO_3$ is a large-gap band insulator that becomes metallic upon electron doping already at extremely small charge-carrier concentrations $\simeq 5 \times 10^{17}\mathrm{cm}^{-3}$. The observed T^2 resistivity in this material challenges conventional theories for electron–electron scattering. We report on a study of charge transport in the related compound $EuTiO_3$ where the carrier density is tuned via reduction. Because of a lower electric permittivity, the metal–insulator transition (MIT) in $EuTiO_{3-\delta}$ occurs at higher carrier densities compared to doped $SrTiO_3$. The critical carrier concentration n_c for the MIT is discussed in the context of the so-called Mott criterion and compared with other doped perovskite compounds with a quantum-paraelectric parent. Similar to doped $SrTiO_3$, $EuTiO_{3-\delta}$ shows a distinct AT^2 resistivity, where the prefactor A scales with n. Using a simple three-band model, the $A(n)$ behavior in doped perovskite titanates can be described over a large range of n.

Funded by DFG via CRC1238 and via ANR-DFG LO 818/6-1 and HE 3219/6-1.

HL 4.10 Mon 12:00 HSZ 201

Magnetic Phase diagram and thermal expansion studies of $NiTiO_3$ — •Kaustav Dey[1], Sven Sauerland[1], Johannes Werner[1], Rabindranath Bag[2], Surjeet Singh[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute of Physics , Heidelberg University, Germany — [2]IISER Pune, Maharashtra, India

We report the magnetic phase diagram of $S = 1$ magnetodielectric $NiTiO_3$ single crystals grown by the optical floating zone technique. The high-quality single crystals have been studied by specific heat, by magnetometry up to 60 T, and by thermal expansion and magnetostriction measurements up to 15 T, respectively. The compound evolves long-range antiferromagnetic order at $T_N = 22.5$ K with spins lying in the $ab-$plane. Pronounced anomalies in the thermal expansion coefficients $(\alpha_i, (i = a, b))$ at T_N indicate strong magnetoelastic coupling in $NiTiO_3$. Magnetic length and entropy changes as detected by α and c_p obey Grüneisen scaling which evidences one dominant (spin) degree of freedom driving the transitions. In addition, the magnetic phase diagram features a spin-reoriented phase below $B_c = 1.2$ T which suggests the presence of a small in-plane anisotropy. Notably, spin-reorientation is associated with a first-order-like anomaly in the magnetostriction. The high-field behavior of magnetization is linear and isotropic with saturation at 36 T thereby facilitating constructing the entire magnetic phase diagram.

HL 4.11 Mon 12:15 HSZ 201

Low-Energy Excitations in $NiTiO_3$ and $Ni_{0.25}Mn_{0.75}TiO_3$ Probed by Antiferromagnetic Resonance — •Martin Jonak, Kaustav Dey, Johannes Werner, Changhyun Koo, and Rüdiger Klingeler — Kirchhoff Institute of Physics, Heidelberg University, Heidelberg, Germany

We study magnetic excitations in $NiTiO_3$ and $Ni_{0.25}Mn_{0.75}TiO_3$ by means of X-band and high-frequency electron spin resonance spectroscopy. Our data for $NiTiO_3$ show that in the antiferromagnetically ordered and spin-reoriented phase, i.e. below T_N and in external magnetic fields above the spin-reorientation field $B_C = 1.13(8)$ T, antiferromagnetic resonance (AFMR) modes are well described by

a two-sublattice model with an easy *ab*-plane. Correspondingly, two zero-field excitation gaps are deduced at $\Delta_1 \approx 15$ GHz and $\Delta_2 = 185(2)$ GHz, respectively. At $B < B_C$, an additional magnon mode is observed, which rules out a simple two-sublattice model, thereby contradicting the presently established picture of the low-field ground state. The strongly Mn-doped $Ni_{0.25}Mn_{0.75}TiO_3$ exhibits at least two antiferromagnetically ordered phases. The low-temperature phase shows AFMR modes of a two-sublattice antiferromagnet with anisotropy gaps $\Delta_1 = 29(1)$ GHz and $\Delta_2 = 139(3)$ GHz.

HL 4.12 Mon 12:30 HSZ 201

Electronic transformations in the semi-metallic transitional oxide Mo_8O_{23} — •Venera Nasretdinova[1], Yaroslav Gerasimenko[1,2], Jernej Mravlje[2], Gianmarco Gatti[3], Petra Sutar[2], Damjan Svetin[1,2], Anton Meden[4], Viktor Kabanov[2], Alexander Kuntsevich[5,6], Marco Grioni[3], and Dragan Mihailovic[1,2] — [1]CENN Nanocenter, Ljubljana, Slovenia — [2]JSI, Ljubljana, Slovenia — [3]Institute of Physics, EPFL, Lausanne, Switzerland — [4]University of Ljubljana, Slovenia — [5]LPI of RAS, Moscow, Russia — [6]HSE, Moscow, Russia

Mo_8O_{23} is a low-dimensional stoichiometric transitional metal oxide from MoO_{3-x} family. Its room-temperature phase associated with charge density wave (CDW) is accompanied by non-monotonic resistivity at low temperatures well below structural transitions. Using tunneling and angle-resolved spectroscopy, transport measurements and density functional calculations we reveal electronic transformations leading to a multi-band correlated ground state [1, 2]. We observe the metal-to-insulator transition at 343 K in resistivity, consistent with CDW onset. At low temperatures, the picture with the only CDW order parameter is broken by the onset of the correlated ground state visible both in transport and spectroscopic probes. Spatially-resolved tunneling spectroscopy studies reveal the emergent electronic texture. We discuss the possible origins of the electronic order that emerge in the absence of any structural or magnetic transitions.

[1] V. Nasretdinova et al., Phys.Rev. B 99, 085101 (2019)
[2] V. Nasretdinova et al., Sci. Rep. 9, 15959 (2019)

HL 4.13 Mon 12:45 HSZ 201

Cr and Ce magnetic ordering in $CeCrO_3$:revisited — •Neetika Sharma[1], Reinhard K. Kremer[1], Clemens Ritter[2], and Fereidoon S. Razavi[3] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany — [2]Institute Laue Langevin, Grenoble 38000, France — [3]Department of Physics, Brock University, St. Catharines, ON, L2S 3A1, Canada

We have investigated the magnetic structure of $CeCrO_3$ using neutron powder diffraction (NPD). $CeCrO_3$ crystallizes with the $GdFeO_3$ structure-type (Pbnm). Earlier neutron diffraction measurements on $CeCrO_3$ have proposed a G-type afm structure for the Cr and a C-type for the Ce sublattice. The analysis of the magnetic structure for the Ce sublattice had been based on one magnetic peak (102) at d $\sim$ 3.152 Å. However, the proposed C-type coupling for Ce will generate primarily two magnetic Bragg peaks (100) at d $\sim$ 5.47 Å and (102) at d $\sim$ 3.152 Å. We have collected NPD patterns on a sample of $CeCrO_3$ using ILL's D20 high-intensity medium resolution diffractometer and did observe the previously reported magnetic Bragg peak at d $\sim$ 3.152 Å, however significantly less intense than reported before. Simulations indicate that only the presence of magnetic coupling of C-type on the Cr- and the Ce- sublattices can lead to a situation where the magnetic peak (102) at d $\sim$ 3.152 Å is a lot stronger than the (100) Bragg peak at d $\sim$ 5.47Å. Following this proposal we have analyzed our neutron diffraction data very carefully at low temperature (1.5K), and conclude a CyGz type magnetic ordering for the Cr sub-lattice with a very small Cy-component and Cy type coupling for Ce - sublattice.

HL 5: Organic semiconductors I (joint session HL/CPP)

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

HL 5.1 Mon 9:30 POT 112

Towards a plastic brain — •Matteo Cucchi, Hans Kleemann, Hsin Tseng, Alexander Lee, and Karl Leo — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Technische Universität Dresden, 01062 Dresden, Germany

Interconnectivity, fault tolerance and dynamic evolution of the circuitry have been long sought-after objectives of bio-inspired electronics and engineering. The massive parallelization of the neuronal circuitry grants the human brain superior efficiency and capabilities in cognitive learning and pattern recognition compared to digital, transistor-based machines. Here, we developed a technique to grow conductive networks and artificial synapses based on organic semiconductors. Their dendritic growth, stimulated by an AC signal, resembles the formation of new synapses in the nervous system (synaptogenesis). Moreover, their functions in saline solution emulate numerous brain features over multiple orders of magnitude in the time domain, such as learning, forgetting, time-dependent-spiking plasticity, and Pavlovian conditioning. We employ the artificial synapses to show a new device-concept capable of recognizing numerical patterns and explore possible pathways towards biocompatibility, neuroprosthetics and brain-inspired computing.

HL 5.2 Mon 9:45 POT 112

Dibenzopentacene single crystals: growth, characterization and exciton dispersion — •Lukas Graf, Fupin Liu, Bipasha Debnath, and Martin Knupfer — IFW Dresden

Pentacene and its hydrocarbon relatives continue to attract researchers world-wide, as they promise applications due to their relatively high charge carrier mobilities and their intriguing photophysical behavior including singlet fission processes. We have studied a relatively unexplored member of this family, Dibenzopentacene (DBP).

Single crystals of DBP have been grown using the vapor phase transport method, which to the best of our knowledge are the first DBP single crystals reported so far. We have determined the DBP crystal structure using X-ray diffraction and complementary electron diffraction experiments. The electronic excitations of DBP have been investigated using electron energy-loss spectroscopy (EELS). We present results on the strongly anisotropic electronic excitations across the band gap, and in addition their momentum behavior, i.e. their dispersion. An analysis of this exciton dispersion using a simple model from the literature allowed to gain first information on the charge carrier hopping parameters in DBP.

This is supported by the DFG (KN393/25, KN293/26).

HL 5.3 Mon 10:00 POT 112

Self-alignment OTFT structures — •Jörn Vahland, Hans Kleemann, and Karl Leo — TU Dresden, IAP

Organic thin film transistor (OTFT) parameters have significantly improved in regard to static transistor performance, e.g. contact resistance and mobility. The dynamic performance, though, is mainly governed by the device capacitance. A large device capacitance restricts the switching frequency and might ultimately lead to inefficient circuits. Historically, this limitation has been overcome in inorganic device architectures by employing a so-called self-aligned gate structure, which allows structuring of source- and drain-electrode with virtually no overlap to the gate, yielding low overlap capacitance.

The transfer to OTFTs is not trivial, since subtractive process steps such as etching need to be selective to various materials within a typical device stack i.e. the semiconductor and the gate dielectrics. First implementations of self-alignments for OTFTs employ process steps which are unfortunately not scalable (such as through-plane exposure or lift-off), effectively prohibiting such devices in actual circuits.

We propose a coplanar OTFT in top gate configuration where selective etching processes and additional passivation layers are used in order to form a truely self-aligned organic transistor. We discuss the scaling of the overlap capacitance and highlight the potential of such self-aligned devices for high-frequency operation. Furthermore, we discuss the influence of etching process on the channel properties, and describe how charge carrier mobility and on/off ratio of the transistor can be preserved.

HL 5.4 Mon 10:15 POT 112

Exciton dispersion in rubrene single crystals — •Tobias Lettmann and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, 48149 Münster

Rubrene single crystals are proposed as components of various organic (opto-)electronic devices. Their electronic (quasiparticle) bandstructure shows an anisotropic behaviour with a relatively strong dispersion of several 100 meV along the Γ-Y direction, whereas the bands are almost flat along the Γ-X direction [1].

Corresponding to the electronic bands, excitons can also exhibit dispersion of their excitation energies as a function of their total momentum (related to their centre-of-mass motion). This dispersion and its anisotropy might be relevant for excitonic hopping transport. In this talk we use the GW/BSE approach of many-body perturbation theory (MBPT) to calculate the excitonic bandstructure of rubrene single crystals in order to investigate if the anisotropy is still present or mitigated by excitonic effects.

[1] S. Yanagisawa et al., Phys. Rev. B **88**, 115438 (2013)

HL 5.5 Mon 10:30 POT 112

Conductivity studies at the crystal-film charge transfer interfaces — •Bipasha Debnath[1], Michael Bretschnieder[1], Shu-Jen Wang[2], Martin Knupfer[1], Yulia Krupskaya[1], and Bernd Büchner[1] — [1]Leibniz Institute for Solid State and Material Research Dresden, Dresden, Germany — [2]Dresden Integrated Center for Applied Physics and Photonic Materials (IAP), Dresden, Germany

The charge transfer occurs at the interface of two organic semiconductor materials known as donor and acceptors. The alignment of the electron affinity of one material with the ionization potential of other material leads to enhance electrical conductivity at their interface by exchanging charge carriers between them. Herein, we try to explore the underlying mechanism of charge transfer with a systematic study by preparing interfaces between Rubrene and F6-TCNNQ, as donor and acceptor semiconductor materials, respectively. By thermally evaporating F6-TCNNQ film on the surface of highly-ordered Rubrene single-crystals, the charge transfer interfaces are fabricated. The electrical characterization of these interfaces reveals enhanced conductivity. Furthermore, temperature-dependent measurements demonstrate thermally activated conductivity. The fundamental properties such as charge carrier density and mobility are investigated through additional Hall-effect measurements. This work is financially supported by DFG (KR 4364/4-1)

30 min. break.

HL 5.6 Mon 11:15 POT 112

Investigation of biodegradable devices — •Kevin Krechan[1], Daniel Firzlaff[2], Hans Kleemann[1], Karl Leo[1], and Kathrin Harre[2] — [1]Technische Universität Dresden, Deutschland — [2]HTW Dresden, Deutschland

In an aging society there is an increasing need for innotative health care and monitoring solutions. Sensor solutions for health monitoring are vital for improved treatment quality and the reduction of costs.

In particular, there is a strong need to continuous postoperative in-vivo surveillance systems. However, such sensor systems are required to be bio-compatible and ideally biodegradable in order to undesired postoperative complications.

In this contribution we discuss sensor concepts for e.g. in-vivo pressure or ion sensing based on bio-compatible organic semiconductor materials. Most importantly, we make use of biodegradable collagen-based substrate materials and discuss their decomposition behavior as well as the associated challenges during the fabrication of the sensor system. Overall, we believe that our approaches will enable the development of fully degradable sensor tags in future.

HL 5.7 Mon 11:30 POT 112

High-gap donor-acceptor blends exhibiting both efficient emission and charge-generating properties — •Xiangkun Jia[1], Sascha Ullbrich[1], Johannes Benduhn[1], Vasileios C. Nikolis[1], Jinhan Wu[1], Yuan Liu[1], Axel Fischer[1], Donato Spoltore[1], Sebastian Reineke[1], and Koen Vandewal[1,2] — [1]Technische Universität Dresden, Dresden, Germany — [2]Hasselt University, Hasselt, Belgium

We demonstrate that the intermolecular charge-transfer (CT) states at the donor-acceptor interfaces are crucial for the operation of organic optoelectronics. Such D-A based OLEDs show electroluminescence external quantum yields (EQE_{EL}) of up to 16%, while in contrast, D-A systems for state-of-the-art OSCs typically only feature $EQE_{EL} \approx 0.01 - 0.0001\%$. The dominating non-radiative recombination in the latter is the main reason for their large voltage losses and low power-conversion efficiencies. Here, we adopt high-gap materials to increase the energy of CT states. This blend shows a fill factor of 70% and an internal quantum efficiency of 83% upon solar illumination, comparable to well performing OCSs. Meanwhile, its non-radiative voltage loss is reduced to $0.10V$ and EQE_{EL} reaches 1.5%. This work therefore shows that efficient photogeneration of free carriers and a high electroluminescence quantum yield do not necessarily need to be mutually exclusive in organic semiconductors.

HL 5.8 Mon 11:45 POT 112

Quantifying the Damage Induced by Monoatomic Ion Beam Etching during X-ray Photoemission Spectroscopy Depth Profiling of Conjugated Polymers — •Yvonne Jasmin Hofstetter[1,2] and Yana Vaynzof[1,2] — [1]Integrated Center for Applied Physics and Photonics, Dresden, Germany — [2]Center for Advancing Electronics Dresden, Dresden, Germany

X-ray photoemission spectroscopy (XPS) depth profiling using monoatomic Ar+ ion etching sources is commonly used to probe the vertical compositional profiles of polymer-based organic photovoltaic devices, focusing on compositional variations across interfaces and vertical phase separation within bulk-heterojunction active layers. The damage induced by the monoatomic etching is generally considered to be very shallow and is assumed to not significantly alter the XPS signal acquired at each step of the depth profile. Herein, we quantify the damage depth for a variety of conjugated polymers for monoatomic Ar+ ion beams of variable energy from 0.5 to 4 keV. Our results indicate that even when etching with the lowest available ion beam energy for as little as 3 s, the damage inside the polymer bulk material significantly exceeds the XPS probing depth (approx. 10 nm). We find that the damaged material exhibits a distorted composition which strongly changes the resulting XPS depth profile. In contrast, we find that Ar gas cluster ion beam etching is significantly less damaging and preserves compositional information demonstrating its superior suitability for XPS depth profiling of organic materials.

HL 5.9 Mon 12:00 POT 112

Momentum dependent investigation of electronic excitations in β-metal-phthalocyanines — •Louis Philip Doctor and Martin Knupfer — Leibniz Institut für Festkörper- und Werkstoffforschung, Helmholtz Str. 20, 01069 Dresden

This work presents an investigation of the electronic excitations of β-metal-phthalocyanines. We prepared 120 nm thick thin films by physical vapour deposition, which afterwards underwent an annealing process. Infrared spectroscopy revealed that the annealed films were in the β-phase. The films were further characterised in the visible regime. The prominent feature in this regime is the Q-band, which consists of four peaks arising from the HOMO to LUMO transition split by solid-state effects. Furthermore, the dispersion of the Q-band was measured using electron energy loss spectroscopy. We found a complex momentum dependent behaviour. Most interesting is the negative dispersion of the lowest-lying excitation, which also has a tremendous effect on the performance of optoelectronic devices. This redshift partially correlates with the intermolecular distance and the charge carrier transfer integrals. The latter were determined by a theoretical model, which describes the interaction of Frenkel and charge transfer excitons in metal-phthalocyanines. Our results clearly indicate a prominent influence of charge transfer excitons to the lowest electronic excitations.

HL 5.10 Mon 12:15 POT 112

Comparing Charge Generation and Extraction in Y6 and LM11 Devices — •Seyed Mehrdad Hosseini[1], Yingping Zou[2], and Safa Shoaee[1] — [1]Institute of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Straße 24-25, Potsdam-Golm D-14476, Germany — [2]College of Chemistry and Chemical Engineering, Central South University, Changsha 410083, P.R. China

In the last few years, non-fullerene acceptors (NFA) have dominated organic solar cells. Whilst in thin films, exceptional fill-factor (FF) can be obtained, in thicker junctions however, FF is usually affected. Reduced FF is the manifestation of voltage-dependent charge photogeneration and/ or inefficient free charge extraction3. In this study, we compare two NFAs, named Y6 and LM11, when blended with PM6. Our results show that although PM6:LM11 device has a higher open-circuit voltage (Voc) than PM6:Y6, lower FF limits the efficiency. We employed time-delayed collection field (TDCF) measurements to reveal the reason behind the poorer FF in PM6:LM11 device by studying charge generation and recombination in both systems.

HL 6: Heterostructures, interfaces and surfaces (joint session HL/O)

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

HL 6.1 Mon 9:30 POT 151

Determining the band alignment of copper oxide-gallium oxide heterostructures — •Sebastian Leonard Benz, Martin Becker, Angelika Polity, Sangam Chatterjee, and Peter Jens Klar — Institute for Experimental Physics I and Center for Materials Research (LaMa), Justus Liebig University Giessen, Germany

The copper oxides cuprite (Cu_2O) and tenorite (CuO) are ideal candidates for solar cells as they promise high conversion efficiencies according to the Shockley-Queisser limit[1]. However, both cannot readily be doped n-type, hampering charge-carrier extraction of the photoexcited electron-hole pairs. The combination of the copper oxides with gallium sesquioxide is considered an excellent heterojunction system for overcoming this challenge. In such a pn junction, the p-type copper oxide layer will act as absorber and the transparent n-type gallium sesquioxide as window layer. In these devices, the band alignment at the internal interface is crucial for the device performance. Here, we study the band alignments of different copper oxide-gallium sesquioxide heterostructures by X-ray photoelectron spectroscopy. Within the experimental margin of error, Cu_2O-α-Ga_2O_3 appears to offer the most favourable band alignment for photovoltaic applications.

[1] William Shockley and Hans J. Queisser (March 1961). Journal of Applied Physics. 32 (3): 510*519.

HL 6.2 Mon 9:45 POT 151

Nanometer Scale Characterization of Al/TiOx/SiOx Electron Selective Passivating Contacts Utilizing Advanced TEM Methods — •Christoph Flathmann[1], Tobias Meyer[1], Valeriya Titova[2,3], Jan Schmidt[2,3], and Michael Seibt[1] — [1]University of Goettingen, IV. Physical Institute, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Institute for Solar Energy Research Hamelin (ISFH), Emmerthal, Am Ohrberg 1, 31860, Germany — [3]Institute of Solid-State Physics, Leibniz University Hannover, Hannover, Appelstraße 2, 30167, Germany

One promising possibility to further increase photovoltaic efficiency and to enable new solar cell designs is the development of carrier selective passivating contacts. A particularly interesting electron selective passivating contact consists of an n-type crystalline Si base with tunnel silicon oxide (SiO_x), atomic layer deposited sub-stoichiometric titanium oxide (TiO_x) and aluminum as a rear contact. It is commonly assumed that SiO_x ensures high chemical interface passivation, whilst oxygen vacancies in the TiO_x result in an increased open circuit voltage. However, the detailed interplay of structure, composition and electrical properties is not entirely understood yet. We, therefore, apply various STEM techniques, such as EDX, EELS and 4D-STEM, to characterize such contacts for differently treated samples. The analytical methods show strong interdiffusion at the interfaces; in particular, intermixing of Al and TiO_x appears to be important for contact quality. Furthermore, the capabilities of medium resolution 4D-STEM to elucidate properties of such interfaces are explored.

HL 6.3 Mon 10:00 POT 151

direct insight into the structure-property relation of interfaces from first-principles crystal structure prediction — •lin sun[1], miguel a. l. marques[2,3], and silvana botti[1,3] — [1]Institut für Festkörpertheorie und Optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Institut für Physik - Martin-Luther-Universität Halle, D-06099 Halle, Germany — [3]European Theoretical Spectroscopy Facility

In this work we develop an efficient and accurate computational scheme aimed at a full understanding of heterogeneous materials. Our approach is a variant of the minima-hopping method for global crystal structure prediction. Specifically, we implement a constraint library and we enable variations of the atomic density in proximity to the interface. DFT and DFTB calculations supply necessary energy and forces to the minima-hopping algorithm. With this method, we find a rich polymorphism in the reconstructions of tilt boundaries in polycrystalline silicon, with recurring bonding patterns that we classify in increasing energetic order. In several cases, we succeed in identifying atomic arrangements that are significantly more stable than previously predicted structures, while in other cases we show that the algorithm can recover, without experimental input, geometries that had been built by hand to match experimental data. We extend then the calculations to other group IV elements, and compare lowest energy reconstructions of C, Si, Ge and Sn grain boundaries. Finally, a clear relation between bonding patterns and electrically active interface states is unveiled and discussed.

HL 6.4 Mon 10:15 POT 151

Effect of KF and RbF post-deposition treatments on the electronic structure of the CdS/Cu(In,Ga)Se2 interface in thin-film solar cells investigated by Kelvin Probe and Photoelectron Yield Spectroscopy — •Marin Rusu[1], Tim Kodalle[2], Leo Choubrac[1], Sergiu Levcenco[1], Nicolas Barreau[3], Christian Kaufmann[2], Rutger Schlatmann[2], and Thomas Unold[1] — [1]Struktur und Dynamik von Energiematerialien, Helmholtz-Zentrum Berlin für Materialien und Energie, Lise-Meitner Campus, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]PVcomB, Helmholtz-Zentrum Berlin für Materialien und Energie, Schwarzschildstr. 3, 12489 Berlin, Germany — [3]Institut des Matériaux Jean Rouxel (IMN)-UMR6502, Université de Nantes, 2 rue de la Haussinière, 44322 Nantes Cedex 3, France

We investigate the impact of potassium fluoride (KF) and rubidium fluoride (RbF) post-deposition treatments on electronic features of the Cu(In,Ga)Se2 (CIGSe) layer and CdS/CIGSe interface in a sequential time-dependent CdS thickness evolvement over the chemical bath deposition (CBD) process. Kelvin Probe and Photoelectron Yield Spectroscopy methods have been employed. Although we observe similarities with the reported data, we observe additional distinct features. We find that after an initial CBD stage the valence band maximum of the CIGSe surface is significantly shifted (by 180-620 mV) towards the Fermi level. In addition, K and Rb act as compensating dopants in CdS. Energy level diagrams are proposed and discussed.

HL 6.5 Mon 10:30 POT 151

Template-Guided Programmable Janus Heteronanostructure Arrays for Efficient Plasmonic Photocatalysis — •Zhiqiang Zeng, Rui Xu, Huaping Zhao, and Yong Lei — Technische Universität Ilmenau, 98693, Ilmenau, Germany.

Janus heteronanostructures (HNs), as an important class of anisotropic nanomaterials, could facilitate synergistic coupling of diverse functions inherited by their comprised nanocomponents. Nowadays, synthesizing deterministically targeted Janus HNs remains a challenge. Here, a general yet scalable technique is utilized to fabricate an array of programmable Janus HNs based on anodic aluminum oxide binary-pore templates. By designing and employing an overetching process to partially expose four-edges of one set of nanocomponents in a binary-pore template, selective deposition and interfacing of the other set of nanocomponents is successfully achieved along the exposed four-edges to form a densely packed array of Janus HNs on a large scale. In combination with an upgraded two-step anodization, the synthesis provides high degrees of freedom for both nanocomponents of the Janus HNs, including morphologies, compositions, dimensions, and interfacial junctions. Arrays of TiO2-Au and TiO2/Pt NPs-Au Janus HNs are designed, fabricated, and demonstrated about 2.2 times photocurrent density and 4.6 times H2 evolution rate of that obtained from their TiO2 counterparts.

30 min. break.

Invited Talk HL 6.6 Mon 11:15 POT 151

Exciton-Polariton Topological Insulator — •Sebastian Klembt — Technische Physik, Wilhelm-Conrad-Röntgen-Research Center for Complex Material Systems, and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Topological insulators (TIs) constitute a striking example of materials in which topological invariants are manifested in robustness against perturbations. The most striking characteristic is the emergence of topological edge states at the interface between areas with distinct topological invariants. The observable physical effect is unidirectional, robust edge transport, immune to disorder or defects. TIs have at first been observed in the integer quantum Hall effect in fermionic systems of correlated electrons. However, during the past decade the concepts of topological physics have been introduced into numerous fields be-

yond condensed matter, including photonic systems. Recently, TIs were proposed in exciton-polariton systems organized as honeycomb lattices, under the influence of a magnetic field. Exciton-polaritons are the new eigenstate quasiparticles resulting from the strong coupling of quantum well excitons to light in an optical microcavity mode. Here, we demonstrate experimentally the first exciton-polariton TI and as such the first symbiotic light-matter TI. In polaritonic honeycomb lattices, we show the existence of a C = 2 Chern TI, manifesting in a chiral, topologically protected edge mode. Notably, due to the driven-dissipative nature of polaritons this is an open system, with a strong non-linearity still preserving the topological mode.

HL 6.7 Mon 11:45 POT 151

Quantum spin Hall quantum point contacts — •Niccolo Traverso Ziani[1], Bjoern Trauzettel[2], Christoph Fleckenstein[2], Lorenzo Privitera[2], and Maura Sassetti[1] — [1]Università degli Studi di Genova, Genova, Italy — [2]Universitaet Wuerzburg, Wuerzburg, Deutschland

The edges of two-dimensional topological insulators are fashinating systems. In order to fully exploit their potential, gaps need to be induced. While superconducting gaps can be implemented, magnetic and interaction-related ones seem to be experimentally challenging. We propose a wide range of possibilities enabled by the gaps that can open when constrictions between helical edges[1] are created. Jackiw-Rebbi charges[2], Majorana bound states[3], parafermions[4] and Floquet bound states[5] are addressed.

[1] J. Strunz, J. Wiedenmann, C. Fleckenstein, L. Lunczer, W. Beugeling, V. L. Mueller, P. Shekhar, N. Traverso Ziani, S. Shamim, J. Kleinlein, H. Buhmann, B. Trauzettel, and L. W. Molenkamp, Nat. Phys. (2019).

[2] C. Fleckenstein, N. Traverso Ziani, and B. Trauzettel EPL (Europhysics Letters) 121, 57003 (2018).

[3] C. Fleckenstein, N. Traverso Ziani, and B. Trauzettel, in preparation

[4] C. Fleckenstein, N. Traverso Ziani, and B. Trauzettel, Phys. Rev. Lett. 122, 066801 (2019)

[5] C. Fleckenstein, N. Traverso Ziani, L. Privitera, M. Sassetti, and B. Trauzettel, arXiv:1908.11719

HL 6.8 Mon 12:00 POT 151

Correlation of optical properties and interface morphology in type-II semiconductor heterostructures — •Luise Rost, Jannick Lehr, Milan Maradiya, Wolfgang Stolz, and Wolfram Heimbrodt — Department of Physics and Materials Sciences Center, Philipps-Universität Marburg, Germany

The (Ga,In)As/GaAs/Ga(As,Sb) material system is used for lasers operating over a wide spectral range in the infrared. To further optimize the design of such heterostructures, it is important to have deep understanding of the influence of the interface morphology and the charge carrier dynamic through the interface. Here (Ga,In)As/GaAs/Ga(As,Sb) type-II double quantum well heterostructures has been grown by metall-organic vapor phase epitaxy. A growth interruption procedure was used to intentionally modify the morphology of the internal interfaces. The heterostructures were investigated using continuous wave and time-resolved photoluminescence spectroscopy. A correlation was revealed between the interface morphology and optical and kinetic properties. AFM images of the as grown interface surfaces show substantially smoother interfaces both on vertical as well as lateral length scales. We will illustrate that for every used material there is a matching growth interruption time to further enhance the optical response of such a type-II heterostructure.

HL 6.9 Mon 12:15 POT 151

First-principles study of the structural and electronic properties of the GaAsxP1-x surface — •Marsel Karmo and Erich Runge — TU ILmenau, Weimarer Str.32, 98693 ILmenau

GaAsP is a III-V semiconductor alloy, which forms crystals in zincblende structure. Due to its high electron mobility, it is an important material in optoelectronics, mainly for solar cells. For the latter, it is important to understand the surface relaxation and reconstruction in the P-rich MOVPE process. We use the Vienna Ab initio Simulation Package (VASP) to perform first-principles calculations to identify the composition-dependent surface reconstructions and bonding-sites for adsorbates.

HL 6.10 Mon 12:30 POT 151

Copper iodide thin films: Dynamic AFM studies of local electrical properties — •Tillmann Stralka, Chang Yang, Holger von Wenckstern, and Marius Grundmann — Solid State Physics, Leipzig, Germany

The search for high-performance p-type transparent conductive materials has been a major challenge in decades [1]. Copper iodide (CuI) or alloys based on CuI [2] could offer a solution, since CuI does outperform all other known p-type TCMs, concerning transmittance in the visible spectrum as well as electrical conductivity at room temperature [3]. In this contribution polycrystalline CuI thin films grown by sputtering, are investigated. Hereby we try to understand the impact of grains and grain boundaries (GBs) on transport mechanisms. Topographic features as GBs lead to a depletion of majority charge carriers and even a localized inversion (two dimensional electron gas) within GBs [4]. To acquire morphological and electrical properties with a high spatial resolution we employ atomic force microscopy, which additionally offers different modes to characterize electrical properties (such as: capacitance, conductivity and work function). These measurements will be conducted and evaluated with a novel approach that offers voltage spectroscopy and localization of sub-nm sized objects at the same time and furthermore correlate topographic features with electrical properties.

[1] M. Grundmann et al., J.Phys.D.Apps.Phys., 49(213001), 2016 [2] T. Jun et al., Adv. Mater. 30(1706573), 2018 [3] C. Yang et al., PNAS 113(412929) [4] M. Kneiß et al., Adv. Mater. Interfaces, 5(6), 2018

HL 6.11 Mon 12:45 POT 151

Stability and Tunneling Transport Properties of $NiSi_2$-Si Interfaces — •Florian Fuchs[1,2,3,4], Sibylle Gemming[2,3], and Jörg Schuster[1,2,3,4] — [1]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany — [2]Chemnitz University of Technology, Chemnitz, Germany — [3]Center for Advancing Electronics Dresden (cfaed), Dresden, Germany — [4]Forschungsfabrik Mikroelektronik, Berlin, Germany

Metal-semiconductor interfaces are of huge importance for applications and are considered for various modern device architectures. We study the interface between $NiSi_2$ and silicon on the basis of density functional theory. Different crystal orientations and strain states are investigated systematically. The energetically most favorable interface orientation is worked out, which can explain recent experimental observations [1]. Using atomistic quantum transport simulation, the tunneling transport through the interface is calculated [2]. The transport is related to underlying properties including the Schottky barrier height and the effective mass. This is done on the basis of the Wentzel-Kramers-Brillouin approximation, which can describe the tunneling transport reasonably well. Finally, the Schottky barrier height and its strain dependence is discussed in the context of the metal-induced gap states model.

[1] Khan et al., *Appl. Sci.* **9**, 3462 (2019)
[2] Fuchs et al., *J. Phys.: Condens. Matter* **31**, 355002 (2019)

HL 7: Focus Session: When theory meets experiment: Hybrid halide perovskites for applications beyond solar I (joint session HL/CPP)

Hybrid halide perovskites are by now well established solar absorber and emitter materials, with power conversion efficiencies of single cell devices exceeding 20%. We have observed - with notable exceptions - a widening gap between experimental and theoretical efforts in the literature on halide perovskites. Further, a large fraction of the literature focuses on properties relevant for optoelectronic applications, while we envision a much wider scope for these materials, e.g in spintronic and electro-chemical applications. The purpose of this focus session is to provide a platform for theorists and experimentalists

working in this field, to interact, present state-of-the-art methods, and exchange their ideas on future directions for this technologically relevant class of materials beyond the current focus on optoelectronics.

Organizers: Linn Leppert (Universiät Bayreuth) and Felix Deschler (TU Munich)

Time: Monday 9:30–12:00 Location: POT 251

Invited Talk HL 7.1 Mon 9:30 POT 251

Anharmonic semiconductors - Lessons Learned from Halide perovskites — •Omer Yaffe — Weizmann Institute of Science, Rehovot, Israel

In semiconductor physics, the dielectric response, charge carrier mobility and other electronic material properties at finite temperatures, are always treated within the framework of the harmonic approximation. This approach is very successful in capturing the properties of tetrahedrally bonded semiconductors such as silicon and GaAs.

In my talk, I will show that 2D and 3D halide perovskites are fundamentally different due to their strongly anharmonic lattice dynamics. Large amplitude, local polar fluctuations induced by lattice anharmonicity localize the electronic states and enhance the screening of electric charge within the material. In other words, in some aspects, halide perovskites behave more like a liquid than a crystalline solid. I will also discuss the implications of these findings on other families of semiconductors such as organic and rock-salt semiconductors.

Invited Talk HL 7.2 Mon 10:00 POT 251

Lattice Screening of Excitons in Lead Halide Perovskites from First Principles — •Marina R. Filip[1], Jonah B. Haber[2], and Jeffrey B. Neaton[2,3,4] — [1]Department of Physics, University of Oxford — [2]Department of Physics, UC Berkeley — [3]Molecular Foundry and Materials Science Division, Lawrence Berkeley National Laboratory — [4]Kavli Energy NanoSciences Institute at Berkeley

Dielectric screening in semiconducting and insulating crystals generally originates both from electrons and polar phonons. Since photoexcited electron-hole pairs interact within this dielectric environment, both the electronic and lattice components of the screening can have important contributions to excitonic properties; for lead-halide perovskites, this is suggested from both theoretical and experimental evidence [1,2]. However, standard ab initio GW-BSE methodology for calculating optical excitations does not capture dynamic lattice polarization effects. In this talk I will present our extension of the GW-BSE method, to include lattice contributions to the screening. I will show that in heteropolar semiconductors with weakly bound excitons, dynamic lattice polarization can significantly reduce the exciton binding energy, and I will demonstrate this effect for the CsPbX3 (X = Cl, Br, I) perovskites. Furthermore, I will discuss more generally the lattice contribution to the exciton binding energy in heteropolar semiconductors, as it emerges from a generalization of the Wannier-Mott model to include dynamical lattice polarization effects. [1] Miyata et al, Nat. Phys. 11, 582 (2015) [2] Umari et al, JPCL, 9, 3, 620 (2018). Work supported by the US DoE in the C2SEPEM center; computational resources from NERSC.

15 min. break.

Invited Talk HL 7.3 Mon 10:45 POT 251

Structural dynamics and disorder in halide perovskites — •David Egger — Department of Physics, Technical University of Munich, 85748, Garching, Germany

Halide perovskites (HaPs) are highly promising materials for several optoelectronic applications. HaPs are also very interesting scientifically because of the peculiar structural dynamics that occur in the material. These include the appearance of massive structural disorder and anharmonic effects already at room temperature, which challenge our currnent understanding of coupling between lattice vibrations and optoelectronic properties in a semiconductor.

In this talk, I will present our recent explorations of the consequences of the unusual structural phenomena in HaPs for their optoelectronic properties. Theoretical calculations based on density functional theory, molecular dynamics, and tight-binding modeling will be used to examine the impact of structural dynamics on pertinent device-relevant observables. Consequences of the structural dynamics and anharmonicity in HaPs will be discussed for the charge-carrier mobility, Urbach energy, and defect energetics. It will be shown that the impact of the unusual structural dynamics on the optoelectronic properties of HaPs cannot be neglected when understanding these materials microscopically and designing new functional compounds.

HL 7.4 Mon 11:15 POT 251

Optoelectronic properties of lead-free double-perovskites from first principles — •Raisa I. Biega[1], Marina R. Filip[2,3], Linn Leppert[1], and Jeffrey B. Neaton[2,3,4] — [1]Institute of Physics, University of Bayreuth, Bayreuth, Germany — [2]Department of Physics, University of California, Berkeley, USA — [3]Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, USA — [4]Kavli Energy NanoSciences Institute, Berkeley, USA

Power conversion efficiencies of single junction solar cells with lead-based halide perovskite absorbers have exceeded 25%. However, stability concerns have stimulated efforts for finding substitutes with similar optoelectronic properties, i.e., small band gaps, low effective masses and small exciton binding energies. Double perovskites containing alternating mono- and trivalent metal cations have emerged as one such alternative. Here we present first principles calculations of the electronic structure and excited states of the double perovskites Cs_2AgBX_6 (B=Bi, Sb and X=Br, Cl). We use density functional theory and *ab initio* Green's function-based many-body perturbation theory within the GW and Bethe-Salpeter equation approach to calculate band structures and absorption spectra of these materials. Our results provide insights into the nature of optical excitations and suitability for photovoltaic and other light harvesting applications.

We acknowledge computational resources provided by NERSC, a DOE Office of Science User Facility supported by the U.S. Department of Energy and financial support by the DFG Programs SFB840 and GRK1640.

HL 7.5 Mon 11:30 POT 251

First principles calculations for blue-emitting organic-inorganic halide perovskites — •Ivor Loncaric[1], Luca Grisanti[1], Jasminka Popovic[1], and Aleksandra Djurisic[2] — [1]Rudjer Boskovic Institute, Zagreb, Croatia — [2]The University of Hong Kong

Ruddlesden-Popper halide perovskite (RPP) materials are of significant interest for light-emitting devices since their emission wavelength can be controlled by tuning the number of inorganic layers n. However, RPP films typically contain phases with different n which hinders the achievement of pure blue emission from n=2 films. Furthermore, energy funneling phenomenon, which involves energy transfer from lower n (higher energy) to higher n (lower energy) domains resulting in a brighter, but red-shifted emission, represents the further difficulty in obtaining pure blue emission from n=2 RPP emitters. By performing DFT calculations at room temperature we obtained an improved understanding of the effect of spacer cation on RPP properties. The calculations can be compared to real experimental conditions and give an insight into the feasibility of the stabilization of n=2 perovskite phase.

HL 7.6 Mon 11:45 POT 251

Computing temperature-dependent band gap distributions of halide perovskites with a first-principles tight-binding approach — •Maximilian J. Schilcher[1], Matthew Z. Mayers[2], Liang Z. Tan[3], David R. Reichman[2], and David A. Egger[1] — [1]Department of Physics, Technical University of Munich, 85748 Garching, Germany — [2]Department of Chemistry, Columbia University, New York, NY 10027, USA — [3]Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

Due to their remarkably soft lattice and large temperature-induced nuclear fluctuations, it is challenging to understand the microscopic origin of the fascinating optoelectronic properties of halide perovskites (HaPs). In order to reveal their electronic and optical characteristics, one can apply well-established theoretical methods, such as density functional theory (DFT). However, conventional DFT calculations are limited in addressing the impact of complex structural effects in HaPs that require the simulation of large supercell sizes and nuclear dynamical phenomena.

In this work, we employ a recently developed tight-binding (TB) approach [1], which is parametrized on the basis of DFT calculations, and apply it to trajectories obtained from efficient molecular dynamics

calculations at various temperatures. We compute dynamic band-gap distributions for several HaPs to estimate the influence of temperature on these distributions, in order to explain the electronic and optical characteristics of HaPs around room temperature.

[1] M. Z. Mayers, et al., Nano Lett. 18, 8041-8046 (2018).

HL 8: Nitrides: Devices

Time: Monday 9:30–11:30 Location: POT 51

HL 8.1 Mon 9:30 POT 51

Extreme laser background suppression for resonant fluorescence of a quantum emitter — •Meryem Benelajla[1,2], Elena Kammann[1], and Khaled Karrai[1] — [1]attocube systems AG, Eglfinger Weg 2, 85540 Haar bei München — [2]LPCNO INSA CNRS UPS, 135 Av. Rangueil , 31077 Toulouse, France

Semiconductor nanostrustures are promising candidates for developing a broad range of single photon technologies. Relevant demonstrations in this field has been carried out by resonantly coupling a laser beam to a quantum emitter. However, such challenging measurements require the suppression of laser background by several order of magnitudes.One way to do that is to use cross polarization confocal microscopy. Normally, high quality commercial crossed polarizers allows a laser suppression down to 5 to 6 orders of magnitudes. Surprisingly, when used in combination with a confocal microscope, the extinction ratio is boosted up to 9 order of magnitudes. This unexpected but very welcome enhancement finds its origin in the Imbert-Fedorov effect, now commonly referred to as Spin Hall effect of light, which manifests itself in the reflectivity of a Gaussian laser beam off a mirror. In this presentation, we will discuss in details the physics and optics of such a remarkable effect, which we mapped in details for the first time.

HL 8.2 Mon 9:45 POT 51

Realizing tunnel junctions in MOVPE-grown AlGaN-based UVC LEDs emitting at 233 nm — •Verena Montag[1], Luca Sulmoni[1], Frank Mehnke[1], Martin Guttmann[1], Christian Kuhn[1], Norman Susilo[1], Johannes Glaab[2], Tim Wernicke[1], Markus Weyers[2], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Berlin

A highly conductive and UV-transparent p-AlGaN layer is needed to overcome the strong absorption and the poor current spreading of p-contacts in deep UV LEDs. However, transparent p-AlGaN layers exhibit high sheet and contact resistances resulting in very large operating voltages. A promising alternative to standard p-contacts is the injection of holes into the AlGaN quantum well by tunnel heterojunctions (TJs) allowing for low resistivity n-layers and n-contacts on both sides of the device. This way, a transparent top n-AlGaN layer can be used as an excellent current spreading layer together with a metal reflector enhancing the light extraction. We have successfully demonstrated fully transparent AlGaN-based TJ-LEDs emitting at 233 nm grown entirely by MOVPE. A thin GaN interlayer was implemented to enhance carrier tunneling at the TJ interface. Typically, the operation voltages, the output powers and the external quantum efficiencies of a 0.15 mm^2 TJ-LED featuring a 8 nm thick GaN interlayer are 24 V, 83 μW and 0.16%, respectively, measured on wafer at 10 mA in cw operation.

HL 8.3 Mon 10:00 POT 51

GaN:Ge as transparent conductive nitride contact layer for blue tunnel-junction LEDs — •Christoph Berger, Silvio Neugebauer, Cleophace Seneza, Hartmut Witte, Jürgen Bläsing, Armin Dadgar, and André Strittmatter — Otto-von-Guericke-Universität Magdeburg

Using germanium as a shallow donor for n-type GaN films grown by metalorganic vapor-phase epitaxy, we achieve very high electron concentrations of up to 2 x 10^{20} cm^{-3} and low specific bulk resistivities down to 3 x 10^{-4} Ωcm. Under optimized growth conditions, no degradation of the crystalline quality is observed and layers exhibit high optical transparency making highly doped GaN:Ge very attractive for different application fields. One promising application of such n^{++}-layers is the achievement of transparent conductive nitride (TCN) contacts with excellent current spreading on top of LEDs, edge emitting laser diodes or vertical-cavity surface-emitting lasers (VCSELs). Such intrinsic TCN contacts offer significant lower absorption than conventionally used Iindium Tin Oxide layers, which is helpful to increase the output power of light emitting devices or to decrease the threshold current for VCSELs. Therefore, we realized tunnel-junction LEDs by capping conventional pn-LED structures with TCN contacts using GaN:Ge layers. We will discuss structural, electrical and optical characteristics of fabricated tunnel junction LEDs and compare them with standard LEDs.

HL 8.4 Mon 10:15 POT 51

Effects of degradation on the electrooptical properties of UVB-LEDs measured by temperature dependent electroluminescence spectroscopy — •Jakob Höpfner[1], Priti Gupta[1], Martin Guttmann[1], Jan Ruschel[2], Johannes Glaab[2], Tim Kolbe[2], Arne Knauer[2], Tim Wernicke[1], Markus Weyers[2], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics, Berlin, Germany — [2]FBH, Berlin, Germany

The operation of UVB-LEDs induces changes in their electrooptical behaviour, especially a reduction in the emission power. As the lifetime of a device is a key property for its application, it is important to understand the processes governing their degradation behavior. We report an investigation on UVB-LEDs emitting at 310 nm before and after aging (1000 h at 100 mA (67 A cm^{-2}) and heatsink temperature of 70 °C) using temperature(T)–dependent electroluminescence spectroscopy from 20 K – 340 K. Before aging, the external quantum efficiency (EQE) at 10 mA gradually increases with decreasing temperature from 0.8 % at 340 K to 1.8 % at 150 K and then levels off. This is similar to the expected change in radiative recombination efficiency (η_{rad}) with decreasing temperature due to the reduction of the non-radiative recombinations, indicating that EQE(T) is dominated by η_{rad}. After aging, the EQE reduces to 0.45 % (340 K) and the EQE(T) shows a constant increase with decreasing temperature peaking at 1.4 % (80 K). Below 80 K, a sharp droop in EQE is observed in the case of aged LED. These findings indicate a reduction in both η_{rad} and injection efficiency as degradation mechanism in aged LEDs.

HL 8.5 Mon 10:30 POT 51

Speeding up LED design using experimental device data in the nextnano software — •Maria Cecilia da Silva Figueira, Alex Trellakis, Takuma Sato, Carola Burkl, and Stefan Birner — nextnano GmbH, Lichtenbergstr. 8, 85748 Garching b. München, Germany

We present a simple but a very efficient way to speed up the design or optimization of new devices, by importing experimental data of a previous design or prototype directly into a simulator.

The commercial nextnano software is a semiconductor nanodevice simulation tool that has been developed for predicting and understanding a wide range of electronic and optical properties of quantum structures such as internal quantum efficiency (IQE) or the emission spectrum. A very valuable feature of nextnano is the possibility to include experimental profiles for simplifying the process of writing the required input files for the new structure.

As a case study, an UVB LED structure developed at RIKEN was simulated after importing the doping profiles measured with SIMS into the nextnano software. A methodology was developed in order to identify the best characteristics of a new layer in the structure ("Final Barrier"), simulating strain and self-consistent Schrödinger-Poisson-Current equations. As result of the optimization process the internal quantum efficiency was estimated around 66% for an AlGaN Final Barrier with molar fraction 14% of Al content, thickness between 6 to 8 nm, operating at 6.7 V.

HL 8.6 Mon 10:45 POT 51

Thermal management of ultraviolet LEDs and VCSELs: computer-aided multiphysics optimization — •Giulia Cardinali[1,2], Filip Hjort[2], Michael Alexander Bergmann[2], Johan Gustavsson[2], and Åsa Haglund[2] — [1]Department of Electronics and Telecommunications, Politecnico di Torino, Turin, Italy — [2]Department of Microtechnology and Nanoscience, Chalmers Univer-

sity of Technology, Gothenburg, Sweden

Thermal management is crucial to push the power conversion efficiency above the current limit of 10% in UV LEDs and to enable lasing in UV VCSELs. Numerical simulations have been used to study thermal transport in AlGaN-based vertical-cavity surface-emitting lasers (VCSELs) with dielectric distributed Bragg reflectors (DBRs) and thin-film flip-chip LEDs. The VCSELs technology suffers from poor thermal dissipation through to the DBRs: AlN or diamond heat spreading layers showed to be the most effective way to reduce the internal temperature while maintaining a short optical cavity length. Transfer matrix simulations show a resonance wavelength shift rate with temperature of 6 $\times$ 10^{-3} nm/K, one order of magnitude lower than the value reported for GaN VCSELs with thermally conductive bottom epitaxial DBR. In UVB LEDs to enhance the vertical heat transport the mesa should be in contact with the carrier over the whole area by avoiding air gaps. In that way, thermal performance becomes less dependent upon the exact alignment during the flip-chip bonding process.

HL 8.7 Mon 11:00 POT 51

Characterization of GaN-based FinFETs Grown by Molecular Beam Epitaxy — •Fabian Becker, Florian Pantle, and Martin Stutzmann — Walter Schottky Institut and Physics Department, Technische Universität München, Garching, Germany

Gallium nitride (GaN) is a promising candidate for high power and high frequency electronic applications due to its superior material properties like a high electronic breakdown field, large bandgap, high electron mobility and high electron saturation velocity. An approach to overcome spacial limitations of planar devices is the utilization of vertical 3D structures like nanofins. GaN fin-shaped field effect transistors (FinFETs) gain increasing interest due to a higher active channel area and a better controllability of the gate. Further, GaN nanofins selectively grown by molecular beam epitaxy (MBE) are expected to have a higher crystal quality and reduced defect densities compared to their counterparts fabricated by top-down etching techniques.

Here, we present the fabrication and electrical characterization of MBE-grown GaN FinFETs with various fin dimensions on different substrates. In addition, the nanofins are evaluated by scanning electron microscopy and characterized by Raman and photoluminescence spectroscopy.

HL 8.8 Mon 11:15 POT 51

AlGaN-based UVC-LEDs on AlN/sapphire templates with low threading dislocation density — •Daniel Hauer Vidal[1], Norman Susilo[1], Arne Knauer[2], Sylvia Hagedorn[2], Johannes Enslin[1], Tim Wernicke[1], Markus Weyers[2], and Michael Kneissl[1] — [1]Technische Universität Berlin, Berlin, Deutschland — [2]Ferdinand-Braun-Institut, Berlin, Deutschland

AlGaN-based ultraviolet light emitting diodes (UV LEDs) near 265 nm have applications for the desinfection of water, surfaces and medical equipment. However, most devices are grown on AlN/sapphire templates, which have a high threading dislocation density (TDD). One method to reduce the TDD to around 2×10^9 cm^{-2} are epitaxially laterally overgrown (ELO) AlN/sapphire-templates. They are produced by overgrowing a sapphire template with 0.8 μm of AlN. This layer is then patterned with 1.5 μm thick ridges and subsequently overgrown with several μm of AlN until coalescence. Recently a new approach was developed using high temperature annealing (HTA). In this method a AlN/sapphire template is face to face annealed at temperatures above 1500°C. The annealing step leads to a restructuration of the AlN layer, which produces templates with TDDs at around 1×10^9 cm^{-2}. Another method to reduce the TDD within the active region is to manipuilate the growth mode using different susbtrat off-cut angles. In this study we compare UVC-LEDS grown by metalorganic vapor phase epitaxy on HTA, ELO AlN/sapphire and their combination HTA-ELO. Finally UVC-LEDs are realised on HTA-ELO showing an emission power of 47 mW at 350 mA and 265 nm.

HL 9: 2D semiconductors and van der Waals heterostructures I (joint session HL/DS/O)

Time: Monday 9:30–13:00 Location: POT 81

HL 9.1 Mon 9:30 POT 81

Demonstration of a broadband Photodetector Based on a Two-Dimensional Metal-Organic Framework — •Himani Arora[1,2], Renhao Dong[3], Tommaso Venanzi[1,2], Jens Zscharschuch[1], Harald Schneider[1], Manfred Helm[1,2], Xinliang Feng[3], Enrique Cánovas[4], and Artur Erbe[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Faculty of Physics & Center for Advancing Electronics Dresden, Technische Universität Dresden, 01062 Dresden, Germany — [3]Faculty of Chemistry and Food Chemistry & Center for Advancing Electronics Dresden, Technische Universität Dresden, 01062 Dresden, Germany — [4]Instituto Madrileño de Estudios Avanzados en Nanociencia (IMDEA Nanociencia), 28049 Madrid, Spain

Electrically-conducting metal-organic frameworks (MOFs) have gained considerable attention in last years. In this regard, we report a novel semiconducting Fe3(THT)2(NH4)3 (THT, 2,3,6,7,10,11-triphenylenehexathiol) two-dimensional MOF. The developed MOF films reveal a free-charge band-like transport with a record-high Hall mobility of 230 cm2 V-1 s-1 at room temperature. We further demonstrate a proof-of-concept photodetector based on Fe3(THT)2(NH4)3 MOF films, operative in UV-to-NIR range. Due to IR bandgap of the MOF samples (0.45 eV), the photodetectors are best operated at cryogenic temperatures by suppressing the noise from thermally-activated charge carriers to obtain a clear signal from optically generated carries. Our work reports the first proof-of-concept MOF photodetector, revealing MOFs as promising candidates for optoelectronics.

HL 9.2 Mon 9:45 POT 81

Theory of synchrotron-based spectroscopic techniques on two-dimensional materials — •Dominik Christiansen, Malte Selig, and Andreas Knorr — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

High energy radiation enables the spectroscopic analysis of core level electronic excitations.

First, we develop a theoretical framework for X-ray absorption spectroscopy (XAS) including electronic and structural information obtained from near-edge XAS and extended XAS [1]. Analysing graphene as exemplary material, we show that the characteristic behaviour of the XAS spectra can be derived from the semi-empirical tight-binding approach by considering the spatially non local light-matter interaction.

Second, we develop a theory of exciton dynamics in time and angle resolved photoemission spectroscopy investigating the exciton formation and thermalization in ultrathin transition-metal dichalcogenides [2,3].

[1] B. Buades *et al.*, Optica **5**, 000502 (2018)
[2] D. Christiansen *et al.*, Phys. Rev. B **100**, 205401 (2019)
[3] M. Selig *et al.*, 2D Mater. **5**, 035017 (2018)

HL 9.3 Mon 10:00 POT 81

The Ultimate Radiative Emission Rate of van der Waals materials — •Mark Kamper Svendsen[1], Yaniv Kurman[2], Ido Kaminer[2], and Kristian Sommer Thygesen[1] — [1]Techincal University of Denmark, Kgs. Lyngby, Denmark — [2]Technion University, Haifa, Israel

We consider the coupling between intersubband transitions in few layer transition metal dichalcogenide(TMD) stacks and graphene plasmons. Specifically, we consider few layer TMD quantum wells[1] of different thicknesses, squeezed in between a metallic substrate and a graphene sheet. Using a new, non-perturbative combined MQE-DFT time domain methodology to calculate the state evolution, we find radiative rates exceeding 1 THz and extreme Purcell factors of more than 1E6. Interestingly, we find that for certain combinations of the TMD stack width and graphene Fermi level, graphene plasmon launching becomes the dominant method of emission. This could potentially point to interesting new possibilities in graphene plasmonics.

[1] Schmidt, P., Vialla, F., Latini, S. et al. Nano-imaging of intersubband transitions in van der Waals quantum wells. Nature Nanotech 13, 1035*1041 (2018) doi:10.1038/s41565-018-0233-9

HL 9.4 Mon 10:15 POT 81

Excitation-induced optical nonlinearities and charge car-

rier localization in atomically thin TMD semiconductors — •Daniel Erben[1], Alexander Steinhoff[1], Michael Lorke[1,2], Christian Carmesin[1], Matthias Florian[1], and Frank Jahnke[1] — [1]Institute for Theoretical Physics, University of Bremen — [2]BCCMS, University of Bremen

To interpret the nonlinear optical properties of atomically thin transition metal dichalcogenides (TMD), the density of photoexcited carriers is of central importance. However, in experiments the excited carrier density is practically not accessible. For the case of above band-gap optical pumping of TMD monolayers, we utilize the semiconductor Bloch equations to determine the excitation density as function of the optical pump fluence. Our theory includes Pauli-blocking, band-gap renormalization, dephasing and screening of the Coulomb interaction due to excited carriers. The excitation density strongly depends on the wavelength of the exciting laser pulse. For pumping at the band gap, Pauli blocking of available phase space and renormalizations of the single particle energies are the dominant sources of a nonlinear density dependence, even at small pump fluence. In another study, we investigate the charge-carrier confinement in TMD nanobubbles. The latter are formed during stacking processes and exhibit quantum light emission upon optical excitation. We demonstrate that the emission originates from strong carrier localization, which is caused by the interplay of surface wrinkling, strain-induced confinement, and local changes of the dielectric environment. These effects combine to a specific localization signature that is found in recent spatially resolved photoluminescence experiments.

HL 9.5 Mon 10:30 POT 81

Near-field photoluminescence of two-dimensional semiconductors — •Vlastimil Křápek, Petr Dvořák, Martin Konečný, Lukáš Kejík, Michal Horák, and Tomáš Šikola — CEITEC, Brno University of Technology, Purkyňova 123, 61200 Brno, Czech Republic

Layered two-dimensional semiconductors are ideal light sources for on-chip integration. They exhibit strong luminescence even at elevated temperature, are very compact, highly tunable, and capable of single-photon emission. Since the wavelength of the light is considerably larger than the physical dimensions of the emitter, near-field handling of the emission with a deeply subwavelength spatial resolution would be of great importance. Here we present fully near-field photoluminescence experiment of two-dimensional semiconductors, with a surface plasmon interference device (SPID) used for the excitation and scanning near-field optical microscopy (SNOM) for the collection.

A SPID is formed by an opaque gold layer with the thickness of about 200 nm with the subwavelength grooves serving as sources of surface plasmon polaritons (SPP) [1]. We characterize the electric near field of SPP by SNOM, demonstrating the ability of SPP to excite the semiconductor placed on the SPID. We also demonstrate the polarization sensitivity of the experiment [1,2]. Next, we put various layered two-dimensional semiconductors on top of the SPID and characterize their SPP-excited luminescence by SNOM, demonstrating subwavelength spatial resolution.

[1] P. Dvořák et al., Opt. Express **25**, 16560 (2017).
[2] P. Dvořák et al., Nanoscale **10**, 21363 (2018).

HL 9.6 Mon 10:45 POT 81

2D Semiconductors in moving and standing phonon fields — •Tobias M. Petzak, Emeline D. S. Nysten, and Hubert J. Krenner — Lehrstuhl für Experimentalphysik 1, Institut für Physik, Universität Augsburg, Universitätstr. 1, 86159 Augsburg, Germany

In this work, we prepare two-dimensional layers of transition metal dichalcogenides (TMDCs) such as MoS_2, $MoSe_2$, WS_2 or WSe_2 via micromechanical exfoliation and transfer them into the propagation path of a Surface Acoustic Wave (SAW) directly on a $LiNbO_3$ substrate via viscoelastic stamping. The electric field of the SAW couples to the electron system of the monolayer semiconductors and, thus, we gain insight into the dynamics of photogenerated charges in the sample in a non-invasive, completely contact-free, way.

Additionally, we coupled WSe_2 monolayers to the phononic modes of a high quality factor SAW resonator. This resonator-based spectroscopy increases the sensitivity of our technique. In spectrally resolved experiments using the resonator we are able to resolve the absorption edge of the 2D semiconductor which is in agreement with photoluminescence data. The latter results mark the first major step toward highly sensitive SAW spectroscopy employing SAW resonators.

30 min. break

HL 9.7 Mon 11:30 POT 81

Interlayer excitons in $MoSe_2/WSe_2$ heterobilayers — •Johannes Michl[1], Oliver Iff[1], Maximilian Waldherr[1], Sefaattin Tongay[2], Martin Kamp[1], Sven Höfling[1], and Christian Schneider[1] — [1]Technische Physik, Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Arizona State University

Two dimensional materials such as monolayers of transition metal dichalcogenides (TMDs) offer a wide range of possibilities for investigation due to their unique optical properties, resulting from the exotic valley physics and the strong Coulomb interaction. By stacking two different TMDs, a van der Waals heterostructure is formed. This heterobilayer can exhibit a type-II band alignment, enabling formation of interlayer excitons, with the electron and the hole residing in separate layers. As the heterobilayer is formed, spatially periodical moiré potentials occur due to the lattice mismatch and twist of the different monolayer materials. The moiré potential is predicted to have a great impact on the interaction of light with the interlayer excitons. We discuss the observation of interlayer excitons in $MoSe_2/WSe_2$ heterobilayers performing μ-PL measurements. Due to the weaker coupling strength between the electron and hole in the spatially separated arrangement, the luminscence from the interlayer excitons is shifted around 200 nanometers. The interlayer excitonic resonance is further characterized by a distinct, non-trivial peak structure, which indicates the involvement of a moiré superpotential.

HL 9.8 Mon 11:45 POT 81

Interlayer excitons and band alignment in MoS_2/GaSe heterostructures. — •Christian Wagner[1,2], Mahfujur Rahaman[2], Dietrich R.T. Zahn[2], and Sibylle Gemming[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany

We study the influence of the $(GaSe)_n/(MoS_2)_m$ heterostack composition on the band alignment and the interlayer exciton energy using *ab initio* calculations.

The electronic interaction between individual layers in a 2D heterostack is often reasonably described by a perturbation of the physical effects of the isolated layers by additional electrostatic doping and screening. In terms of optical properties, however, the formation of bound interlayer excitons composed of electrons from one layer and holes from the neighboring layer is possible. These states are measured experimentally by photoluminescence and photocurrents, e.g. in the case of MoS_2 on GaSe due to its type-II band alignment [1].

The interlayer excitons can be approximately located in k-space and energy from density functional theory by relating the band structures of the heterostack to the band structure of the individual layers. This is allowed due to the weak hybridization of electronic states between the two materials. Furthermore, the many-body description allows extracting the exciton binding energies and oscillator strengths in order to obtain the respective spectral signatures.

[1] M. Rahaman *et al.*, J. Phys.: Condens. Matter **31**, 114001 (2019)

HL 9.9 Mon 12:00 POT 81

Biexcitons in 2D transition metal dichalcogenide from first principle: binding energies and fine structure — •Abderrezak Torche and Gabriel Bester — Institut für Physikalische Chemie, Universität Hamburg, Grindelallee 117, D-20146 Hamburg, Germany

Reducing the dimensionality of a system enhances quasiparticles interaction and leads to the formation of Coulomb bound complexes which govern most of the optical properties of semiconductors. Among these complexes, biexcitons are of special interest. Theoretically, first principle treatment of biexcitons, on the same theoretical footing as excitons and trions, is now possible thanks the the newly developed methodology of Ref. [1] which uses a hybrid approach combining configuration interaction and green function methods for the description of many-electrons many-holes excitations. This methodology is applied here to study the binding and fine structure of biexcitons in different transition metal dichalcogenides. The resulting binding energies agree better with experimental values a compared to previous effective mass treatment. The fine structure of biexcitons is shown to be highly dependent on temperature and become very dense (e.g. have many sub-peaks that are separated by hundreds of micro-eV to few meV) at room temperature.

[1] Torche, A., and Bester, G. (2019).PRB,100(20), 201403.

HL 9.10 Mon 12:15 POT 81

In-plane anisotropy of the photon-helicity induced linear Hall effect in few-layer WTe_2 — •Simon Steinhauser[1,2], Paul Seifert[1,2], Florian Sigger[1,2], Jonas Kiemle[1,2], Kenji Watanabe[3], Takashi Taniguchi[3], Christoph Kastl[1,2,4], Ursula Wurstbauer[1,2,5], and Alexander Holleitner[1,2] — [1]Walter Schottky Institut and Physics Department, Technical University of Munich, Am Coulombwall 4a, D-85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstrasse 4, D-80799 München, Germany — [3]Advanced Materials Laboratory, Tsukuba, Ibaraki 305-0044, Japan — [4]Molecular Foundry, Lawrence Berkeley National Laboratory, One Cyclotron Road, Berkeley, California 94720, USA — [5]Institute of Physics, University of Münster, Wilhelm-Klemm-Strasse 10, D-48149 Münster, Germany

Using Hall photovoltage measurements, we demonstrate that a linear transverse Hall voltage can be induced in few-layer WTe_2 under circularly polarized illumination. We find that the photon-helicity induced Hall effect is strongly anisotropic with respect to the crystal axis. Our results are consistent with the Berry curvature and its dipolar distribution due to the breaking of inversion symmetry. We also studied how the Hall voltage changes with varying layer numbers. Time resolved optoelectronic autocorrelation spectroscopy shows the comparatively long spin lifetime of carriers caused by the momentum-indirect electron and hole pockets in WTe_2.

HL 9.11 Mon 12:30 POT 81

Characterization of interlayer excitons in $MoSe_2$-WSe_2 heterostructures in high magnetic fields — •Johannes Holler[1], Michael Kempf[3], Jonas Zipfel[1], Mariana Ballottin[2], Anatolie Mitioglu[2], Philipp Nagler[1], Michael Högen[1], Alexey Chernikov[1], Peter Christianen[2], Christian Schüller[1], and Tobias Korn[3] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]High Field Magnet Laboratory (HFML EMFL), Radboud University Nijmegen, Netherlands — [3]Institut für Physik, Universität Rostock, Germany

In the recent years, the research on transition-metal dichalchogenides (TMDCs) and especially their heterostructures has increased a lot. These heterostructures are fabricated by stacking two different TMDCs on top of each other. With the right material combination, a type-II band alignment can be achieved and electrons and holes are spatially separated forming so-called interlayer excitons (IEXs).

Here, we study these IEXs in $MoSe_2$-WSe_2 heterostructures. In low-temperature PL measurements in magnetic fields of up to 30T, we observe a giant valley-selective splitting and a resulting near-unity valley polarization. In time-resolved measurements, we track the buildup of IEX valley polarization in the magnetic field. We also find a clear dependence of the magnetic-field behavior of the IEX on the stacking angles.

HL 9.12 Mon 12:45 POT 81

Defect-related photoluminescence of WS_2 monolayers — •Marcel Ney, Aswin Asaithambi, Lukas Madauss, Marika Schleberger, Axel Lorke, and Günther Prinz — Faculty of Physics and CENIDE, University Duisburg-Essen, Germany

Two-dimensional transition metal dichalcogenide (TMD) monolayers interact efficiently with visible light due to the direct band gap nature at the K-point in momentum space. The result of the quantum confinement effects in two dimensions is a strong electron-hole Coulomb interaction, leading to a large exciton binding energy, which makes this material very promising for optoelectronic devices.
We will present low-temperature photoluminescence-spectroscopy (PL) measurements, which show the influence of laser-irradiation with different excitation powers on WS_2 monolayers grown on a standard Si/SiO_2 substrate via a chemical vapor deposition (CVD) process.
In the PL investigations, we observed a defect-related emission D_1, which can be assigned to adsorbate-decorated defect complexes [1]. The nature of this defect-related state investigated by laser-power-dependent measurements, will be presented in this contribution. During a laser excitation cycle, a laser-activated emission with a higher energy than the defect-related emission D_1, occurs. Furthermore, another defect-related emission D_2 was observed. Due to the annealing properties after laser-irradiation we identify this emission as a monosulfur vacancy decorated with physisorbed adsorbates [2].
[1] Z. He et al., ACS Nano 10, 5847 (2016)
[2] V. Carozo et al., Science Advances 3, e1602813 (2017)

HL 10: Focus: High-resolution Lithography and 3D Patterning (Part I) (joint session KFM/HL/CPP)

Chair: Robert Kirchner (TU Dresden)

Time: Monday 9:30–12:50 Location: TOE 317

Invited Talk HL 10.1 Mon 9:30 TOE 317

Novel device integration - combining bottom-up and top-down approaches — •Artur Erbe — Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Scaling electronic devices to smallest structure sizes well below 10nm will require novel developments for the fabrication of single components. Smallest functional devices can be assembled using chemical methods leading to, e.g., single molecules with electronic functionalities. Reliable contacting of single molecules using metallic contacts is, however, an extremely challenging task which has not been solved so far. We have therefore developed techniques which use self-assembly for the creation of conducting nanostructures in order to create small, self-assembled circuits which then can be contacted reliably using standard lithographic methods. In this talk, we demonstrate how single organic molecules can be contacted using mechanically controllable break junctions. In addition, we show how DNA Origamis can be used for the self-assembly of metallic nanowires, which are contacted using electron beam lithography and electrically characterized. Further integration of such nanostructures into standard silicon electronics may be achieved by connecting them with 1d- or 2d-semiconductors. We have therefore developed transistors based on 2d-materials and silicon nanowires using electron beam lithography and dry etching (i.e. using a classical top-down approach), which are reconfigurable. With the combination of these devices with self-assembled nanostructures, a large variety of electronic nanocircuits can be constructed in future applications.

HL 10.2 Mon 10:00 TOE 317

Fabrication of NbC Josephson-junction arrays by focused-ion-beam-induced deposition — •Fabrizio Porrati, Felix Jungwirth, Sven Barth, and Michael Huth — Goethe-University, Institute of Physics, Frankfurt a. M.

In this work, a Ga focused-ion-beam is used in combination with the precursor Nb(NMe2)3(N-t-Bu) to fabricate 2D Josephson-junction arrays made of NbC nanodots with typical diameter of 40 nm. Square-arrays with lattice constant between 70 nm and 100 nm are characterized by transport measurements. The ratio Ej/Ec between Josephson coupling energy and the charging energy can be varied by tuning either the dot thickness or the inter-dot distance. As a consequence, a superconductor to insulator transition takes place, as shown by temperature-dependent resistivity measurements. In the Josephson regime, the arrays show magnetic frustration. The resistance as function of the magnetic field exhibits an oscillating behavior with a period of 380 mT for the square-array with lattice constant of 70 nm.

HL 10.3 Mon 10:20 TOE 317

Avoiding amorphization during semiconductor nanostructure ion beam irradiation — •G. Hlawacek[1], X. Xu[1], W. Möller[1], H.-J. Engelmann[1], N. Klingner[1], A. Gharbi[2], K.-H. Heinig[1], S. Facsko[1], and J. von Borany[1] — [1]Ion Beam Physics and Materials Research, Helmholtz—Zentrum Dresden – Rossendorf, Dresden, Germany — [2]CEA-Leti, Grenoble, France

Ion beam induced amorphization of semiconductor nanostructures limits the applicability of ion beam processing to semiconductor nanostructures. Here, we present an approach that not only avoids this amorphization but in addition allows to tailor the lateral device di-

mensions of pillars and fins used in modern GAA and Fin-FET designs. Si nanopillars (diameter: 25–50 nm) have been irradiated by either 50 keV broad beam Si^+ or 25 keV focused Ne^+beam from a helium ion microscope (HIM) at various temperatures using fluences of 2×10^{16} cm^{-2} and higher. While at room temperature strong deformation of the nanopillars has been observed, the pillar shape is preserved above 325°C. This is attributed to ion beam induced amorphization of Si at low temperatures allowing plastic flow due to the ion hammering effect and surface capillary forces. Plastic deformation is suppressed for irradiation at elevated temperatures. Above 325°C, as confirmed by diffraction contrast in BF-TEM, the nanopillars remain crystalline, and are continuously thinned radially with increasing fluence down to 10 nm. This is due enhanced forward sputtering through the sidewalls of the pillar, and agrees well with 3D ballistic computer simulations.

Supported by the H-2020 under Grant Agreement No. 688072.

HL 10.4 Mon 10:40 TOE 317

Grayscale Lithography: Creating complex 2.5D structures in thick photoresist by direct laser writing — •Dominique Collé — Heidelberg Instruments, Heidelberg, Germany

Heidelberg Instruments's lithography systems make it possible to expose any pattern directly without fabricating a mask, which results in a significantly shorter prototyping cycle. The use of a digital mask also allows some quick modification of the design when necessary. The possibility to modulate the energy of each pixel exposed brings the control over the 3rd dimension. This localized dose modulation can be represented as gray tones in a design between black (no dose / no depth in the resist) and white (highest dose / maximum depth in the resist) with up to 1024 different gray tones. Grayscale lithography opens a new world of application from texturing to micro-optic. Micro lenses array, light diffusers, Fresnel lenses, blazed gratings and diffractive optic elements are some typical micro-structures made with grayscale lithography.

20 min. break

Invited Talk HL 10.5 Mon 11:20 TOE 317

Shapeable materials technologies for high resolution patterning of 3D microelectronic devices — •Daniil Karnauschenko — Institute for Integrative Nanosciences, Leibniz IFW, Helmholtz str. 20, 01069 Dresden, Germany

Electronic devices are continually evolving to offer improved performance, smaller sizes, lower weight, and reduced costs, often requiring state of the art manufacturing and materials to do so. An emerging class of materials and fabrication techniques, inspired by self-assembling biological systems shows promise as an alternative to the more traditional methods that are currently used in the microelectronics industry. Mimicking unique features of natural systems, namely flexibility and shapeability, the geometry of initially planar microelectronic structures can be tailored. Heavily relying on cylindrical geometry, fabrication of microwave helical antennas, coils, resonators and magnetic sensors is challenging, when conventional fabrication techniques are applied. Involving high resolution lithographic patterning and self-assembly strategies realization of these spatially non-trivial devices in a compact form and with a reduced number of fabrication steps become feasible. This spatial self-assembly process, triggered by an external stimulus, offers a possibility of an improved performance while reducing overall manufacturing complexity of devices and components by harnessing the relative ease in which it can produce microscopic 3D geometries such as a *Swiss-roll* architecture. These benefits can lead to tighter a system integration of electronic components including active electronics with reduced costs fabricated from a single wafer.

HL 10.6 Mon 11:50 TOE 317

Coupling Single Mode Fibers to Single Quantum Emitters using Femtosecond 3D Printing Technology — •Ksenia Weber[1], Simon Thiele[2], Simon Ristok[1], Sarah Fischbach[3], Jan Hausen[3], Lucas Bremer[3], Mark Saritson[4], Simone Protalupi[4], Alois Herkommer[2], Stefan Reitzenstein[3], Peter Michler[4], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Stuttgart — [2]Institute for Applied Optics and Research Center SCoPE, University of Stuttgart, Stuttgart — [3]Institute of Solid State Physics, Technische Universität Berlin — [4]Institut für Halbleiteroptik und Funktionelle Grenzflächen and Research Center SCoPE, University of Stuttgart

We propose a method to efficiently couple single photon quantum emitters to optical single mode fibers. Due to the undirected emission of single photon sources, such as quantum dots or defect centers in crystals, coupling into optical fibers which is essential for long range quantum communication is typically associated with high losses. To overcome this limitation, femtosecond two-photon lithography can be used to directly fabricate a combination of a microlens and an optical fiber holder onto a quantum emitter. A single mode optical fiber is then integrated into the fiber holder. Due to the high precision of the femtosecond 3D printing process, the position of the fiber core can be adjusted with sub-micrometer accuracy to match the focal point of the microlens. Light from the emitter which is focused by the microlens can therefore efficiently be coupled into the fiber. We present a number of different optical layouts and discuss their pros and cons.

HL 10.7 Mon 12:10 TOE 317

Optical properties of photoresists for femtosecond 3D printing: Refractive index, extinction, luminescence - dose dependence, aging, heat treatment and comparison between 1-photon and 2-photon exposure — •Michael Schmid, Dominik Ludescher, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Femtosecond 3D printing has emerged as an important technology for manufacturing nano- and microscopic optical devices and elements. Detailed knowledge of the dispersion in the visible and near-infrared spectral range is crucial for the design of these optical elements. Here we provide refractive index measurements for different UV-doses, aging times, heat treatment and 2-photon exposed structures for the photoresists IP-S, IP-Dip, IP-L, OrmoComp, IP-Visio, and PO4. We use a modified and automized Pulfrich refractometer setup, utilizing critical angles of total internal reflection with an accuracy of $5\cdot10^{-4}$ in the visible and near-infrared spectral range. We compare Cauchy and Sellmeier fits to the dispersion curves. We also give Abbe numbers and Schott Catalog numbers of the almost entirely polymerized resists. Additionally, we provide quantitative extinction and luminescence measurements for all photoresists.

HL 10.8 Mon 12:30 TOE 317

Acoustic Impedance Matching on Ultrasonic Devices using Additive Manufacturing — •Severin Schweiger, Sandro Koch, Marcel Krenkel, and Marco Kircher — Fraunhofer Institute for Photonic Microsystems, Dresden, Germany

Acoustic impedance matching layers are attached to ultrasonic transducers to increase acoustic energy transmission into the load medium. A capacitive micromachined ultrasonic transducer (CMUT) emits sound via electrostatic deflection of a flexible electrode. Especially air-coupled CMUTs with protective or focusing layers exhibit a notable impedance mismatch. We propose a new approach to fabricate impedance matching metamaterials with low load-side specific acoustic impedance values, by employing a photolithographic additive manufacturing technology using two photon absorption. It will enable improved impedance matching, which has a beneficiary effect on acoustic bandwidth, efficiency and sensitivity of the CMUT. The center operating frequency of the CMUT can be influenced via this process as well. The technology also allows for direct fabrication of microstructures on the chip, foregoing any adhesion layers that disturb the impedance matching and enabling the protective and/or focusing aspects of the layer. This contribution will show analytic and FEM simulations of CMUTs with matching layers. Fabricated impedance matching layer samples and on chip fabrication will be presented as well. Electric impedance and acoustic measurements are in progress and will be featured accordingly.

HL 11: Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions I (joint session O/HL/CPP/DS)

Electronic-structure calculations from first principles have become an indispensable and ubiquitous tool in materials modeling, design, and discovery. One of the outstanding challenges in this area is to study materials at finite temperature, in order to achieve a more realistic description of materials properties and to enable direct comparison with experimental data. To address this challenge it will be necessary to move beyond the static-ions approximation, and to devise systematic approaches for incorporating the effects of electron-phonon coupling, phonon-phonon interactions, and phonon-assisted quantum processes in state-of-the-art electronic-structure methods. The invited lectures will cover recent progress in the broad area of electron-phonon physics from the point of view of first-principles calculations. More generally, the symposium will also cover other areas of first-principles computational materials science (basic methods and applications).

Claudia Draxl (Humboldt-Universität zu Berlin, Germany), Feliciano Giustino (University of Texas at Austin, USA), Matthias Scheffler (Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany)

Time: Monday 10:30–12:45 Location: GER 38

Invited Talk HL 11.1 Mon 10:30 GER 38

Predominance of non-adiabatic effects in zero-point renormalization of electronic energies. — •Xavier Gonze[1,2], Anna Miglio[1], Véronique Brousseau-Couture[3], Gabriel Antonius[4,5], Yang-Hao Chan[4], Steven Louie[4], Giantomassi Matteo[1], and Michel Côté[3] — [1]UCLouvain, Belgium. — [2]Skoltech, Moscow, Russia. — [3]Dept. Physique, U. Montréal, Canada. — [4]Dept. Physics, U. California Berkeley & Materials Sci. Div. NBNL Berkeley, CA, USA. — [5]Dept. Chim., Bio. & Physique, U. Québec Trois-Rivières, Canada.

Electron-phonon interaction induces variation of bandgaps with temperature, and zero-point motion renormalization (ZPR) even at 0K. Ignored in most calculations, ZPR has been evaluated recently for several materials, often relying on the adiabatic approximation, reasonably valid for materials without infrared (IR) activity, but eagerly applied to other materials. We present the first large-scale (29 materials) first-principles evaluation of ZPR beyond the adiabatic approximation [1]. For materials with light elements the ZPR is often larger than 0.3 and up to 1.1 eV: it is useless to go beyond G0W0 without including ZPR in such materials. For IR-active materials, global agreement with experimental data is obtained only with nonadiabatic effects. They even dominate ZPR for many materials. A generalized Fröhlich model that represents accurately nonadiabatic effects accounts for more than half the ZPR for a large set of materials.

[1] A. Miglio, V. Brousseau-Couture, G. Antonius, Y.-H. Chan, S.G. Louie, M. Giantomassi, M. Côté, and X. Gonze. Submitted.

HL 11.2 Mon 11:00 GER 38

A generalized first-principles formalism for the electron-phonon renormalization of electronic energy eigenvalues — •Jae-Mo Lihm[1,2,3] and Cheol-Hwan Park[1,2,3] — [1]Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea — [2]Center for Correlated Electron Systems, Institute for Basic Science, Seoul 08826, Korea — [3]Center for Theoretical Physics, Seoul National University, Seoul 08826, Korea

The interaction between electrons and phonons induce a temperature-dependent renormalization of electronic energy eigenvalues [1]. The perturbative theory of Allen, Heine, and Cardona (AHC) [2] enables an efficient first-principles calculation of the renormalized electronic eigenenergies. The temperature dependence of the electronic bandgap, optical responses, and topological properties of real materials have been investigated within the AHC formalism. In this study, we generalize the AHC formalism [3] so that it could be applied to a broader class of materials. We demonstrate our formalism by calculating the temperature-dependent electronic energy eigenvalues of representative materials.

[1] F. Giustino, Rev. Mod. Phys. 89, 015003 (2017)

[2] P. B. Allen and V. Heine, J. Phys. C 9, 2305 (1976); P. B. Allen and M. Cardona, Phys. Rev. B 24, 7479 (1981); 27, 4760 (1983).

[3] J.-M. Lihm and C.-H. Park, unpublished.

HL 11.3 Mon 11:15 GER 38

Electron-phonon interactions beyond the Born-Oppenheimer approximation in Kohn Sham theory — •Nikitas Gidopoulos — Department of Physics, Durham University, South Road, Durham, DH1 3LE, U.K.

I shall present our work on non-adiabatic corrections to the electron-phonon matrix elements, in density functional theory beyond the Born Oppenheimer approximation, where the Kohn-Sham single-particle potential contains a non-adiabatic correction term [1]. This term depends self-consistently on the nuclear vibrational wave function. The standard expansion of the non-adiabatic KS potential around the nuclear equilibrium positions yields electron-phonon matrix elements beyond the BO approximation.

[1] NI Gidopoulos, EKU Gross, Phil. Trans. R. Soc. A 372, 20130059 (2014). http://dx.doi.org/10.1098/rsta.2013.0059

HL 11.4 Mon 11:30 GER 38

Renormalized second-order perturbation theory for the band gap and single-particle excitations of solids — •Maria Dragoumi[1], Sergey V. Levchenko[2,1], Igor Ying Zhang[3,1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, DE — [2]Skolkovo Institute of Science and Technology, Moscow, RU — [3]Fudan University, Shanghai, CN

We report an efficient implementation of renormalized second-order single-particle energies for periodic systems in an all-electron numeric atomic orbital framework. Starting from second-order perturbation theory, which is single-electron self-interaction free as a virtue of the first-order and second-order exchange diagrams, we use the Dyson equation to sum up infinite number of diagrams [1,2]. In our implementation we use Ewald summation for the long-range part of the Coulomb interaction. This results in an integrable singularity in k-space, which has to be carefully evaluated in order to ensure proper convergence with k-point mesh density. For this purpose we develop an approach based on a generalization of the Gygi-Baldereschi method. The dependence on the starting point of the perturbation theory is examined. The new approach shows a competitive or even superior performance for the description of band-energies compared to the current state-of-the-art methods such as hybrid functionals and G^0W^0 approximation. Thus, with a good starting point this method becomes a powerful tool for the prediction of band energies for a variety of materials.

[1] J. Sun and R. J. Bartlett, J. Chem. Phys. 104, 8553 (1996).

[2] A. Grüneis *et al.*, J. Chem. Phys. 133, 074107 (2010).

HL 11.5 Mon 11:45 GER 38

Band structure of semiconductors and insulators from Koopmans-compliant functionals — •Riccardo De Gennaro[1], Nicola Colonna[2], and Nicola Marzari[1] — [1]Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — [2]Laboratory for Neutron Scattering and Imaging (LNS), Paul Scherrer Institute, 5232 Villigen, Switzerland

Koopmans-compliant functionals provide a novel orbital-density-dependent framework for an accurate evaluation of spectral properties, obtained imposing a generalized piecewise-linearity condition on the total energy of the system with respect to the occupation of each orbital. In crystalline materials, due to the orbital-density-dependent nature of the functionals, minimization of the total energy leads to a ground-state set of variational orbitals that are localized and break

the periodicity of the underlying lattice. Despite that, thanks to the Wannier-like character of the variational orbitals, we show that the Bloch symmetry is still preserved and it is possible to describe the electronic energies through a band structure picture. In this talk I will present results for some benchmark semiconductors and insulators, obtained by unfolding the electronic bands obtained with Gamma-point-only calculations.

HL 11.6 Mon 12:00 GER 38

Dynamical vertex corrections beyond GW from time-dependent density-functional theory — •Georg S. Michelitsch[1,2], Lucia Reining[1,2], and Matteo Gatti[1,2] — [1]Laboratoire des Solides Irradiés, École Polytechnique, F-91128 Palaiseau, France — [2]European Theoretical Spectroscopy Facility (ETSF)

Strong many-body effects in solid state materials are the reason for features such as satellites in electronic excitation spectra. Many-body perturbation theory approaches based on the Green's function formalism are the state-of-the-art in their understanding, commonly applied in terms of the GW approximation to the self-energy, which neglects the so-called vertex correction in Hedin's equations. Although successful for some observables such as band gaps, this approximation cannot sufficiently well describe satellite peaks observed in experiment. Vertex corrections beyond GW can be taken into account thanks to time-dependent density-functional theory[1]. However, only adiabatic approximations have been considered so far. Here we make use of a non-adiabatic approximation[2] to investigate dynamical vertex corrections within a model self-energy. We compare our results to calculations where a static vertex is included and report first successes in terms of a correction to the satellites in the spectral function of sodium.

[1] R. Del Sole et al. *Phys. Rev. B*, 49, 8024 (1994)
[2] M. Panholzer et al. *Phys. Rev. Lett.*, 120, 166402 (2018)

HL 11.7 Mon 12:15 GER 38

Large-scale benchmark of exchange-correlation functionals for the determination of electronic band gaps of solids — •Pedro Borlido[1], Thorsten Aull[2], Ahmad Huran[2], Fabien Tran[3], Miguel Marques[2], and Silvana Botti[1] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [3]Institute of Materials Chemistry, Vienna University of Technology, Getreidemarkt 9/165-TC, A-1060 Vienna, Austria

We compile a large dataset designed for the efficient benchmarking of exchange-correlation functionals for the calculation of electronic band gaps.The dataset comprises information on the experimental structures and band gaps of 472 non-magnetic materials, and includes a diverse group of covalent-, ionic-, and van der Waals-bonded solids.

We used it to benchmark a set of 30 functionals sampling the entirety of Jacob's Ladder. This includes well established functionals such as PBE, mBJ and HSE06, as well as several other less known functionals.

The comparison of experimental and theoretical band gaps shows that mBJ is at the moment the best available density functional, closely followed by HSE06. Other functionals such as HLE16, HLE17, AK13 and TASK also show overall good performance.

HL 11.8 Mon 12:30 GER 38

Assessment of Approximate Methods for Anharmonic Free Energies — •Venkat Kapil[1], Edgar Engel[2], Mariana Rossi[3], and Michele Ceriotti[1] — [1]Swiss Federal Institute of Technology, Switzerland — [2]Department of Physics, University of Cambridge, UK — [3]MPI for Structure and Dynamics of Matter, Hamburg, Germany

Quantitative estimations of thermodynamic stabilities, measured by free energies, must take into account thermal and quantum zero-point nuclear motion. While these effects are easily estimated within a harmonic approximation, corrections arising from the anharmonic nature of the interatomic potential are often crucial and their accurate computations require expensive path integral simulations. Consequently, different approximate methods for computing affordable estimates of anharmonic free energies have been developed. Understanding which of the approximations involved are justified for a given system is complicated by the lack of comparative benchmarks. We here assess the accuracy of some of the commonly used approximate methods: vibrational self-consistent field and self-consistent phonons by comparing anharmonic corrections to Helmholtz free energies against reference path integral calculations. We study a diverse set of systems, ranging from simple weakly anharmonic solids to flexible molecular crystals with freely-rotating units and conclude that efforts towards obtaining computationally-feasible anharmonic free-energies of molecular systems must focus at reducing the expense of path integral methods. *Kapil, Venkat, et al. Assessment of Approximate Methods for Anharmonic Free Energies. JCTC, 2019, doi:10.1021/acs.jctc.9b00596.*

HL 12: 2D Materials I: Electronic Structure, Excitations, etc. (joint session O/CPP/HL)

Time: Monday 10:30–13:45 Location: WIL C107

Invited Talk HL 12.1 Mon 10:30 WIL C107

A microscopic view of graphene quantum Hall edge states with STM and AFM measurements — •Joseph A. Stroscio — NIST, Gaithersburg, MD 20899, USA

2D heterostructed devices with electrostatic pn junction boundaries provide a convenient geometry for the examination of Quantum Hall edge states with microscopic probes. In this talk I will review our work in circular and rectangular geometries to examine the quantum Hall edge states which form in high magnetic field using scanning tunneling microscopy (STM) and atomic force microscopy (AFM) measurements. In circular graphene pn junctions a concentric series of compressible and incompressible rings form due to electron interactions, and show single electron charging when probed by scanning tunneling spectroscopy. In a rectangular Hall bar geometry defined by pn junction boundaries, the compressible strips form the topological protected edge states in the quantum Hall effect. For the graphene Hall bar device, we utilize simultaneous AFM, STM, and quantum transport measurements at mK temperatures. The Kelvin probe force microscopy (KPFM) mode of AFM detects the chemical potential transitions when Landau levels are being filled or emptied as a function of back gate potential. In particular, symmetry breaking states can be resolved at filling factors ν = *1 inside the N=0 Landau level manifold, showing the lifting of the graphene four-fold degeneracy due to spin and valley. With KPFM we can map the dispersion of the Landau levels across the quantum Hall edge boundary as a function of density and spatial position, including resolving the ν = *1 edge modes.

HL 12.2 Mon 11:00 WIL C107

Energy dissipation on suspended graphene quantum dots — •Alexina Ollier[1,2], Marcin Kisiel[1], Urs Gysin[1], and Ernst Meyer[1] — [1]Department of Physics, University of Basel,Klingelbergstr. 82, 4056 Basel, Switzerland — [2]Swiss Nanoscience Institute, Klingelbergstrasse 82, 4056 Basel

Here we report on a low temperature (T=5K) measurement of striking singlets or multiplets of dissipation peaks above graphene nanodrums surface. The stress present in the structure leads to formation of few nanometer sized graphene quantum dots ribbons (GQDRS) and the observed dissipation peaks are attributed to tip-induced charge state transitions in quantum-dot- like entities. The dissipation peaks strongly depend on the external magnetic field (B=0T-2T), the behavior we attributed to crossover from quantum dot carrier confinement to the confinement by magnetic field.

HL 12.3 Mon 11:15 WIL C107

The edge morphology and electronic properties of ballistic sidewall zig-zag graphene nanoribbons on SiC (0001) — •T.T.Nhung Nguyen[1], H. Karakachian[2], J. Aprojanz[1], U. Starke[2], A. Zakharov[3], C. Polley[3], and C. Tegenkamp[1] — [1]TU Chemnitz, Germany — [2]Max Planck Institute, Germany — [3]MAX IV Lab, Sweden

Epitaxial graphene nanoribbons grown on SiC(0001) mesa structures were shown to reveal ballistic transport at room temperature. The subsequent improvement of preparation parameters allows us to fabricate large scale zig-zag type ribbons with 40nm in widths with a pitch size down to 200 nm. We analyzed the electronic structure of the ribbons and their edges by ARPES and STM/STS. Indeed, ARPES reveals

clearly the Dirac cone from the ribbon. The Fermi energy coincides with the Dirac point. This finding is corroborated by STS, revealing an elastic tunneling gap of around 130meV. STM shows that the zig-zag edge merges into the SiC substrate. Exactly at the position of this edge, a metallic state is seen at 0V. The gradual decrease of its intensity within 3nm comes along with a peak splitting. Moreover, the valence and conduction band states reveal close to the edge a larger gap of around 300 meV. We assign these findings to a hybridization of the zig-zag GNR edge with SiC. Furthermore, we propose that the ballistic transport is rather mediated by a 1D interface state rather than by a GNR edge state. The interface state mimics massive particles, which is consistent with the energy positions of electron transmission peaks found in GNR nanoconstrictions of various lengths.

HL 12.4 Mon 11:30 WIL C107

Attosecond-fast current control at graphene-based interfaces — •Tobias Boolakee, Christian Heide, Heiko B. Weber, and Peter Hommelhoff — Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen

Epitaxially grown monolayer graphene on bulk n-doped silicon carbide (SiC) forms a Schottky contact with remarkable electronic and optical properties. We show that charge transfer across the graphene-SiC solid-state interface takes place within (300 ± 200) attoseconds (1 as = 10^{-18} s), which is the fastest charge transfer observed across a solid-state interface [1]. To reveal the attosecond dynamics, we apply femtosecond laser pulses and use saturable absorption in graphene as an intrinsic clock to determine how long an excited state stays excited before charge transfer and thermalization depopulate this state. Recent experimental results and a simple theoretical modelling based on rate equations and on a quantum mechanical model will be presented [2,3].

[1] Heide, C. et al. accepted in Nat. Photon.
[2] Higuchi, T. et al. Nature **550**, 224–228 (2017).
[3] Heide, C. et al. New J. Phys. **21** (2019).

HL 12.5 Mon 11:45 WIL C107

Sideband generation & pseudospin-flip excitations in graphene using tr-momentum microscopy — •Marius Keunecke[1], David Schmitt[1], Christina Möller[1], Davood Momeni Pakdehi[2], Hendrik Nolte[1], Wiebke Bennecke[1], Marie Gutberlet[1], Matthijs Jansen[1], Marcel Reutzel[1], Klaus Pierz[2], Daniel Steil[1], Hans Werner Schumacher[2], Sabine Steil[1], and Stefan Mathias[1] — [1]Georg-August-Universität Göttingen. I. Physikalisches Institut, 37077 Göttingen, Germany — [2]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

The coherent control of quantum states is a promising route towards new emerging phases in solids. One of these phases are the so called Floquet-Bloch states, created by a periodic driving laser. Other light-matter coupled states (Volkov states) arise close to the surface of a solid and are understood as a final state dressing by the laser light. In graphene, the driving by circularly polarized light is predicted to open up a bandgap at the dirac point and thus creating a Floquet topological insulator [1]. In our experiment, the electronic bandstructure of ML graphene on SiC (0001) is mapped during photo-excitation using a momentum microscope in combination with a 1 Mhz femtosecond HHG lightsource (26.6 eV). Different pump wavelengths and polarizations are used to disentangle the excited states dynamics and the sideband generation at high momenta. We will discuss the nature of the generated sidebands and the photoinduced anisotropic hot carrier distributions. [1] M. A. Sentef et al., Nat. Commun. 6, 7047 (2015)

HL 12.6 Mon 12:00 WIL C107

Melting the low temperature gap in monolayer VSe_2, in time resolved ARPES — •Deepnarayan Biswas[1,2], Alfred Jones[1], Paulina Majchrzak[1,3], Klara Volckaert[1], Charlotte Sanders[1,3], Igor Marković[2], Federico Andreatta[1], Akhil Rajan[2], Yu Zhang[3], Gabriel Karras[3], Tsung-Han Lee[4], Chang-Jong Kang[4], Byoung Ki Choi[5], Richard Chapman[3], Adam Waytt[3], Emma Springate[3], Jill Miwa[1], Philip Hofmann[1], Phil D. C. King[2], Young Jun Chang[5], Nikola Lanata[1], and Søren Ulstrup[1] — [1]Aarhus University, Denmark — [2]University of St Andrews, UK — [3]Central Laser Facility, UK — [4]Rutgers University, USA — [5]University of Seoul, Republic of Korea

The group V transition metal dichalcogenide VSe_2 shows a charge density wave (CDW) transition at 110 K with $(4 \times 4 \times 3)$ charge ordering in its bulk form. In contrast, recent experiments on monolayer (ML) VSe_2 have shown an enhanced transition at $\sim$ 140 K with very different charge ordering. Moreover, this transition is accompanied by a full gapping of the Fermi surface. Here, we have used time and angle resolved photoelectron spectroscopy (TR-ARPES) to understand the electron dynamics in ML VSe_2 above and below the transition temperature. We have also modelled the ARPES intensity using a modified BCS self energy and density functional theory calculated bare bands. We find the gapped phase vanishes upon pumping and takes unusually long time to recover (more than 10 ps). This behaviour points toward a hot electron relaxation bottleneck coupled with an electronic phase transition in this sample.

HL 12.7 Mon 12:15 WIL C107

Time-dependent momentum distributions of bright and dark excitons in bulk WSe2 — •Shuo Dong[1], Samuel Beaulieu[1], Dominik Christiansen[2], Maciej Dendzik[1], Tommaso Pincelli[1], Rui Patrick Xian[1], Julian Maklar[1], Malte Selig[2], Andreas Knorr[2], Martin Wolf[1], Laurenz Rettig[1], and Ralph Ernstorfer[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany

Transition metal dichalcogenide semiconductors feature exceptional optoelectronic properties. The investigation of excited states in k-space provides access to optically-bright and dark states on equal footing. Here, we perform the momentum-resolved excited-state mapping in the entire first Brillouin zone of bulk WSe2 using time-resolved momentum microscopy. Upon resonant excitation of band gap, the bright excitons with trARPES signal in the K valleys rapidly scatter to finite-momentum dark excitons in the Σ valleys. We analyze the shape and size of momentum distribution of the excited state. Under the plane wave final state approximation, the Fourier transform of photoemission signal yields real-space image of excitonic wave function. Combined with a microscopic theoretical description of exciton dynamics, the momentum-resolved valley carrier distribution provides information of fundamental exciton properties, like size, binding energy and exciton-phonon coupling.

HL 12.8 Mon 12:30 WIL C107

Sub-picosecond photo-induced displacive phase transition in two-dimensional $MoTe_2$ — •Bo Peng[1,2], Hao Zhang[2], Heyuan Zhu[2], Bartomeu Monserrat[1], and Desheng Fu[3] — [1]TCM Group, Cavendish Laboratory, University of Cambridge, United Kingdom — [2]Department of Optical Science and Engineering, Fudan University, China — [3]Department of Optoelectronics and Nanostructure Science, Shizuoka University, Japan

Photo-induced phase transitions (PIPTs) provide an ultrafast, energy-efficient way for precisely manipulating the topological properties of transition-metal ditellurides, and can be used to stabilize a topological phase in an otherwise semiconducting material. By first-principles calculations, we demonstrate that the PIPT in monolayer $MoTe_2$ from the semiconducting 2H phase to the topological 1T' phase can be driven purely by electronic excitations. The photo-induced electronic excitation changes the electron density, and softens the lattice vibrational modes. These pronounced softenings lead to structural symmetry breaking within sub-picosecond timescales, which is far shorter than the timescale of a thermally driven phase transition. The transition is predicted to be triggered by photons with energies over 1.96 eV, corresponding to an excited carrier density of 3.4×10^{14} cm^{-2}, which enables a controllable phase transformation by varying the laser wavelength. Our results provide insight into the underlying physics of the phase transition in 2D transition-metal ditellurides, and show an ultrafast phase transition mechanism for manipulation of the topological properties of 2D systems.

HL 12.9 Mon 12:45 WIL C107

Understanding electron beam damage in 2D materials from first-principles calculations: Effects of chemical etching and electronic excitation — •Silvan Kretschmer[1] and Arkady V. Krasheninnikov[1,2] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Department of Applied Physics, Aalto University School of Science, Aalto, Finland

Two-dimensional (2D) materials are routinely characterized nowadays in the transmission electron microscope (TEM). The high-energy electron beam in TEM can create defects in the target, and as the influence of defects on materials properties is expected to be stronger in systems with reduced dimensionality, understanding defect production

in 2D materials is of particular importance. Irradiation-induced defects can appear through three mechanisms, namely ballistic or knock-on damage (1), ionization and electronic excitations (2) and beam-induced chemical etching (3). Only the first channel is well understood, while observations of defects formation in 2D transition metal dichalcogenides below the knock-on threshold point out that other mechanism should be important. Here we investigate the role of beam-induced chemical etching and electronic excitations in defect production by using ab-initio molecular dynamic simulations and advanced first-principles simulation techniques based on the Ehrenfest dynamics combined with time-dependent density-functional theory. We demonstrate that the adsorption of small beam-induced radicals and electronic excitations dramatically lower the displacement threshold.

HL 12.10 Mon 13:00 WIL C107

Interaction of highly charged ions with single, bi- and trilayer graphene — •Anna Niggas[1], Janine Schwestka[1], Sascha Creutzburg[2], Benjamin Wöckinger[1], Tushar Gupta[3], Bernhard C. Bayer-Skoff[3], Friedrich Aumayr[1], and Richard A. Wilhelm[1,2] — [1]TU Wien, Institute of Applied Physics, Vienna, Austria — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany — [3]TU Wien, Institute of Materials Chemistry, Vienna, Austria

The interaction of highly charged ions (HCIs) with surfaces has been in the focus of many groups over the last decades. Recently, the rise of 2D materials has provided access to study the neutralisation dynamics of HCIs as they have not reached their equilibrium charge state inside atomically thin materials yet.

In our experiment, we use Xe ions (Xe^{1+} to Xe^{44+}) with energies in the range of 1-400 keV as projectiles and we then record the exit charge states of the ions after transmission through 2D materials. Additionally, we are able to determine the energy loss during the interaction through time of flight measurements, the yield and energy of emitted secondary electrons and forward sputtered target atoms in coincidence.

We now focus especially on the dependence of the neutralisation process on the thickness of the target. Thus, we employ single, bi- and trilayer graphene to mimic graphite with adjustable thickness. In order to ensure that this target structure is not affected by contaminations, it is crucial to implement cleaning procedures. Possible *in-situ* techniques and their effects will also be discussed in this context.

HL 12.11 Mon 13:15 WIL C107

Neutralization of ions transmitted through graphene and MoS_2 monolayers — •Sascha Creutzburg[1,7], Janine Schwestka[2], Anna Niggas[2], Heena Inani[3], Anthony George[4], Lukas Madauss[5], Stefan Facsko[1], Jani Kotakoski[3], Marika Schleberger[5], Andrey Turchanin[4], Pedro L. Grande[6], Friedrich Aumayr[2], and Richard A. Wilhelm[1,2] — [1]HZDR, Ion Beam Center, Dresden, Germany — [2]TU Wien, Institute of Applied Physics, Vienna, Austria — [3]University Vienna, Faculty of Physics, Vienna, Austria — [4]Friedrich Schiller University Jena, Institute of Physical Chemistry, Germany — [5]University Duisburg-Essen, Faculty of Physics and CENIDE, Germany — [6]Federal University of Rio Grande do Sul, Porto Alegre, Brazil — [7]TU Dresden, Germany

Ion irradiation is a widely used technique for material modification. The use of ion irradiation for defect engineering in 2D materials requires a high sensitivity of energy deposition in the surface during the ion's impact. Ions of high charge states (e.g. Xe^{30+}) deposit their potential energy of up to tens of keV in shallow surface depths triggering nanostructure formation. In fact, nanostructure formation in 2D materials, like carbon nanomembranes or MoS_2, due to the impact of Xe ions of charge states larger than 28 was observed. In contrast, no nanostructures on graphene were found, even after irradiation with Xe^{40+} ions. Here, we investigated the ion's neutralization during the transmission through freestanding graphene and MoS_2 monolayers. We deduce the lost energy of the ions (kinetic and potential) in experiment and put our results into context of nanostructuring.

HL 12.12 Mon 13:30 WIL C107

Ab-initio Exciton-polaritons: Cavity control of two-dimensional Materials — •Simone Latini[1], Enrico Ronca[1], Hannes Hübener[1], Umberto De Giovannini[1], and Angel Rubio[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter and Center for Free Electron Laser Science, 22761 Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth avenue, New York NY 10010

We put forward a novel way of controlling the optical features of two-dimensional materials by embedding them in a cavity. The cavity light-matter interaction leads to the formation of exciton-polaritons, mixed states of matter and light. We demonstrate a reordering and mixing of bright and dark excitons leading to the direct optical observation of the latter. In type II van-der-Waals heterostructure, we show that the cavity provides control on the stabilization of inter- over intralayer excitons. Our theoretical predictions are based on a newly developed non-perturbative many-body framework that involves the ab-initio solution of the coupled quantized electron-photon Schrödinger equation in a quantum-electrodynamics plus Bethe-Salpeter approach. Within this framework we are able to investigate exciton-polariton states and predict their dispersion and response in a strong cavity light-matter coupling regime. Our method lends itself to the investigation of more complex polaritonic, so called phonoriton, a mixture of excitons, phonons and photons. In particular we were able to identify elusive phonoritonic spectral features observed in a state-of-the-art pump and probe experiment.

HL 13: Focus Session: Spin-Charge Interconversion (joint session MA/HL)

While classical spintronics has traditionally relied on ferromagnetic metals as spin generators and spin detectors, a new approach called spin-orbitronics exploits the interplay between charge and spin currents enabled by the spin-orbit coupling (SOC) in non-magnetic systems. Efficient spin-charge interconversion can be realized through the direct and inverse Edelstein effects at interfaces where broken inversion symmetry induces a Rashba SOC. Although the simple Rashba picture of split parabolic bands is usually used to interpret such experiments, it fails to explain the largest conversion effects and their relation to the actual electronic structure.

Organizer: Ingrid Mertig (University Halle-Wittenberg)

Time: Monday 15:00–18:15 Location: HSZ 04

Invited Talk HL 13.1 Mon 15:00 HSZ 04

SrTiO3-based 2-dimensional electron gases for ultralow power spintronics — •Manuel Bibes — CNRS/Thales, Palaiseau, France

The MESO transistor is a spin-based non-volatile device proposed by Intel in which magnetic information is written by a magnetoelectric element and read out by a spin-orbit element through the inverse spin Hall effect or the inverse Edelstein effect (IEE). In this talk, I will show that the 2DEG that forms at the interface of SrTiO3 (STO) with LaAlO3 or reactive metals such as Al may be exploited to interconvert spin and charge currents through the direct and inverse Edelstein effects with high efficiencies. I will first present spin to charge conversion experiments using the spin-pumping technique to inject a spin current in the 2DEG. By applying a gate voltage, we tune the position of the Fermi level in the multi-orbital electronic structure of STO, which results in a strong variation of the IEE amplitude with sign changes. This can be modelled through a tight-banding modelling of the band structure measured by ARPES. Importantly, a finite conversion effect persists at room temperature, with a figure-of-merit competitive for MESO-based electronics. In a second part, I will present gate-controlled, all-electrical spin current generation and detection in planar nanodevices free from ferromagnets and only based on a STO 2DEG. Here, the spin current is generated by the direct 2D spin Hall effect from

a charge current running in the 2DEG, transported through the device over several microns and reconverted into a charge current by the inverse 2D spin Hall effect.

Invited Talk HL 13.2 Mon 15:30 HSZ 04

Spin-to-charge current conversion for logic devices — •Felix Casanova — CIC nanoGUNE, San Sebastian, Basque Country, Spain

The integration of logic and memory in spin-based devices, such as the recent MESO proposal by Intel [1], could represent a post-CMOS paradigm. A key player is the spin Hall effect (SHE), which allows to electrically create or detect pure spin currents without using ferromagnets (FM). Understanding the different mechanisms giving rise to SHE allows to find and optimize promising materials for an efficient spin-to-charge conversion (SCC). We unveiled these mechanisms in prototypical materials Pt and Ta [2]. A radically different approach is by engineering a van der Waals heterostructure which combines graphene with a transition metal dichalcogenide. We recently demonstrated SHE in graphene due to spin-orbit proximity with MoS2 [3]. The combination of long-distance spin transport and SHE in different parts of the same material gives rise to an unprecedented SCC efficiency.

Finally, I will present a novel and simple FM/Pt nanodevice to readout the in-plane magnetic state of the FM electrode using SHE [4]. The spin-orbit based detection allows us to independently enhance the output voltage (needed to read the in-plane magnetization) and the output current (needed for cascading circuit elements) with downscaling of different device dimensions, which are necessary conditions for implementing the MESO logic [1].

[1] Manipatruni et al., Nature 565, 35 (2019); [2] Sagasta et al., PRB 94, 060412 (2016); ibid. 98, 060410 (2018); [4] Safeer at al., Nano Lett. 19, 1074 (2019); [5] Pham et al., submitted.

Invited Talk HL 13.3 Mon 16:00 HSZ 04

Spin-charge interconversion in graphene/TMD Van der Waals heterostructures — •Bart Van Wees — Zernike Institute for Advanced materials, University of Groningen, The Netherlands

I will give an introduction into spin transport, spin relaxation and spin-charge conversion in Van der Waals heterostructures made of (single) layer graphene and (single layer) transition metal dichalcogenides (TMDs). Due to their proximity, the strong anisotropic spin orbit interaction in the TMD results in anisotropic, valley-Zeeman and Rashba type spin orbits field in the graphene . As a result the spin relaxation in graphene becomes strongly anisotropic, with out-of-plane oriented spins having a factor 10 or more longer spin life times than in-plane oriented spins [1,2]. The proximity induced spin orbit interaction also gives the possibility of gate tuneable spin change interconversion mechanisms such as spin Hall effect (and its inverse) and Rashba Edelstein effect (and its inverse). I will explain how these effects are observed experimentally [3,4,5], and how they can be optimized for future 2D spintronics applications.

1] T.S. Ghiasi et al., Nano Lett. 17, 7528-7532 (2017)
2] L.Benitez et al., Nature Physics 14, pages303-308(2018)
3] C.K. Safeer et al., Nano Lett. 19, 2, 1074-1082 (2019)
4] T.S. Ghiasi et al., Nano Lett. 19,9, 5959-5966 (2019)
5] L. A. Benítez et al, https://arxiv.org/abs/1908.07868

15 min. break.

Invited Talk HL 13.4 Mon 16:45 HSZ 04

Ferroelectric control of the spin-to-charge conversion in the ferroelectric Rashba semiconductor GeTe — Sara Varotto[1], Luca Nessi[1], Stefano Cecchi[2], Paul Noel[3], Simone Petrò[1], Alessandro Novati[1], Raffaella Calarco[2], Matteo Cantoni[1], Laurent Vila[3], Jean-Philippe Attané[3], Riccardo Bertacco[1], and •Christian Rinaldi[1] — [1]Dipartimento di Fisica, Politecnico di Milano, via Colombo 81, 20133 Milano, Italy — [2]Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany — [3]Univ. Grenoble Alpes, CNRS, CEA, Grenoble INP, IRIG-SPINTEC, F-38000 Grenoble, France

Scalable and energy efficient spin-orbit logic has been very recently pointed out by Intel as technologically suitable computing alternative to CMOS devices [1]. It comprises an electrically driven memory element, with the spin-orbit-based detection of the state performed by spin-to-charge conversion. In this talk, we show that the ferroelectric Rashba semiconductor Germanium Telluride offers memory as well as spin-orbit readout in a silicon-compatible semiconductor. GeTe possesses a giant bulk Rashba-like spin texture, which can be reversed by its non-volatile ferroelectricity [2]. Here we demonstrate the switchability of bulk GeTe through gate electrodes, enabling the electric control of spin textures. Spin pumping measurements in Fe/GeTe heterostructures revealed the ferroelectric control of the spin to charge conversion, paving the way to single-compound spin-orbit logic devices.

[1] S. Manipatruni, Nature 565, 35 (2019); [2] C. Rinaldi et al., Nano Letters 18, 2751 (2018)

Invited Talk HL 13.5 Mon 17:15 HSZ 04

Theory of spin-to-charge conversion in a topological oxide two-dimensional electron gas — •Annika Johansson[1], Börge Göbel[1,2], Ingrid Mertig[1], and Manuel Bibes[3] — [1]Martin Luther University Halle-Wittenberg, Halle, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany — [3]Unité Mixte de Physique CNRS/Thales, Université Paris-Sud, Université Paris-Saclay, Palaiseau, France

$SrTiO_3$ (STO)-based two-dimensional electron gases (2DEGs) provide a highly efficient spin-to-charge conversion [1], also known as inverse Edelstein effect [2,3]. Recently, an extremely large spin-to-charge conversion efficiency was demonstrated in the 2DEG at the interface between STO and Al [4]. The application of a gate voltage leads to a strong variation and even sign changes of the spin-to-charge conversion.

We explain this unconventional gate dependence of the (inverse) Edelstein effect from a theoretical perspective by Boltzmann transport calculations within a multiorbital tight-binding model. By a band-resolved analysis of the Edelstein signal we relate the experimentally observed spin-to-charge conversion to the band structure as well as the topological character and the spin texture of the 2DEG.

[1] E. Lesne *et al.*, Nat. Mater. **15**, 1261 (2016)
[2] V. M. Edelstein, Solid State Commun., **73**, 233 (1990)
[3] K. Shen *et al.*, Phys. Rev. Lett. **112**, 096601 (2014)
[4] D. Vaz *et al.*, Nature Materials **18**, 1187 (2019)

Invited Talk HL 13.6 Mon 17:45 HSZ 04

Nonlinear magnetoresistance from surface states of a topological insulator — •Giovanni Vignale[1], Pan He[2], Dapeng Zhu[2], Shuyuan Shi[2], Hyunsoo Yang[2], Steven S.-L Zhang[3,4], and Olle Heinonen[3] — [1]Department of Physics and Astronomy, University of Missouri-Columbia, Missouri 65211, USA — [2]1Department of Electrical and Computer Engineering, and NUSNNI, National University of Singapore, 117576, Singapore — [3]2Materials Science Division, Argonne National Laboratory, Lemont, Illinois 60439, USA — [4]3Department of Physics, Case Western Reserve University, Cleveland, Ohio 44106, USA

Surface states of topological insulators exhibit the phenomenon of spin-momentum locking, whereby the orientation of an electron spin is determined by its momentum. We have discovered a close link between the spin texture of these states and a new type of nonlinear magnetoresistance, which depends on the relative orientation of the current with respect to the magnetic field as well as the crystallographic axes, and scales linearly with both the applied electric and magnetic fields. The nonlinear magnetoresistance originates from the conversion of a non-equilibrium spin current into a charge current under the application of an external magnetic field. Additionally, we find that the transverse component of the nonlinear resistance exhibits a pi/2 phase shift with respect to its longitudinal counterpart, in marked contrast to the usual pi/4 phase difference that exists between the linear planar Hall effect and the anisotropic magnetoresistance in typical topological insulators and transition metal ferromagnets.

HL 14: Topological Insulators 2 (jointly with DS, MA, HL, O) (joint session TT/HL)

Time: Monday 15:00–16:45 Location: HSZ 103

HL 14.1 Mon 15:00 HSZ 103

Simulating Floquet topological phases in static systems — •Selma Franca[1], Fabian Hassler[2], and Ion Cosma Fulga[1] — [1]IFW Dresden and Würzburg-Dresden Cluster of Excellence ct.qmat, Helmholtzstr. 20, 01069 Dresden, Germany — [2]JARA-Institute for Quantum Information, RWTH Aachen University, 52056 Aachen, Germany

We show that the transport properties of static, higher-order topological insulators (HOTIs) can be used to simulate the behavior of time-periodic (Floquet) topological insulators, without the need for external driving. We consider D-dimensional HOTIs with gapless corner states, which are weakly probed by means of a transport measurement. The unitary reflection matrix describing back-scattering from the HOTI boundary is topologically equivalent to a $(D-1)$-dimensional nontrivial Floquet operator. To characterize the topology of the resulting unitary, we introduce the concept of "nested" scattering matrices, showing that they correctly determine its topological invariants. Our results provide a route to engineer topological unitaries in the lab, using HOTIs and measurement techniques that have already been demonstrated in experiment. Unlike previous methods used to simulate Floquet systems, the resulting phase is expected to be robust against decoherence, since it occurs in the absence of any external driving field.

HL 14.2 Mon 15:15 HSZ 103

Boundary State Engineering and Topological Charge Pumps in non-Hermitian Floquet systems — •Bastian Höckendorf, Andreas Alvermann, and Holger Fehske — Institut für Physik, Universität Greifswald, Greifswald, Germany

In Hermitian topological systems, the bulk-boundary correspondence strictly constraints boundary transport to values determined by the topological properties of the bulk. We demonstrate that this constraint can be lifted in non-Hermitian Floquet insulators. Provided that the insulator supports an anomalous topological phase, non-Hermiticity allows us to modify the boundary states independently of the bulk, without sacrificing their topological nature. Non-Hermitian boundary state engineering specifically enables the enhancement of boundary transport relative to bulk motion, helical transport with a preferred direction, and chiral transport in the same direction on opposite boundaries [1]. Through dimensional reduction, the Floquet insulator reduces to a one-dimensional Floquet chain which possesses a topological phase with unidirectional transport. The topological signature of this phase are non-contractible loops in the spectrum of the Floquet propagator that are separated by an imaginary gap. We define the corresponding topological invariant as the winding number of the Floquet propagator relative to the imaginary gap and then establish that the charge transferred over one period equals the winding number. In fundamental difference to the situation for static or Hermitian chains, the chain acts as a topological charge pump [2].
[1] Phys. Rev. Lett. **123**, 190403 (2019)
[2] arXiv:1911.11413

HL 14.3 Mon 15:30 HSZ 103

Experimental evidence for spin-momentum locking in topological insulator nanoribbons — •Jonas Kölzer[1], Abdur Rehman Jalil[1], Daniel Rosenbach[1], Kristof Moors[1,2], Dennis Heffels[1], Peter Schüffelgen[1], Tobias W. Schmitt[1,3], Gregor Mussler[1], Thomas L. Schmidt[2], Detlev Grützmacher[1], Hans Lüth[1], and Thomas Schäpers[1] — [1]Peter Grünberg Institut, Forschungszentrum Jülich and JARA Jülich-Aachen Research Alliance, 52425 Jülich, Germany — [2]University of Luxembourg, Physics and Materials Science Research Unit,Avenue de la Faïencerie 162a, 1511 Luxembourg, Luxembourg — [3]JARA-FIT Institute Green IT, RWTH Aachen University, 52056 Aachen, Germany

Crosses and triple junctions of nanoribbons are at the center of most of the Majorana braiding schemes proposed, since a minimum of three leads is geometrically required for braiding. Topological insulators are a promising class of materials for realizing Majorana states when combined with a superconductor. Making use of these states in a braiding scheme would allow fault tolerant quantum computing. An experimental realization of a Bi_2Te_3 nanoribbon triple junction which is grown selectively using molecular beam epitaxy is presented. The magneto-transport characteristics of the topological insulator triple junctions at low temperatures are analyzed and compared to the theoretical prediction derived from tight binding transport simulations. The experimental data not only suggests the contribution of surface state transport, but it also provides evidence for spin-momentum locking in topological insulators.

HL 14.4 Mon 15:45 HSZ 103

Meta-magnetism of weakly-coupled antiferromagnetic topological insulators — •Aoyu Tan[1,3], Valentin Labracherie[1,3], Narayan Kunchur[1], Anja Wolter[1], Joseph Dufouleur[1], Bernd Buechner[1,2], Anna Isaeva[1,2], and Romain Giraud[1,3] — [1]Leibniz Institute for Solid State and Materials Research, IFW Dresden, 01069 Dresden, Germany — [2]Faculty of Physics, TU Dresden, 01062 Dresden, Germany — [3]Univ. Grenoble Alpes, CEA, CNRS, Spintec, 38000 Grenoble, France

The magnetic properties of van der Waals magnetic topological insulators $MnBi_2Te_4$ and $MnBi_4Te_7$ are investigated by magneto-transport measurements. We evidence that the relative strength of the inter-layer exchange coupling J to the uniaxial anisotropy K controls a transition from an A-type antiferromagnetic order to a ferromagnetic-like metamagnetic state. A bi-layer Stoner-Wohlfarth model allows us to describe this evolution, as well as the typical angular dependence of specific signatures, such as the spin-flop transition of the uniaxial antiferromagnet and the switching field of the metamagnet. In micron-size magnets, the single-domain switching-field astroid are however partly truncated by the nucleation of domain walls along the easy-axis direction.

HL 14.5 Mon 16:00 HSZ 103

Analytic continuation of Bloch states and the significance for universal boundary physics — Mikhail Pletyukhov[1], Dante Kennes[1], Jelena Klinovaja[2], Daniel Loss[2], and •Herbert Schoeller[1] — [1]RWTH Aachen University, Germany — [2]University of Basel, Switzerland

For generic tight-binding models in one dimension with non-degenerate bands we present an analytic continuation of Bloch states to complex quasimomentum [1], useful for an understanding of boundary physics in half-infinite systems. We show that the pole positions provide the oscillation frequency and localization length of edge states and the branching points define the corresponding quantities for the total density. Each edge state is shown to have a fingerprint in the bulk density which cancels exactly the edge state density. The remaining part of the density is shown to have a pre-exponential power-law with universal exponent -1/2. Introducing a phase variable which continuously shifts the boundary, we derive topological constraints for the edge modes and show that the pole positions oscillate around the branch cuts. We find that the phase dependence of the model parameters can always be chosen such that no edge mode crosses the chemical potential when shifting the boundary by one lattice site. This provides a rigorous proof for universal properties of the boundary charge found in Ref.[2].
[1] M. Pletyukhov et al., arXiv:1911.06886.
[2] M. Pletyukhov et al., arXiv:1911.06890.

HL 14.6 Mon 16:15 HSZ 103

Strong topology and Dirac semimetal phase in cubic half-Heusler under strain — •Sanjib Kumar Das[1], Jorge Facio[1], Ion Cosma Fulga[1], and Jeroen van den Brink[1,2] — [1]IFW Dresden, Helmholtzstrasse 20, 01069 Dresden — [2]Department of Physics, Technical University Dresden, 01062 Dresden, Germany

Theoretically, many half-Heusler compounds exhibit topological phases under strain. Depending on sign of the strain, they can host either a Dirac semimetal or a topological insulating phase. Strain along a suitable direction can split the quadratic band crossing of the bulk band structure, and hence open up a topological gap in these materials. By combining density functional theory(DFT) and tight-binding model calculations, we show that one such cubic half-Heusler material hosts strong topological and Dirac semimetallic phases under compressive or tensile strain, respectively. We hope that our work will motivate further experiments in this direction.

HL 14.7 Mon 16:30 HSZ 103

Fractional corner charges in a 2D super-lattice Bose-Hubbard model — •Julian Bibo[1,4], Izabella Lovas[1,4], Yizhi You[3], Fabian

Grusdt[1,2,4,5], and Frank Pollmann[1,4] — [1]Technische Universität München — [2]Ludwig-Maximilians-Universität München — [3]Princeton Center for Theoretical Science — [4]Munich Center for Quantum Science and Technology — [5]Department of Physics and Institute for Advanced Study, Technical University of Munich

Higher order topological insulators (HOTIs) represent a novel class of topological phases protected by a combination of spatial and internal symmetries. While many non-interacting system have been introduced and studied, it is unclear to which extend the results obtained in non-interacting systems transfer to their strongly-interacting counter parts. In our work, we introduce an experimentally accessible model, a 2D super-lattice Bose-Hubbard model on a square lattice at half-filling, that realizes a robust higher order topological phase protected by charge conservation and fourfold rotation symmetry. Excitingly, our model predicts the presence of symmetry protected fractional charges e/2 to occur at the corners. The presence and robustness of the predicted fractional corner charges is confirmed using the Density Renormalisation Group Ansatz (DMRG). Finally, we propose a way to measure the characteristic fractional corner charges and also provide simulations for the measurement.

HL 15: Graphene (jointly with DY, MA, HL, DS, O) (joint session TT/DY/HL)

Time: Monday 15:00–18:30 Location: HSZ 201

HL 15.1 Mon 15:00 HSZ 201

Edge state crossing behaviour in a multi-band tight-binding model of graphene — •Thorben Schmirander, Marta Prada, and Daniela Pfannkuche — I. Institut für theoretische Physik Universität Hamburg, Hamburg, Deutschland

The description of Dirac electrons in the band structure of graphene is commonly performed using effective tight binding models [1]. These effective models use single-orbital Hamiltonians with modified hopping parameters in order to account for the influence of the higher energy orbitals in graphene. We go beyond such effective models by including d-orbitals in an atomistic tight-binding model. The inclusion of the d-orbitals results in a breaking of electron-hole symmetry which in turn changes the dispersion of the states around the Fermi energy. When considering a finite graphene sample, edge states occur, which cross the band gap and connect the Dirac cones at the K and K' point. These edge states are the key to the topological properties of graphene, because they may exhibit the Spin Hall effect [3]. The band gap crossing is discussed by comparing different expectation values computed from the edge states. These expectation values change under different influences, such as strain or an external electric field. Apart from qualitatively treating these influences on the crossing of the band gap, electron-electron interactions are included via a self-consistent mean-field approach.
[1] van Miert, G., Juricic, V. and Morais Smith, C. Phys. Rev. B 90 195414 (2014)
[2] van Gelderen, R. and Morais Smith, C., Phys. Rev. B 81 125435 (2010)
[3] Kane, C. L . and Mele, E. J., Phys. Rev. Lett. 95, 226801 (2005)

HL 15.2 Mon 15:15 HSZ 201

Graphene grain boundaries for strain sensing: a computational study — •Delwin Perera and Jochen Rohrer — Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany

Graphene has been celebrated as a material with exceptional properties at various fronts of electronics. In this contribution we investigate the strain sensing capabilities of graphene containing grain boundaries by using the non-equilibrium Green function formalism. Our work is inspired by an enhanced piezoresistivity of nanocrystalline graphene found experimentally in 2015 [1]. We investigate how different structural realizations of the grain boundary impact the transport properties. In particular, we compute strain gauge factors solely from *ab initio* electronic structure calculations as a function of the grain boundary topology. Thereby, we can compare this popular figure of merit for strain gauges with experimental values.
[1] Riaz *et al.*, Nanotechnology **26**, 325202 (2015)

HL 15.3 Mon 15:30 HSZ 201

Virtual experiments on negative refraction across graphene pn junctions — •Wun-Hao Kang and Ming-Hao Liu — Department of Physics, National Cheng Kung University, Tainan, Taiwan

Graphene is a promising 2D material exhibiting optics-like properties due to its relativistic electronic structure linear in momentum. When charge carriers pass through a bipolar junction, the group velocity component parallel to the interface changes sign, leading to a negative refraction angle and hence effectively a negative refraction index in Snell's law. Many groups have been working on negative refraction in graphene, both theoretically and experimentally. However, most studies focus on the design of Veselago lensing. Here, we revisit a recent experiment [1] and perform quantum transport simulations for the same device geometry, based on the scalable tight-binding model [2]. Under ideal conditions, our result shows clear conductance peaks due to electron focusing, which is a combined effect of Klein tunneling and negative refraction. To single out the effect of negative refraction, we have further proposed a simpler design for future experiments.
[1] G.-H. Lee et al., Nat. Phys. **11**, 925–929 (2015)
[2] M.-H. Liu et al., Phys. Rev. Lett. **114**, 036601 (2015)

HL 15.4 Mon 15:45 HSZ 201

Electronic properties in a Bernal bilayer graphene monitored by selective functionalization — •Ahmed Missaoui[1,3], Jouda khabthani[1], Didier Mayou[2], and Guy Trambly de Laissardière[3] — [1]Laboratoire de la Physique de la Matière Condensée, Faculté des Sciences de Tunis, Université de Tunis El Manar, Tunis, Tunisia — [2]Institut Néel, CNRS, Univ. Grenoble Alpes, France — [3]Laboratoire de Physique théorique et Modélisation, CNRS , Univ. de Cergy- Pontoise, France

The absence of a band gap in the monolayer graphene presents a great limitation of the fields of application. In a Bernal bilayer of graphene we can exceed its limits with induce a tunable band gap here by applying a gate voltage. In this context, we study the electronic properties of bilayer graphene in the presence of adsorbates such as hydrogene. We used a tight binding modelisation and DFT calculations for our study. We analyze [1] the effects of a selective distribution of adosrbats between the two sublattices A and B [2] on band structure and the microscopic conductivity with Kubo formalisim. The results show that in some cases depending on Fermi energy value and specific adsorbate distribution a gap appears, and in others cases, a linear dispersion with an increase in conductivity with the concentrations is reported.
[1] Jyoti. Katoch et al., Phys. Rev. Lett. 121, 136801 (2018)
[2] A. Missaoui et al., J. Phys. : Condens. Matter 30, 195701 (2018)

HL 15.5 Mon 16:00 HSZ 201

Zero-magnetic-field Hall effects in artificially corrugated bilayer graphene — •Sheng-Chin Ho[1], Ching-Hao Chang[1,2], Yu-Chiang Heish[1], Shun-Tsung Lo[1], Botsz Huang[1], Carmine Ortix[3,4], and Tse-Ming Chen[1,2] — [1]Department of Physics, National Cheng Kung University, Tainan, Taiwan — [2]Center for Quantum Frontiers of Research & Technology (QFort), National Cheng Kung University, Tainan 701, Taiwan — [3]Institute for Theoretical Physics, Center for Extreme Matter and Emergent Phenomena, Utrecht University, Princetonplein 5, NL-3584 CC Utrecht, Netherlands — [4]Dipartimento di Fisica E. R. Caianiello, Universita di Salerno, IT-84084 Fisciano, Italy

We propose a new scheme that uses a lithographically-defined strain technology to modify the interlayer coupling and intralayer interaction of bilayer graphene (BLG). In this deformed BLG system, we demonstrate an unusual pseudo-magnetoresistance anisotropy and the so-called nonlinear Hall effect. These observations are the consequence of the Fermi surface anisotropy and tilted mini-Dirac cones, which originate from the non-zero first-order moments of the pseudo-magnetic field in both real- and momentum-spaces, i.e., the pseudo-magnetic field dipole and Berry curvature dipole. This new approach enables us to turn a simple bilayer graphene into an exotic phase of matter with nontrivial band dispersion generated by the strain engineering, on par with the creation of metamaterials or state-of-art twistronics engineering.

HL 15.6 Mon 16:15 HSZ 201

Spin-caloritronic transport in hexagonal graphene nanodots

— Thi Thu Phùng[1], Robert Peters[2], •Andreas Honecker[1], Guy Trambly de Laissardière[1], and Javad Vahedi[1,3] — [1]Laboratoire de Physique Théorique et Modélisation, CNRS (UMR 8089), Université de Cergy-Pontoise, France — [2]Department of Physics, Kyoto University, Japan — [3]Department of Physics and Earth Sciences, Jacobs University Bremen, Germany

First, we investigate magnetism in the Hubbard model for hexagonal graphene dots. Employing static respectively dynamic mean-field theory (DMFT) we show that magnetism can be generated at the zigzag edges beyond a critical interaction of the on-site Coulomb interaction U that decreases with increasing dot size. Building on these results, we apply the Landauer formalism in the framework of the non-equilibrium Green function method to calculate the spin and charge currents through these dots as a function of temperature. We show that in the "*meta*" configuration of a hexagonal dot subject to weak Coulomb interactions, a pure spin current can be driven just by a temperature gradient in a temperature range that is promising for device applications.

15 min. break.

HL 15.7 Mon 16:45 HSZ 201

Lévy flights and Hydrodynamic Superdiffusion on the Dirac Cone of Graphene — •Egor Kiselev[1] and Jörg Schmalian[1,2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany

We show that the hydrodynamic collision processes of graphene electrons at the neutrality point can be described in terms of a Fokker-Planck equation with a fractional derivative, corresponding to a Lévy flight in momentum space. Thus, electron-electron collisions give rise to frequent small-angle scattering processes that are interrupted by rare large-angle events. The latter give rise to superdiffusive dynamics of collective excitations. We discuss the relevance of our results to experiments with injected electron beams, and show how the superdiffusive behavior makes it possible to obtain analytical results for transport coefficients relevant to the hydrodynamics of graphene electrons.

HL 15.8 Mon 17:00 HSZ 201

Gate-controllable graphene superlattices: Numerical aspects — •Szu-Chao Chen, Wun-Hao Kang, and Ming-Hao Liu — Department of Physics, National Cheng Kung University, Tainan, Taiwan

We study transport properties of gate-controllable graphene superlattices by performing quantum transport simulations based on the scalable tight-binding model and calculations of miniband structures within the continuum method [1]. Good agreement between transport simulations and the corresponding miniband structures confirms the reliability of our calculations for electrostatic superlattices in graphene. Combined with realistic potential profiles obtained from finite-element-based electrostatic simulations, our transport simulations agree well with recent transport experiments for gate-controllable square superlattices. This work therefore paves the way toward exploring gate-controllable graphene superlattices of arbitrary lattices, such as honeycomb or Lieb.
[1] S.-C. Chen et al., arXiv:1907.03288 (2019).

HL 15.9 Mon 17:15 HSZ 201

Localization at the Van Hove singularity — •Peter Silvestrov[1] and Jakub Tworzydło[2] — [1]Institute for Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany — [2]Institute of Theoretical Physics, Warsaw University, Hoża 69, 00–681 Warsaw, Poland

Van Hove singularities are found in the electron spectrum of many 2-dimensional materials of current interest, including graphene systems (twisted bilayer and monolayer on a substrate), transitional dichalcogenides, and 2-dimensional superconductors. They appear due to saddle points in the energy bands at certain momenta. Even though the effective kinetic energy corresponding to such saddle point is unbounded from both above and below, we show that exponentially localized electronic states generically appear here in the presence of a smooth potential $U(x, y)$ with sufficiently diverse landscape. We also consider high order Van Hove singularities, where we predict a discrete spectrum of non-exponentially localized states.

HL 15.10 Mon 17:30 HSZ 201

The optical conductivity of strongly interacting Dirac fermions: a bosonization approach to the Kadanoff-Baym self-consistent resummation — •Sebastián Mantilla and Inti Sodemann — Max Planck Institute for the Physics of Complex Systems

The optical conductivity of 2D Dirac fermions at low energies is controlled by fundamental constants of nature $\sigma_0 = e^2/16\hbar$. However, Coulomb interactions produce a non-trivial dependence of the conductivity with the frequency. We use a bosonization approach to implement exactly a self-consistent Kadanoff-Baym resummation of the electron-hole propagator by mapping the momentum space lattice onto a Heisenberg-type model of interacting spins and employ this approach to determine the frequency dependence of the optical conductivity for Coulomb repulsions. We recover the perturbative renormalization group results at small coupling and extend its predictions to strong coupling. We discuss the relevance of our results to Dirac materials such as graphene and 3D topological insulator surface states.

HL 15.11 Mon 17:45 HSZ 201

Geometric-dissipative origin of the light-induced Hall current in graphene I — •Marlon Nuske[1,3], Lukas Broers[1], and Ludwig Mathey[1,2,3] — [1]Zentrum für optische Quantentechnologien, Universität Hamburg, 22761 Hamburg, Germany — [2]Institut für Laserphysik, Universität Hamburg, 22761 Hamburg, Germany — [3]CUI: Advanced Imaging of Matter, 22761 Hamburg, Germany

We determine the origin of the light-induced Hall current in graphene recently reported by J. McIver, et al., Nature Physics (2019). The Hall current derives from the total Berry curvature of the occupied states of the light-induced Floquet bands, in addition to the kinetic contribution deriving from the band velocities. The occupation of these states of the light-driven material emerges as a steady state that is determined by dissipative processes balancing out the optical driving force. For low electric field strength we propose an intuitive explanation of the Hall current within a two-level Rabi picture.

HL 15.12 Mon 18:00 HSZ 201

Geometric-dissipative origin of the light-induced Hall current in graphene II — •Lukas Broers[1], Marlon Nuske[1,3], and Ludwig Mathey[1,2,3] — [1]Zentrum für optische Quantentechnologien, Universität Hamburg, 22761 Hamburg, Germany — [2]Institut für Laserphysik, Universität Hamburg, 22761 Hamburg, Germany — [3]CUI: Advanced Imaging of Matter, 22761 Hamburg, Germany

Inspired by the recent experiments by J. McIver, et al., Nature Physics (2019), we investigate the light-induced Hall current in graphene. We show that this Hall current derives from the Berry curvature and band velocity contributions of the occupied Floquet-states. To support this proposal we determine the energy and momentum resolved single particle correlation function. The resulting steady state momentum and energy distribution supports the interpretation as a Floquet induced mechanism. We find that for low driving intensity the main contribution to the Hall current emerges from the resonantly driven electron states of the Dirac cone. With increasing driving intensity, additional higher order resonances contribute, giving rise to the full Floquet-driven effect. We demonstrate this within a Master equation formalism, and obtain good quantitative agreement with the experimentally measured Hall current.

HL 15.13 Mon 18:15 HSZ 201

Lightwave valleytronics in graphene — •Hamed Koochaki Kelardeh[1], Alexandra Landsman[2], and Takashi Oka[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Ohio State University, Columbus, USA

We propose a valley-selective device based on graphene at a few-femtosecond timescale with charge separation at different sublattices, and correspondingly at nonequivalent valleys. We characterize the maximality condition of valley polarization and investigate the parameters and condition upon which we can coherently control the carriers and store data via valley degree of freedom. The valley polarization is controlled by the amplitude as well as the carrier-envelope phase of the pulse - one cycle optical field - and the curvature of the electron trajectory in the reciprocal space. We believe the results of our study will step forward the Valleytronics and shed light on ultrafast data storage and processing with uttermost reliability and robustness.

HL 16: Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions II (joint session O/HL/CPP/DS)

Time: Monday 15:00–17:30 Location: GER 38

HL 16.1 Mon 15:00 GER 38

Satellites in optical and loss spectra — •Pier Luigi Cudazzo — Faculty of Science, Technology and Communication, RU Physics and Materials Science, Campus Limpertsberg, Université du Luxembourg, 162 A, avenue de la Faïencerie, L-1511 Luxembourg

Coupling of excitations leads to intriguing effects on the spectra of materials. We propose a cumulant formulation for neutral electronic excitations which opens the way to describe effects such as double plasmon satellites or exciton-exciton and exciton-phonon coupling. Our approach starts from the GW plus Bethe-Salpeter approximation to many body perturbation theory which is based on a quasiparticle picture, and it adds coupling of excitations through a consistent inclusion of dynamically screened interactions. This requires to consider scattering contributions that are usually neglected. The result is formulated in a way that highlights essential physics, that can be implemented as a post processing tool in first principles codes, and that suggests which kind of materials and measurements should exhibit strong effects. This is illustrated using a model.

HL 16.2 Mon 15:15 GER 38

The XPS limit within the one-step model of photoemission: temperature and photon energy effects — •Laurent Nicolaï[1], Vladimir Strocov[2], Juraj Krempaský[2], Federico Bisti[2], Jürgen Braun[3], Hubert Ebert[3], Charles Fadley[4], Ajith Kaduwela[5], Nicholas Pike[6,7], Matthieu J. Verstraete[7], and Ján Minár[1] — [1]Univiversity of West Bohemia, Plzeň, Czech Rep. — [2]Paul Scherrer Institut, Villigen, Suisse — [3]Ludwig-Maximilians-Universität, Germany — [4]Berkeley, California, USA — [5]University of California, USA — [6]University of Oslo, Norway — [7]Université de Liège & European Theoretical Spectroscopy Facility, Belgium

Angle-Resolved Photoemission Spectroscopy (ARPES) is the method of choice for characterising the electronic structure of a given material. A complete understanding of the experimental spectra requires theoretical analyses as well. However, the development of theoretical tools in order to reproduce experimental conditions remains, to this day, a challenge. Using the one-step model of photoemission[1] as implemented in the SPRKKR package[2], our calculations incorporate temperature- and phonon energy-dependent effects via inclusion of both bulk[3] and surface phonons. We also investigate the photon energy range over which the Angle-Integrated PhotoEmission (AIPES) spectra can be compared to the corresponding Weighed Density of States (WDOS).

[1] Braun, Rep. Prog. Phys. 59, 1267-1338 (1996), [2] H. Ebert, D. Ködderitzsch and J. Minár, Rep. on Prog. in Phys. 74, 096501 (2011), [3] L. Nicolaï and J. Minár, AIP Conf. Proc. 1996, 020033 (2018)

HL 16.3 Mon 15:30 GER 38

Ab Initio Linear and Pump-Probe Spectroscopy of Naphthalene Crystals — •Alan Lewis[1] and Tim Berkelbach[2,3] — [1]MPSD, Hamburg, Germany — [2]Columbia University, New York City, USA — [3]Flatiron Institute, New York City, USA

Linear and non-linear spectroscopies are powerful tools used to investigate the energetics and dynamics of electronic excited states of both molecules and crystals. While highly accurate ab initio calculations of molecular spectra can be performed relatively routinely, extending these calculations to periodic systems is challenging. Here, we present calculations of the linear absorption spectrum and pump-probe two-photon photoemission spectra of the naphthalene crystal using equation-of-motion coupled-cluster theory with single and double excitations (EOM-CCSD). Molecular acene crystals are of interest due to the low-energy multi-exciton singlet states they exhibit, which have been studied extensively as intermediates involved in singlet fission. Our linear absorption spectrum is in good agreement with experiment, predicting a first exciton absorption peak at 4.4 eV, and our two-photon photoemission spectra capture the behavior of multi-exciton states, whose double-excitation character cannot be captured by current methods. The simulated pump-probe spectra provide support for existing interpretations of two-photon photoemission in closely-related acene crystals such as pentacene.

HL 16.4 Mon 15:45 GER 38

All-electron real-time TDDFT implementation with Ehrenfest molecular dynamics — •Ronaldo Rodrigues Pela[1,2] and Claudia Draxl[1,2] — [1]Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany — [2]European Theoretical Spectroscopy Facility (ETSF)

Linearized augmented planewaves with local-orbitals (LAPW+lo) are arguably the most precise basis set to represent Kohn-Sham states. When employed within real-time time-dependent density functional theory (RT-TDDFT), they promise ultimate precision achievable for exploring the evolution of electronic excitations in time scales ranging from attoseconds to picoseconds. In this work, we present the implementation of RT-TDDFT in the full-potential LAPW+lo code exciting [1]. For relaxing the nuclear degrees of freedom, we include Ehrenfest molecular dynamics [2]. We benchmark our implementation by analyzing the electric current density and the ion dynamics of Si, C, SiC, and two dimensional BN under the exposure to laser pulses. We compare our results with those obtained using the octopus code [3] and find a satisfactory level of agreement.

References

[1] A. Gulans et al. J. Phys.: Condens. Matter **26**, 363202 (2014).
[2] G. Kolesov et al. J. Chem. Theory Comp. **12**, 466 (2015).
[3] X. Andrade et al. Physical Chemistry Chemical Physics **17**, 31371 (2015).

HL 16.5 Mon 16:00 GER 38

Ab initio study of nonradiative recombination for defects in MoS2 via multiphonon emission — •Simone Manti[1], Lukas Razinkovas[2], Audrius Alkauskas[2], and Kristian Thygesen[1] — [1]Computational Atomic-scale Materials Design (CAMD), Department of Physics, Technical University of Denmark, Kongens Lyngby, Denmark — [2]Center for Physical Sciences and Technology (FTMC), Vilnius, Lithuania

Carrier capture at point defects determines the lifetime of charge carriers and is therefore a very important process for both electronic and opto-electronic devices. The general theory of nonradiative recombination via the so-called multiphonon emission is rather well established, but most studies to date have mainly focused on the description in bulk materials. In this work, we investigate nonradiative carrier capture for a prototypical 2D material, molybdenum disulphide MoS2. Multiphonon emission is governed by (i) electron-phonon coupling between the band edge states and defect states and (ii) the change in the defect geometry upon carrier capture. Our results provide a preliminary description for nonradiative electron capture at sulphur vacancies in monolayer MoS2. In particular, we reveal the important role of the Jahn-Teller effect on the capture process.

HL 16.6 Mon 16:15 GER 38

Phonon-induced electronic relaxation in a strongly correlated system: the Sn/Si(111) ($\sqrt{3} \times \sqrt{3}$) adlayer revisited — •Peter Kratzer and Maedeh Zahedifar — Faculty of Physics, University Duisburg-Essen

The ordered adsorbate layer Sn/Si(111) ($\sqrt{3} \times \sqrt{3}$) with coverage of one third of a monolayer is considered as a realization of strong electronic correlation in surface physics. Our theoretical analysis shows that electron-hole pair excitations in this system can be long-lived, up to several hundred nanoseconds, since the decay into surface phonons is found to be a highly non-linear process. We combine first-principles calculations with help of a hybrid functional (HSE06) with modeling by a Mott-Hubbard Hamiltonian coupled to phononic degrees of freedom. The calculations show that the Sn/Si(111) ($\sqrt{3} \times \sqrt{3}$) surface is insulating and the two Sn-derived bands inside the substrate band gap can be described as the lower and upper Hubbard band in a Mott-Hubbard model with U=0.75eV. Furthermore, phonon spectra are calculated with particular emphasis on the Sn-related surface phonon modes. The calculations demonstrate that the adequate treatment of electronic correlations leads to a stiffening of the wagging mode of neighboring Sn atoms; thus, we predict that the onset of electronic correlations at low temperature should be observable in the phonon spectrum, too. The deformation potential for electron-phonon coupling is calculated for selected vibrational modes and the decay rate of an electron-hole excitation into multiple phonons is estimated, sub-

stantiating the very long lifetime of these excitations.

HL 16.7 Mon 16:30 GER 38

Spectral properties of the interacting homogeneous electron gas — •Tommaso Chiarotti[1], Nicola Marzari[1], and Andrea Ferretti[2] — [1]Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — [2]Centro S3, CNR–Istituto Nanoscienze, 41125 Modena, Italy

Despite its simplicity, the interacting homogeneous electron gas (HEG) is a paradigmatic test case in the study of the electronic structure of condensed matter. Beside being a model for valence electrons in simple metals, it also provides the basic ingredients for key electronic-structure theories. Here, we propose to study it with many-body perturbation theory (MBPT) using one shot, partial self-consistent, and full self-consistent GW, and analyze the description of its spectral function. For this, a novel numerical implementation of MBPT for the 3D non-relativistic HEG has been developed, with a special focus on the treatment of the full-frequency dependence of the Green's function and self-energies. Results for a broad range of densities (going from r_s from 1 to 10) are presented with particular attention to the calculated density-of-states and the spectral potential.

HL 16.8 Mon 16:45 GER 38

Multipole Polarizabilites of Positronium and Its Interaction with Atoms and Molecules — •Jorge Charry, Dmitry Fedorov, and Alexandre Tkatchenko — University of Luxembourg, 1511 Luxembourg, Luxembourg

Positron – the antiparticle of the electron – has many intriguing fundamental properties and it is also useful in many applications for probing matter. Besides electron-positron annihilation, metastable states of atomic and molecular systems involving binding between electrons and positrons are of great interest [1]. In addition, electrons and positrons can form positronium (Ps) atoms and even larger clusters. The polarization of positron by a residual ion is one of possible mechanisms for the formation of bound states for positron-based chemistry [2]. An accurate description of the polarizability of Ps and its bound state with atoms and molecules is essential to understand such interactions. Here, we extend the direct transition-matrix approach, proposed by Kharchenko to determine the multipole polarizabilities of the hydrogen atom [3], to the case of finite nuclear mass. The obtained analytical results, which are in agreement with our numerical calculations performed by means of the molecular orbital based method [4], show that Ps has unique properties in comparison to other normal atoms. Our results shed light into the fundamental interactions between matter and antimatter. [1] Gribakin *et al.*, Rev. Mod. Phys. **82**, 2557 (2010); [2] Bromley and Mitroy, J. Phys.: Conf. Series **199**, 012011 (2010); [3] Kharchenko, Annal. Phys. **355**, 153 (2015); [4] Reyes *et al.*, Int. J. Quant. Chem. **119**, 1 (2019)

HL 16.9 Mon 17:00 GER 38

Energy gap closure of crystalline molecular hydrogen with pressure — •Vitaly Gorelov[1], Markus Holzmann[2,3], David M. Ceperley[4], and Carlo Pierleoni[5,1] — [1]Maison de la Simulation, CEA-Saclay, Gif-sur-Yvette, France — [2]Univ. Grenoble Alpes, CNRS, LPMMC, Grenoble, France — [3]Institut Laue-Langevin, Grenoble, France — [4]Department of Physics, University of Illinois Urbana-Champaign, USA — [5]Department of Physical and Chemical Sciences, University of L'Aquila, L'Aquila, Italy

We study the gap closure with pressure in Phases III and IV of molecular crystalline hydrogen. Nuclear quantum and thermal effects are considered from first principles with Coupled Electron Ion Monte Carlo. The fundamental electronic gaps are obtained from grand-canonical Quantum Monte Carlo methods properly extended to quantum crystals. Nuclear zero point effects cause a large reduction in the gap ($\sim 2eV$). As a consequence the fundamental gap closes at 530GPa for ideal crystals while at 360GPa for quantum crystals. Since the direct gap remains open until ∼450GPa, the emerging scenario is that upon increasing pressure in phase III (C2/c-24 crystal symmetry) the fundamental (indirect) gap closes and the system enters into a bad metal phase where the density of states at the Fermi level increases with pressure up to ∼450GPa when the direct gap closes. Our work partially supports the interpretation of recent experiments in high pressure hydrogen.

HL 16.10 Mon 17:15 GER 38

Using the powerful electronic structure theory to identify single photon emitters in h-BN. — •Sajid Ali — CAMD, Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

In recent years two-dimensional Van Der Walls material h-BN have gained a considerable interest due to the discovery of single photon emission (in both visible and UV region) from the colour centres in this material. This emission is bright, owing to the natural proximity of the centres to the surface, showing promise for high quantum efficiency applications, linearly polarized and strain tuneable. However, the exact chemical nature of the emitting centres is still unknown.

Here, we have performed first principle calculations to obtain observables that can be directly compared with electron paramagnetic resonance (EPR), Optically Detected Magnetic Resonance (ODMR), photoluminescence spectroscopy (PL) and Raman spectroscopy techniques performed on these h-BN emitters. We identify, based on the comparison of our calculations with the experimental data, the defect centres responsible for single photon emission from hexagonal boron nitride.

HL 17: Materials and devices for quantum technology I

Time: Monday 15:00–17:45 Location: POT 112

HL 17.1 Mon 15:00 POT 112

3D Active Sites of Te in Hyperdoped Si by Hard X-ray Photoelectron Kikuchi Diffraction — •Moritz Hoesch[1], Mao Wang[2], Shengqiang Zhou[2], Olena Fedchenko[3], Christoph Schlüter[1], Katerina Medjanik[3], Sergej Babenkov[3], Aimo Winkelmann[4], Hans-Joachim Elmers[3], and Gerd Schönhense[3] — [1]DESY Photon Science, Hamburg, Germany — [2]Helmholt-Zentrum Dresden-Rossendorf, Germany — [3]JGU, Institut für Physik, Mainz, Germany — [4]Academic Centre for Materials and Nanotechnology, AGH University of Science and Technology, Krakow, Poland

n-type doping of Si by Te in excess of the solubility limit was recently demonstrated to lead to hyperdoped material [1]. The samples are made by ion implantation combined with pulsed laser melting. Our investigation by hard x-ray photoelectron spectroscopy (hXPS) reveals at least two different Te species. At the highest doping concentration we study the photoelectron scattering patterns using hard x-ray photoelectron diffraction (hXPD) [2]. Substitutional site occupation of both Te monomers as well as dimers is identified with increasing binding energy (main features in the XPS spectra). The sharp hXPD patterns allow the detailed analysis of the local surrounding of the dopant atoms [3]. At the highest binding energy an additional species is found and the distinct hXPD pattern at this binding energy suggests the assignment to a small fraction of Te in clusters.

[1] M. Wang et al. Phys. Rev. Appl. 11 054039 (2019) and references therein. [2] O. Fedchenko et al NJP 21, 113031 (2019); [3] O. Fedchenko et al., this conference.

HL 17.2 Mon 15:15 POT 112

UHV Lithography for STM Investigations of 3D Topological Insulators-Superconductor Hybrid Arrays — •Michael Schleenvoigt[1], Tobias W. Schmitt[2], Priyamvada Bhaskar[3], Max Vassen-Carl[1], Abdur R. Jalil[1], Benjamin Bennemann[4], Stefan Trellenkamp[4], Florian Lentz[4], Gregor Mussler[1], Markus Morgenstern[3], Peter Schüffelgen[1], and Detlev Grützmacher[1,2] — [1]Peter Grünberg Institute 9, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-FIT Institute Green IT, RWTH Aachen University, 52062 Aachen, Germany — [3]II. Institute of Physics B, RWTH University, 52056 Aachen, Germany — [4]Helmholtz Nano Facility, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

Majorana Zero Modes (MZMs) are proposed to arise at the interface of a topological insulator (TI) and an s-wave superconductor (SC). Scanning tunneling microscopy and spectroscopy (STM/STS) enable the

investigation of MZMs in such hybrid structures. To achieve high SC-TI interface qualities and protect the exposed TI surfaces, device fabrication calls for ultra-high vacuum (UHV) conditions. I will present a three-step in situ fabrication technique. First, TI arrays consisting of molecular beam epitaxy (MBE) grown (Bi,Sb)2(Te,Se)3 compounds are created via stencil lithography. In the second step, SC islands are deposited on top of the TI arrays. Finally the stencil lithography mask is removed without exposing the structures to ambient conditions to prepare the sample for STM/STS investigations in UHV. Topography and spectroscopy maps verify the viability of the process.

HL 17.3 Mon 15:30 POT 112

Fabrication of Topological Insulator Tunnel Junctions — •Dennis Heffels[1], Tobias W. Schmitt[1,2], Michael Schleenvoigt[1], Kristof Moors[1], Max Vassen-Carl[1], Florian Lentz[1], Benjamin Bennemann[1], Gregor Mussler[1], Peter Schüffelgen[1], and Detlev Grützmacher[1,2] — [1]Peter Grünberg Institute, Forschungszentrum Jülich — [2]JARA-FIT Institute Green IT, RWTH Aachen University

At the end of a one-dimensional topological superconductor Majorana zero modes are predicted to exist. As a possible platform for this exotic superconductivity, heterostructures of $(Bi_xSb_{1-x})_2Te_3$ 3D topological insulators (3D TIs) and s-wave superconductors are currently investigated. For this, tunneling spectroscopy is a powerful tool in order to characterize the superconducting proximity effect and detect signatures of Majorana zero modes as shown already on other hybrid platforms like proximitized III-V semiconductor nanowires. A major challenge in order to use this techique also for 3D TI nanoribbons is the fabrication of suitable tunnel junctions while simultaneously preventing the delicate 3D TI surface from degradation at ambient conditions. In this contribution, I will report on progress of a multi-step *in situ* fabrication technique to assemble tunnel junctions at the ends of proximitized 3D TI nanoribbons.

HL 17.4 Mon 15:45 POT 112

Optical Spectroscopy of the ^{28}Si:P donor bound exciton transition — Eduard Sauter[1], M. Beck[1], N. V. Abrosimov[2], J. Huebner[1], and •M. Oestreich[1] — [1]Leibniz Universität Hannover - Abt. Nanostrukturen — [2]Leibniz Institut für Kristallzüchtung Berlin

The donor bound exciton states of ^{28}Si:P show remarkable ensemble transition linewidths[1]. For a ^{29}Si concentration of less than 50ppm, made possible by the avogadro project[2], the D^0X T_2^* coherence times are unprecedented in a semiconductor[3] and the T_1 spin relaxation can be prolonged to the order of minutes[4]. These material qualities may be exploited for spin qubit manipulation and quantum information storage. Spectroscopy of the ≈ 100Mhz FWHM zero phonon line does provide means to verify existing theory of silicon and semiconductors in general to a high degree of accuracy[5]. This contribution explores some of the existing experiments and the possibilities which the donor bound exciton transition might provide for future experiments.

[1] Karaiskaj, D., et al., Physical review letters 86.26 (2001): 6010.
[2] Becker, P., et al. "Enrichment of silicon for a better kilogram." physica status solidi (a) 207.1 (2010): 49-66.
[3] Tyryshkin, Alexei M., et al., Nature materials 11.2 (2012): 143.
[4] Saeedi, Kamyar, et al. Science 342.6160 (2013): 830-833.
[5] Cardona, Manuel, T. A. Meyer, and M. L. W. Thewalt. "Temperature dependence of the energy gap of semiconductors in the low-temperature limit." Physical review letters 92.19 (2004): 196403.

HL 17.5 Mon 16:00 POT 112

Laser-assisted local metalorganic vapor phase epitaxy of (Al,Ga)As layers — •Max Trippel, Jürgen Bläsing, Matthias Wieneke, Armin Dadgar, and Andrè Strittmatter — Institut für Physik, Otto-von-Guericke Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

Up to now, an unsolved problem of integration between Si and III/V semiconductor materials is the misfit between optimum III/V growth conditions and Si electronics. We propose laser-assisted local III/V epitaxy based on metalorganic vapor phase epitaxy (MOVPE) to resolve the growth-temperature related incompatibility of both worlds. (Al,Ga)As/GaAs(001) and (Al,Ga)As/Si(111) have been investigated first study to mark the differences to full-wafer growth on planar substrates. Our custom made epitaxy system comprises a conventional gas mixing cabinet, a stainless-steel vertical growth reactor, a xyz-movable substrate holder and a temperature-controlled laser-heater. Pyrometric temperature measurement is done in the center of the laser spot being as small as 150 μm in diameter. Initial experiments were devoted to find conditions for epitaxial growth with planar top surfaces. With a 200 μm diameter Gaussian-like laser intensity profile on the substrate surface, circular growth areas of 50-150 μm are obtained for a focal plane position of the substrate. A narrow temperature window exists in which planar growth fronts evolve in the center of the mesa. Below this temperature window, only convex growth fronts appear while above a more complex cross-section of the growth front is observed. Epitaxial growth of AlAs mesas on GaAs substrates is demonstrated.

30 min. break.

HL 17.6 Mon 16:45 POT 112

Developing a stand-alone fiber-coupled single-photon source emitting in the telecom O-band — •Jan Grosse[1], Anna Musiał[2], Nicole Srocka[1], Pawel Mrowinski[1,2], Kinga Zołnacz[2], Oleh Kravets[2], Philipp-Immanuel Schneider[3], Jacek Olszewski[2], Krzysztof Poturaj[4], Grzegorz Wójcik[4], Paweł Mergo[4], Kamil Dybka[5], Mariusz Dyrkacz[5], Michał Dłubek[5], Sven Rodt[1], Sven Burger[3], Lin Zschiedrich[3], Wacław Urbańczyk[2], Grzegorz Sek[2], and Stephan Reitzenstein[1] — [1]Institute of Solid State Physics, Technical University of Berlin, Berlin, Germany — [2]Wrocław University of Science and Technology, Wrocław, Poland — [3]JCMwave GmbH, Berlin, Germany — [4]Laboratory for Optical Fiber Technology, Maria Curie-Skłodowska University, Lublin, Poland — [5]Fibrain Sp. z o. o., Zaczernie, Poland

We report on the development of an advanced SPS demonstrator providing fiber coupled single photons in the telecom O-band around 1300 nm. The quantum emitter consists of redshifted low-density InGaAs QDs grown by MOCVD on top of an AlGaAs/GaAs DBR. The outcoupling of photons is enhanced by micromesas patterned deterministically on pre-selected QDs via in-situ EBL resulting in high single-photon purity with $g^{(2)}(0)$ as low as 3%, and temperature stability of emission up to about 60 K. The on-chip fiber coupling of micromesas uses an optical alignment process based on the interferometric mapping using a special high numerical aperture (NA=0.42) single mode fiber which results in an alignment accuracy of about 50 nm. The chip is cooled to 40 K by a compact Stirling cryocooler.

HL 17.7 Mon 17:00 POT 112

Coherent 2D fluorescence spectroscopy on a single molecule indicates electron transfer related to the optical Gunn effect — •Matthias Nuss, Simon Büttner, Donghai Li, Friedrich Schöppler, Tobias Hertel, and Tobias Brixner — Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

The Gunn effect [1] has changed daily lives through the use of "transferred-electron devices". Further developments would benefit from reduced dimensionalities (single-molecule transistors) with tunable quantized nonlinear electro-optical response. Special challenges are to overcome the "THz gap" and to access quantum effects at room temperature that are limited by ensemble averaging or lifetime. In this regard an optical Gunn behaviour was shown in Si nanowires and GaAs and proposed in single-walled carbon nanotubes (SWCNTs) [2]. We carried out ultrafast two-dimensional (2D) fluorescence spectroscopy [3] on an individual SWCNT. We provide insight into the spatio-temporal evolution of electron phonon-mediated intervalley and annihilation dynamics during ultrafast polaron decay in the phonon sideband of an individual SWCNT. We compare the temperature and power dependence, as well as the fourth-order 2D signal of the fluorescence with simulations, to identify the mechanism for electron transfer and discuss this in the light of the Gunn effect [1].
[1] J. B. Gunn, *Solid State Commun.* **1**, 88-91 (1963).
[2] G. Pennington et al.,*Phys. Rev. B* **68**, 045426 (2003)
[3] S. Goetz et al., *Optics Express* **26**, Nr. 4: 3915-25 (2018).

HL 17.8 Mon 17:15 POT 112

Data storage with irradiation-induced defects in SiC — •M. Hollenbach[1,2], C. Kasper[3], D. Poprygin[3], H. Kraus[4], G. Hlawacek[1], Y. Berencén[1], W. Kada[5], T. Ohshima[6], V. Dyakonov[3], and G.V. Astakhov[1,3] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam and Materials Research,Dresden — [2]Technische Universität Dresden,Dresden — [3]Julius-Maximilians-Universität Würzburg, Experimental Physics VI,Würzburg — [4]Jet Propulsion Laboratory, California Institute of Technology,Pasadena — [5]Gunma University,Kiryu — [6]National Institutes for Quantum and Radiological Science andTechnology,Takasaki

The demand for reducing cost and increasing capacities of storing data has led to a continuous improvement of current technologies such as hard disk drives. One of the disadvantages of the present digital media is the limited life span up to 100 years. However, SiC, as a host material for atomic-scale spin centers, especially the Si vacancy, is a promising approach to overcome this limitation. Due to their intrinsic stability, these centers hold promises for next generation long-term data storing. Here, we show the controlled generation of defects by using either focused H^+ or He^+ irradiation. The depth of the defect-rich layer and the number of created luminescent sites are controlled by the energy and the fluence of the ion beam. We demonstrate three dimensional- and multi-bit coding in SiC by using He ions for the writing process. To read out the written defects, a confocal microscope is used. Annealing experiments allowed us to estimate the defect stability to be far above 100 years.

HL 17.9 Mon 17:30 POT 112

Optical characterization of deterministically fabricated quantum-dot microlenses on (111)B GaAs substrate — •Martin von Helversen[1], Alexey Haisler[2], Sarah Fischbach[1], Dimitry Dimitriev[2], Sven Rodt[1], Vladimir Haisler[2], Ilya Derebezov[2], and Stephan Reitzenstein[1] — [1]Institute of Solid State Physics, Technische Universität Berlin, 10623 Berlin, Germany — [2]Institute of Semiconductor Physics, Siberian Branch of Russian Academy of Sciences, 630090 Novosibirsk, Russia

Entangled photon-pairs are excellent candidates for the implementation of secure quantum key distribution schemes [1]. Among suitable single-photon emitters semiconductor quantum dots (QDs) are promising due to their ability to emit polarization entangled photon-pairs on demand via the radiative biexciton-exciton cascade [2]. This, however, requires QDs with a vanishing fine-structure-splitting (FSS) of the excitonic state. We report on QDs grown via molecular beam epitaxy on (111)B GaAs substrate, where the piezoelectric field is directed along the growth direction and allows for a more symmetric growth compared to QDs on (100)-substrate. We find a reduced FSS of $13 \pm 2\,\mu$eV compared to (100) QDs with reported values of around $30\,\mu$eV [3]. By further integation of these emitters into deterministic microlenses [4], their outcoupling efficiency can be optimized to values of above 40%.

[1] Ekert, A. K., Phys. Rev. Lett. 67(6), 661 (1991).
[2] Benson, O. et al., Phys. Rev. Lett. 84(11), 2513 (2000).
[3] Gammon, D. et al., Phys. Rev. Lett. 76(16), 3005 (1996).
[4] Gschrey, M. et al., Nat. Commun. 6, 7662 (2015).

HL 18: Quantum dots and wires I

Time: Monday 15:00–18:15 Location: POT 151

Invited Talk HL 18.1 Mon 15:00 POT 151

Highly efficient sources of single indistinguishable photons — •Niels Gregersen — DTU Fotonik, Technical University of Denmark, Kongens Lyngby, Denmark

Single-photon sources (SPSs) capable of emitting single indistinguishable photons are key components in optical quantum information processing. The SPS figures of merit include the efficiency ϵ of the photon collection and the indistinguishability η of the emitted photons, and scalable optical quantum information processing requires that the product $\epsilon\eta$ is increased very close to unity. In this presentation, I will review present SPS design strategies including the micropillar design and the photonic nanowire design, and I will discuss the potential for increasing $\epsilon\eta$ towards unity.

HL 18.2 Mon 15:30 POT 151

Real-time optical detection of every individual Auger process in a quantum dot — •Hendrik Mannel[1], Jens Kerski[1], Pia Lochner[1], Annika Kurzmann[1], Philipp Stegmann[1], Jürgen König[1], Arne Ludwig[2], Andreas D. Wieck[2], Axel Lorke[1], and Martin Geller[1] — [1]Faculty of Physics and CENIDE, University Duisburg-Essen, Germany — [2]Chair of Applied Solid State Physics, Ruhr-University Bochum, Germany

Auger recombination is a non-radiative process, where the recombination energy of an electron-hole pair is transferred to a third charge carrier. In nanostructured materials, it is a common effect especially in colloidal quantum dots, where it quenches the radiative emission with an Auger recombination time below nanoseconds. In self-assembled QDs, the Auger recombination has only been observed recently [1]. We use two-color resonant laser excitation of the exciton and trion transition on a single self-assembled quantum dot with magnetic fields from 4 to 10 Tesla to monitor every quantum event of the Auger process in real-time. With full counting statistics we observe that the Auger process can be used to tune optically the charge carrier occupation of the dot by the incident laser intensity. Independently we can change the charge carrier occupation of the dot with the electron tunneling from the reservoir by the gate voltage. This demonstrates the potential of the Auger effect for controlling precisely the charge state in a quantum system by optical means. [1] A. Kurzmann et al., Nano Lett. 16, 3367 (2016).

HL 18.3 Mon 15:45 POT 151

Non-Markovianity in quantum optical signals: Wigner time delay and anomalous population trapping — •Alexander Carmele[1,3], Stephan Reitzenstein[2], and Scott Parkins[3] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin — [2]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin — [3]Department of Physics, University of Auckland, Private Bag 92019, Auckland, New Zealand

In comparison to fundamental atom-photon interfaces, a key factor to the understanding of observed phenomena in semiconductor quantum electrodynamics is the presence of a structured environment. This system-reservoir interaction induces intrinsically non-Markovian dynamics [1]. For example, the Wigner delay of QD light emission is limited not only by twice the radiative lifetime as in the case for isolated atoms but also by the phonon-scattering induced decoherence time to approximately the lifetime of the exciton [2]. Another example is anomalous population trapping in multiple-emitter and multiple-excitation waveguide-QED systems. We show that the Markovian treatment does not capture population trapping dynamics even if local phase differences in the light-matter coupling elements are allowed [3].

[1] A. Carmele and S. Reitzenstein, Nanophotonics **8**, 655 (2019).
[2] M. Strauß et al, Phys. Rev. Lett **122**, 107401 (2019).
[3] A. Carmele et al, arXiv:1910.13414 (2019).

HL 18.4 Mon 16:00 POT 151

A deterministically fabricated spectrally-tunable quantum dot based single-photon source — •Marco Schmidt, Martin v. Helversen, Sarah Fischbach, Arsenty Kaganskiy, Ronny Schmidt, Andrei Schliwa, Tobias Heindel, Sven Rodt, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany

Spectrally-tunable quantum light sources are key building blocks of future quantum information networks. Semiconductor-based quantum dots are among the most promising candidates to fulfill this task. On the one hand, this is because of their excellent properties to generate single, indistinguishable and polarization entangled photons and on the other hand, it is explained by their compatibility with advanced device concepts. We demonstrate a tunable single-photon source based on a deterministically fabricated QD microlens which is positioned on top of a piezoactuator via a gold thermocompression bonding procedure [1]. The combination of deterministic fabrication, spectral-tunability and high photon-extraction efficiency makes the QD-microlens single-photon source an interesting building block for the realization of quantum communication networks. The functionality of the strain tunable system and spectroscopic investigations including PID controlled frequency stabilization will be presented.

[1] M. Schmidt et al., A deterministically fabricated spectrally-tunable quantum dot based single-photon source, Opt. Mat. Express, in press (2019)

HL 18.5 Mon 16:15 POT 151

Preparation of the dark exciton in a semiconductor quantum dot using spatially structured light — •Doris E. Reiter[1], Matthias Holtkemper[1], Guillermo F. Quinteiro[2], and Tilmann Kuhn[1] — [1]Institut für Festkörpertheorie, Wilhelm-Klemm-Str. 10,

48149 Münster, Germany — [2]IMIT and Departamento de Física, FaCENA, Universidad Nacional del Nordeste, Corrientes, Argentina

The ground state manifold of a semiconductor quantum dot hosts optically bright excitons which can be used for single photon generation. However, there are also two optically dark excitons in the ground state manifold, which are potentially interesting for storage. To access these dark excitons, we here propose the excitation of the quantum dot with the longitudinal component of a spatially structured light field. This light field component excites a light hole exciton in an excited state, also called a hot exciton state. In typical quantum dots, the hot exciton states are strongly mixed. We calculate the electronic structure of the quantum dot using a configuration interaction method accounting for Coulomb interaction and valence band mixing. We find a strong mixing between the excited light hole exciton and a hot dark heavy hole exciton. The latter is composed of an electron in the s-shell and a hole in the d-shell, which can relax quickly to its ground state (i.e., the s-shell). In this way we can prepare the dark exciton in the ground state manifold, which due to its optically inactivity exhibits a very long lifetime.

30 min. break.

HL 18.6 Mon 17:00 POT 151

Fiber coupling of quantum dot based entangled photon sources — •Weijie Nie[1], Robert Keil[1], Nand Lal Sharma[1], Caspar Hopfmann[1], Fei Ding[2], and Oliver Schmidt[1,3] — [1]Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany — [2]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, 30167 Hannover, Germany — [3]Chemnitz University of Technology, Reichenhainer Strasse 70, 09107 Chemnitz, Germany

Fiber-based highly efficient entangled photon sources are an essential ingredient for quantum photonic networks. While the realization of fiber-coupled single photon sources has been attempted by various methods, direct fiber coupling of quantum dot based entangled photon sources has not been reported. In our work, we employ quantum dot nanomembranes directly attached to single mode fiber end-faces for efficient photon extraction. A key ingredient of efficient photon collection into fibers is the careful design and implementation of an air gap between fiber end face and quantum dot nanomembrane.

HL 18.7 Mon 17:15 POT 151

Radiative coupling between quantum-dot emitters in bimodal microcavity lasers — •Isa Hedda Grothe and Jan Wiersig — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Germany

In bimodal micropillar lasers with two orthogonally polarized modes the interaction with the common quantum-dot gain medium leads to gain competition between the two modes. This results in superthermal values of the autocorrelation function for the weak, non-lasing mode. [1] For standard nanolasers with a single cavity mode, on the other hand, a strong influence of inter-emitter correlations on the input-output characteristics as well as on the statistics of the emitted light has been described. Sub- and superradiant effects can cause an underestimation of the β-factor here and lead to the occurrence of superthermal bunching below threshold. [2]

In light of these findings we make use of a theoretical semiconductor laser model that includes correlations between the emitters in the description of bimodal microcavity lasers to investigate whether an influence of sub- and superradiant effects on the emission behavior can be observed in these systems as well.

[1] H. A. M. Leymann et al., Phys. Rev. A 87, 053819 (2013).
[2] H. A. M. Leymann et al., Phys. Rev. Appl. 4(4), 044018 (2015).

HL 18.8 Mon 17:30 POT 151

Efficient electronic structure calculations for extended systems of coupled quantum dots for Quantum Cascade Lasers Based on a Quantum Dot Superlattice — •Alexander Mittelstädt and Andrei Schliwa — Institut für Festkörperphysik, Technische Universität Berlin

We present a 'linear combination of atomic orbitals'–type of approximation, enabling accurate electronic structure calculations for systems of up to 20 or more electronically coupled quantum dots. Using realistic single quantum dot wavefunctions as basis to expand the eigenstates of the heterostructure, our method shows excellent agreement with full 8-band $\boldsymbol{k}\cdot\boldsymbol{p}$ calculations, exemplarily chosen for our benchmarking comparison, with an orders of magnitude reduction in computational time. We show that, in order to correctly predict the electronic properties of such stacks of coupled quantum dots, it is necessary to consider the strain distribution in the whole heterostructure. Edge effects determine the electronic structure for stacks of $\lesssim 10$ QDs, after which a homogeneous confinement region develops in the center. The overarching goal of our investigations is to design a stack of vertically coupled quantum dots with an intra-band staircase potential suitable as active material for a quantum-dot-based quantum cascade laser.

HL 18.9 Mon 17:45 POT 151

Exploring the Full Photon Statistics of Bimodal-Micropillar Lasers with a Two-Channel Photon-Number-Resolving Transition-Edge-Sensor — •Ching-Wen Shih[1], Marco Schmidt[1], Wenera Zent[1], Christian Schneider[2], Sven Höfling[2], Jörn Beyer[3], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Berlin, Germany — [2]Technische Physik, Universität Würzburg, Germany — [3]Physikalisch-Technische Bundesanstalt, Berlin, Germany

Photon statistics is no doubt one of the key characteristics of photons in quantum light sources. In this regard, a transition-edge-sensor (TES) is an extremely sensitive calorimeter which can resolve the photon numbers and provide the full photon statistics in one shot. Besides, in the case of quantum-dot micropillar lasers, it has been found out that a slight structural asymmetry in the cross-section of micropillars can lift the degeneracy of two fundamental mode components with perpendicular polarizations. In this work, we report on the joint photon number distribution of both modes in such bimodal-micropillar lasers measured by a two-channel photon-number-resolving TES detector system. While both modes share the common quantum dot gain, photon distributions mixed of thermal and Poissonian characteristics were observed above the lasing threshold, indicating interesting mode switching and gain competition effects. We then further reveal the higher-order correlation functions $g^{(k)}(0)$ with $k \geq 2$ and the cross-correlation functions of both modes as a further confirmation of their behaviors.

HL 18.10 Mon 18:00 POT 151

GaAs based quantum dot structures for VECSEL and MIXSEL applications — •Tanja Finke[1], Vitalii Sichkovskyi[1], Jacob Nürnberg[2], Matthias Golling[2], Ursula Keller[2], and Johann Peter Reithmaier[1] — [1]Institute of Nanostructure Technologies and Analytics (INA), Technische Physik, CINSaT, University of Kassel, Germany — [2]Institute for Quantum Electronics, Ultrafast Laser Physics Laboratory, ETH Zürich, Switzerland

By integration of a semiconductor saturable absorber mirror (SESAM) into a vertical external cavity surface emitting laser (VECSEL), one can form a mode-locked integrated external-cavity surface emitting laser (MIXSEL). InGaAs quantum dots (QDs) were used for the gain and absorber regions and optimized by MBE towards high dot density and narrow photoluminescence (PL) emission. The influence of the growth parameters as well as a post-growth rapid thermal annealing (RTA) on the optical and morphological properties of QDs was studied. Furthermore, distributed Bragg mirrors (DBR) were grown and maximum reflectivity values of 99.8 % could be achieved. All the sections were integrated into a single VECSEL structure. To improve the absorption and fast recovery dynamics of high-quality QD-SESAMs, p-type doping recombination centers close to the QD layers were introduced. The effect of the beryllium δ-doping level and post-growth RTA on the optical properties of the QDs was studied and QD-SESAMs with different designs were characterized by nonlinear reflectivity and pump-probe experiments. A fast recovery time of 2 ps and saturation parameters comparable to QW based SESAMs were achieved.

HL 19: Focus Session: When theory meets experiment: Hybrid halide perovskites for applications beyond solar II (joint session HL/CPP)

Hybrid halide perovskites are by now well established solar absorber and emitter materials, with power conversion efficiencies of single cell devices exceeding 20

Organizers: Linn Leppert (Universiät Bayreuth) and Felix Deschler (TU Munich)

Time: Monday 15:00–17:00 Location: POT 251

Invited Talk HL 19.1 Mon 15:00 POT 251

Double perovskite electronic structures: A chemical perspective — •Adam Slavney[1], Hemamala Karunadasa[2], Linn Leppert[3], and Bridget Connor[2] — [1]Department of Chemistry, Harvard University, Cambridge, Massachusetts, USA — [2]Department of Chemistry, Stanford University, Stanford, California, USA — [3]Institute of Physics, University of Bayreuth, Bayreuth, Germany

Halide double perovskites, of the formula A2BB'X6, are close analogs to the APbX3 lead halide perovskites and have attracted significant interest as possible non-toxic alternatives to the lead materials in perovskite photovoltaics. Double perovskites divide the formally +2 charge on the octahedral B site unevenly over two B sites, allowing for cations with charges from +1 - +4 to be incorporated into the perovskite lattice. I will discuss the results of our experimental and theoretical investigations into double perovskites over the last several years, with a particular emphasis on understanding the differences in electronic structure between single and double perovskites. The double perovskite electronic structure is largely dictated by the combination of the B and B* cations rather than either cation individually and I will provide simple rules which accurately predict the band structure from the chemical formula in nearly every case. Double perovskites electronic structures have features not available in single perovskites including symmetry-forbidden bandgaps and unusually small bandgaps generated by metal-metal charge transfer transitions. Finally, I will discuss some of the defect chemistry of double perovskites and how those lessons can be applied to halide perovskites more broadly.

Invited Talk HL 19.2 Mon 15:30 POT 251

Solid state ionics of hybrid halide perovskites: equilibrium situation and light effects — •Alessandro Senocrate[1,2], Gee Yeong Kim[1], Tae Youl Yang[1], Giuliano Gregori[1], Michael Graetzel[1,2], and Joachim Maier[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]École polytechnique fédérale de Lausanne

In recent years, hybrid halide perovskites have been attracting great attention due to their exceptional photo-electrochemical properties. When used as light-harvesters in solar cells, device efficiencies exceeding 25% can be realized. We showed that a deeper understanding of (i) functionality, (ii) stability, as well as (iii) the possibility to improve the performance require a thorough insight into non-stoichiometry and ion transport.

In this contribution, we study the nature of the ionic conductivity in methylammonium lead iodide ($MAPbI_3$), the archetypal halide perovskite, by means of a great number of electrochemical and nuclear magnetic techniques. To aid the experimental investigation, we include detailed defect chemical modelling describing the effects of varying iodine partial pressure (stoichiometry) and dopant content. By extending this study to the situation under illumination, we observe a striking enhancement of ionic conductivity by more than 2 orders of magnitude in $MAPbI_3$, alongside the expected increase in electronic conductivity. We provide a mechanistic explanation of this astonishing phenomenon and discuss its relevance for the photo-stability of this class of materials.

HL 19.3 Mon 16:00 POT 251

Looking beyond the surface: The band gap of bulk methylammonium lead iodide — Oskar Schuster[1], Peter Wientjes[1], Shreetu Shrestha[2], Ievgen Levchuk[2], Mykhailo Sytnyk[3], Gebhard Matt[2], Andres Osvet[2], Miroslaw Batentschuk[2], Wolfgang Heiss[3], Christoph Brabec[2], Thomas Fauster[1], and •Daniel Niesner[1] — [1]Lehrstuhl für Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Staudtstr. 7, 91058 Erlangen, Germany — [2]Materials Science Department (I-MEET), FAU, Martensstrasse 7, 91058 Erlangen, Germany — [3]Materials Science Department, FAU, Energy Campus Nürnberg, 90429 Nürnberg, Germany

Reported optical properties of lead halide perovskites as basic as the absorption onset and the band gap vary significantly. To unambiguously answer the question whether the discrepancies are a result of differences between bulk and "near-surface" material, we perform bulk-sensitive two-photon absorption with an information depth in the millimeter range on single crystals. In the application-relevant room-temperature tetragonal phase (170 K) we find a bulk band gap of 1.55 ± 0.01 eV. Reference measurements on the surface-near region in a reflection geometry show excitonic transitions at 1.59 ± 0.01 eV, consistent with the literature. The small band gap of the bulk material explains the extended infrared absorption of crystalline perovskite solar cells, the narrow bandwidth of crystalline perovskite photodetectors making use of the spectral filtering at the surface, and the low-energy bands which carry optically driven spin-polarized currents.

HL 19.4 Mon 16:15 POT 251

Double Peak Emission in Lead Halide Perovskites by Self-Absorption — •Konstantin Schötz[1], Abdelrahman M. Askar[2], Wei Peng[3], Dominik Seeberger[1], Tanaji P. Gujar[1], Mukundan Thelakkat[1], Sven Huettner[1], Osman M. Bakr[3], Karthik Shankar[2], Anna Köhler[1], and Fabian Panzer[1] — [1]Universität Bayreuth, Bayreuth, Germany — [2]University of Alberta, Edmonton, Canada — [3]King Abdullah University of Science and Technology (KAUST), Thuwal, Kingdom of Saudi Arabia

Despite the rapidly increasing efficiencies of perovskite solar cells, the optoelectronic properties of this material class are not completely understood. Especially when measured photoluminescence (PL) spectra consist of multiple peaks, their origin is still debated. In this work, we investigate in detail double peak PL spectra of halide perovskite thin films and single crystals with different material compositions. By different optical spectroscopic approaches and quantitative models, we demonstrate that the additional PL peak results from an extensive self-absorption effect, whose impact is intensified by strong internal reflections. This self-absorption accounts for the unusual temperature dependence of the additional PL peak and it implies that absorption until far into the Urbach tail of the perovskite is important. The strong internal reflections entail that even for thin films self-absorption can have a significant contribution to the PL spectrum. Our results allow for a clear assignment of the PL peaks by differentiating between optical effects and actual electronic transitions, which is necessary for understanding the optoelectronic properties of halide perovskites.

HL 19.5 Mon 16:30 POT 251

Surface atomic and electronic structure of $CsPbBr_3$ inorganic perovskite — •Janek Rieger, Felix Trunk, Thomas Fauster, and Daniel Niesner — Lehrstuhl für Festkörperphysik, Friedrich-Alexander University Erlangen-Nürnberg (FAU), Staudtstr. 7, D-91058 Erlangen, Germany

The crystallographic orientation of the surface has a strong impact on the performance of solar cells built from lead-halide perovskites [1]. For a systematic study of the surface carrier-dynamics, we prepare atomically well-defined (001) surfaces of the inorganic perovskite $CsPbBr_3$ by epitaxial growth in ultra-high vacuum. Low-energy electron diffraction was carried out to analyze the resulting samples.

The measured surface unit cell as well as the corresponding phase transitions differ from the bulk-terminated ones. Angle-resolved photoelectron spectroscopy finds a valence-band structure in line with data we obtained from single crystals. Finally, we also investigated the energetics of the conduction-band electrons using two-photon photoelectron spectroscopy. From the positions of the valence-band maximum and the conduction-band minimum we conclude that our $CsPbBr_3$ samples are intrinsic.

[1] S. Y. Leblebici et al., Nat. Energy **1.8**, 16093 (2016).

HL 19.6 Mon 16:45 POT 251

Finite temperature effects on the excited states in layered

BiI_3 — •Ivona Bravic and Bartomeu Monserrat — TCM Group, Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom

Over the last decade layered BiI_3 has been matter of investigation in the optoelectronics community as it exhibits a fundamental band gap similar to that of silicon but behaves like a direct band gap semiconductor. However, the excited state properties of this system remained poorly understood, which is mostly a consequence of the extremely flat band structure and the arising low robustness with respect to dynamical distortions, volume expansion and stacking faults. In order to determine its potential performance in an optoelectronic device at finite temperature, it proves invaluable to establish a fundamental understanding of its excited states and how the aforementioned properties effect those. In this study we reveal the effect of spin-orbit coupling, electron-phonon coupling, exciton-phonon coupling, stacking faults and volume expansion on the optical response and photoluminescence properties of this materials using DFT as well as GW-BSE, proving that it is crucial to account for all these effects to provide a comprehensive understanding of the optoelectronic performance of layered BiI_3, and in general layered van-der Waals materials.

HL 20: 2D semiconductors and van der Waals heterostructures II (joint session HL/DS)

Time: Monday 15:00–18:30 Location: POT 81

Invited Talk HL 20.1 Mon 15:00 POT 81

Resonantly hybridized excitons in moiré superlattices in van der Waals heterostructures — •Alexander Tartakovskii — Department of Physics and Astronomy, University of Sheffield, Sheffield, S3 7RH, UK

Recent years have seen significant effort in exploration of monolayer semiconductors such as transition metal dichalcogenides (TMDs) MoS_2, WS_2, $MoSe_2$, WSe_2 etc. Atomically-thin layers of two-dimensional materials can be assembled in vertical stacks held together by relatively weak van der Waals forces, allowing for coupling between monolayer crystals with incommensurate lattices and arbitrary mutual rotation. The lattice constant difference and the mutual rotation angle present new degrees of freedom for the design of novel meta-materials.

A profound consequence of using these new degrees of freedom is the emergence of an overarching periodicity in the local atomic registry of the constituent crystal structures, known as a moiré superlattice. Here, we show that in semiconducting heterostructures built of incommensurate $MoSe_2$ and WS_2 monolayers, excitonic bands can hybridize, which results in the resonant enhancement of the moiré superlattice effects. $MoSe_2$ and WS_2 are specifically chosen for the near degeneracy of their conduction band edges to promote the hybridization of intra- and interlayer excitons. For $MoSe_2/WS_2$ heterostructures with almost aligned pairs of monolayer crystals, the resonant mixing of the electron states leads to amplified effects of the heterostructure's geometrical moiré pattern on the dispersion of the hybridised excitons.

HL 20.2 Mon 15:30 POT 81

Intralayer and interlayer exciton dynamics in WSe_2/WS_2 van-der-Waals heterostructure — •Manan Shah, Lorenz Maximilian Schneider, and Arash Rahimi-Iman — Department of Physics and Materials Sciences Center, Philipps-Universität, Marburg, 35032 Germany

The van-der-Waals heterostructures (vdW-HS) comprising atomically thin transition-metal dichalcogenides (TMDCs) provide an unprecedented level of freedom for bandgap engineering. However, the HSs give rise to more complex behaviour due to the change in effective dielectric screening, interlayer coupling strength, and moiré potential. The effectiveness of these parameters primarily depends upon the spacing, lattice constant mismatch, and the twist angle between the layers. The hybrid band structure of the vdW-HS system arising from the magnitude of these phenomena is not yet completely understood.

Here, we report a type-II WSe_2/WS_2 HS where the electrons accumulate in the WS_2 monolayer (ML) and the holes accumulate in the WSe_2 ML owing to charge transfer, giving rise to interlayer excitons. This tungsten-based HS is of particular interest due to the presence of energetically favourable spin-forbidden dark A-excitonic states and a strong excitonic binding energy. Our optical-spectroscopy results exhibit the intralayer excitons, intralayer phonon-assisted dark excitons, and interlayer excitons along with the emergence of new excitonic states with a large oscillator strength between the optical bandgap of the constituting MLs [M. Shah et al., *Semiconductors* (in press)].

HL 20.3 Mon 15:45 POT 81

Enabling tailored 2D materials by introducing 1D organic-inorganic perovskites with supramolecular intra-layer interactions — •Philip Klement[1], Natalie Dehnhardt[2], Chuan-Ding Dong[3], Samuel Bayliff[4], Julius Winkler[2], Peter J. Klar[1], Stefan Schumacher[3,5], Sangam Chatterjee[1], and Johanna Heine[2] — [1]Institute of Experimental Physics I and Center for Materials Research (ZfM), Justus Liebig University Giessen, Germany — [2]Department of Chemistry and Material Sciences Center, Philipps-Universität Marburg, Germany — [3]Department of Physics and Center for Optoelectronics and Photonics Paderborn (CeOPP), Paderborn University, Germany — [4]Department of Chemistry and Biochemistry, University of Oklahoma, Norman, USA — [5]College of Optical Sciences, The University of Arizona, Tucson, USA

One of the major current challenges in 2D materials* synthesis is the intentional design of building blocks to introducing superior chemical and physical properties. The limiting factor in this approach is the commonly-believed paradigm that in-plane covalent interactions are strictly necessary to form 2D materials, limiting the number of candidates. Here we show that individual single layers of 2D organic-inorganic perovskites with only 1D covalent intralayer-interactions exist. [BzA]3[BiCl5]Cl (BzA = benzylammonium) is exfoliated down to single layers and reveals extremely strong dimensional effects evidenced by a 0.4 eV shift of the photoluminescence between bulk and single layers. We demonstrate that already 1D covalent interactions render 2D materials possible.

HL 20.4 Mon 16:00 POT 81

Layer-dependent and time-resolved photoluminescence in hBN-encapsulated InSe — •Tommaso Venanzi[1,2], Himani Arora[1,2], Stephan Winnerl[1], Alexej Pashkin[1], Phanish Chava[1,2], Zahkar Kudrynskyi[3], Takashi Tanigushi[4], Kenji Watanabe[4], Artur Erbe[1], Amalia Patane[3], Manfred Helm[1,2], and Harald Schneider[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]Technische Universität Dresden, 01062 Dresden, Germany — [3]School of Physics and Astronomy, University of Nottingham, Nottingham NG7 2RD, UK — [4]National Institute for Material Science, 1-1 Namiki, Tsukuba, 305-0044, Japan

In the last years van der Waals semiconductors have become a subject of intense research. Within this class of materials, InSe shows promising optical and electronic properties. Here we present the optical properties of thin flakes of InSe encapsulated in hBN. The encapsulation in hBN protects the InSe flakes from external contamination assuring long-term stability and reducing the disorder potential in the flake. We have studied the photoluminescence (PL) for different temperatures and number of InSe atomic layers. The relative weights of the exciton and electron-hole contributions to the PL emission are discussed using a lineshape analysis. Our model introduces a PL temperature to include the effects of the disorder potential on the PL emission. Furthermore, we observe a sharp increase of the PL lifetime while decreasing the number of layers. This is due to direct-to-indirect bandgap transition driven by the thickness of the InSe flake.

HL 20.5 Mon 16:15 POT 81

Optical Initialisation and Readout of Spin Defects in hBN — •A. Gottscholl[1], M. Kianinia[2], V. Soltamov[1], C. Bradac[2], C. Kasper[1], K. Krambrock[3], A. Sperlich[1], M. Toth[2], M. Dietz[1], I. Aharonovich[2], and V. Dyakonov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]School of Mathematics and Physical Sciences, Inivertiy of Technology Sydney, Ultimo, NSW 2007, Australia — [3]Departomento de Fisica, Universidade Federal de Minas Gerais, Belo Horizonte, MG, Brazil

The concept of optically addressable spin states in solids is considered as a major building block of upcoming quantum technologies. While several candidates in 3D crystals including diamond and silicon carbide have been extensively studied, the identification of spin-dependent

processes in 2D materials has remained elusive. Optically accessible spin states in hBN are already theoretically predicted, however, they have not been observed experimentally yet. We investigated a bright 850nm defect-related fluorescence in hBN with magnetic resonance techniques and identified it as a negatively charged boron vacancy V_B^-, possessing a spin triplet ground state and a zero field splitting of 3.5 GHz [1]. The defect shows an optically detected magnetic resonance signature at room temperature and can be optically spin polarized at lower temperatures. Our results constitute a leap forward in establishing two-dimensional hBN as a prime platform for scalable quantum technologies.

[1] Gottscholl et al., arXiv:1906.03774

HL 20.6 Mon 16:30 POT 81

Theory of optical absorption in monolayers of transition metal dichalcogenides — •Frank Lengers, Doris E. Reiter, and Tilmann Kuhn — Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm Str. 10, 48149 Münster

Monolayers of transition metal dichalcogenides are attractive materials for optoelectronics due to their strong exciton-light interaction. At the same time the interaction of excitons and phonons plays a crucial role in these systems leading to strong phonon-assisted processes in optical experiments.

In this contribution different theoretical methods for the computation of linear absorption spectra in monolayers of transition metal dichalcogenides are investigated. To be specific, we consider the spectra of $MoSe_2$ using either a correlation expansion in 2nd or 4th Born Approximation or an approximation closely related to the time convolution less master equation used in the theory of open quantum systems. We show that the 2nd Born Approximation gives poor results for elevated temperatures due to the exceptionally strong exciton-phonon interaction. On the other hand the time convolution less approach gives suprisingly good results despite its simplicity when compared to higher-order correlation expansion. This rather easy method can therefore be readily applied to the class of atomically thin solids where strong carrier-phonon interaction plays a vital role.

30 min. break.

HL 20.7 Mon 17:15 POT 81

Band filling and cross quantum capacitance in ion gated semiconducting transition metal dichalcogenide monolayers — •Haijing Zhang[1,2], Christophe Berthod[2], Helmuth Berger[3], Thierry Giamarchi[2], and Alberto Morpurgo[2] — [1]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany — [2]University of Geneva, Geneva, Switzerland — [3]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Ionic liquid gated field-effect transistors based on semiconducting transition metal dichalcogenides are used to study a rich variety of extremely interesting phenomena, while important aspects of how charge carriers are accumulated in these systems remain elusive. Here we present a thorough analysis of charge accumulation in MoSe_2 and WSe_2 monolayers. We identify the conditions when the chemical potential enters different valleys in the monolayer band structure and find that an independent electron picture describes the occupation of states well. Unexpectedly, however, the same analysis of the experiments shows that the total device capacitance cannot be simply described in terms of the series connection of a geometrical capacitance and of a quantum capacitance given by C_Q=e^2/(dμ/dn), as commonly assumed. This unexpected behavior occurs because a cross quantum capacitance contribution is present, which originates physically from mutual screening of the electric field generated by charges on one plate from charges sitting on the other plate. Our findings reveal an important contribution to the capacitance of physical systems that had been virtually neglected until now.

HL 20.8 Mon 17:30 POT 81

Theory of Exciton-Electron Coupling in Two-Dimensional Semiconductors — •Frederik Schirdewahn[1], Dominik Christiansen[1], Andreas Knorr[1], Tommaso Venanzi[2], Stephan Winnerl[2], and Malte Selig[1] — [1]Technische Universität Berlin, Germany — [2]Helmholtz Zentrum Dresden-Rossendorf, Germany

The strong Coulomb interaction in monolayers of doped transition metal dichalcogenides (TMDCs) leads to the formation of tightly bound excitons and electron gas assisted exciton transitions (trions)[1,2]. Here we present a microscopic approach within the Heisenberg equation of motion formalism for the excitonic absorption including trion signatures[3]. We discuss the impact of doping density and temperature on the absorption spectrum. Additionally we present a joint experiment theory study for THz pump VIS probe experiments of doped monolayer $MoSe_2$, where we find a red shift of exciton and trion lines which we trace back to a heating of the electrons due to the THz pulse finding a good comparison between theory and experiment.

[1] G. Plechinger et al., Nat. Commun. 7, 12715 (2016)
[2] T. C. Berkelbach et al., Phys. Rev. B 88, 045318 (2013)
[3] A. Esser et al., phys. stat. sol. (b) 2, 317 (2001)

HL 20.9 Mon 17:45 POT 81

Bosonic Condensation in a hybrid monolayer MoSe2-GaAs-microcavity — •Max Waldherr[1], Nils Lundt[1], Martin Klaas[1], Simon Betzold[1], Matthias Wurdack[2], Anton Nalitov[3], Sefaattin Tongay[4], Elena Ostrovskaya[2], Alexey Kavokin[3], Sven Höfling[1,5], and Christian Schneider[1] — [1]Technische Physik, Physikalisches Institut and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, Germany — [2]Nonlinear Physics Centre, Research School of Physics and Engineering, Australian National University, Canberra, Australia — [3]Physics and Astronomy School, University of Southampton, Highfield, Southampton, UK — [4]School for Engineering of Matter, Transport, and Energy, Arizona State University, Tempe, Arizona, USA — [5]SUPA, School of Physics and Astronomy, St. Andrews, UK

We observe bosonic condensation in a hybrid exciton-polariton system in the strong-coupling regime, with monolayer MoSe2 and GaAs quantum well excitons collectively coupling to a Tamm-plasmon mode. The onset of condensation in the hybrid polariton branch manifests in a superlinear increase of its emission intensity, accompanied by a distinct collapse of the linewidth, a core sign of temporal coherence. At further increasing pumping powers, we observe a continuing blueshift of the resonance originating from particle interactions with uncondensed excitons in the reservoir states. The spin-polarized emission is a clear sign of valley-selective condensation.

HL 20.10 Mon 18:00 POT 81

Micro-photoluminescence studies of defects hosting localized excitons in single-layer MoS_2 — •Oleg Gridenco, Kathrin Sebald, Christian Tessarek, Martin Eickhoff, and Jürgen Gutowski — Institute of Solid State Physics, University of Bremen, D-28359 Bremen, Germany

Beside to free excitons, single-layer transition metal dichalcogenides (TMDs) can also host localized excitons that are bound to defect states and emit with energies smaller than the free-exciton energy. These localized emission centres often appear in as-prepared samples after exfoliation, but they can also be created or enhanced at specific positions by local engineering. In this talk, we will introduce our recent progress in the study of point defects in single-layer MoS_2. Defects were introduced by scanning a Ga^+ ion beam over a certain area of a single-layer using a focused ion beam (FIB) machine. The number of defects was controlled by varying the Ga^+ ion dose. By performing low-temperature micro-photoluminescence (μPL) spectroscopy we investigate the emission properties of localized excitons. Moreover, we found that the intentionally generated defect-related emission centres dominate the optical spectra of MoS_2 at low temperatures. Additionally, light emitted from free or localized excitons needs to be efficiently collected. Here we will discuss how plasmonic nanostructures on top of single-layers are particularly well suited for enhancing the quantum yield of single-layer TMDs.

HL 20.11 Mon 18:15 POT 81

On-demand exchange and spin-orbit in bilayer graphene sandwiched between TMDC and ferromagnet — •Klaus Zollner[1], Martin Gmitra[2], and Jaroslav Fabian[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute of Physics, P. J. Šafárik University in Košice, 04001 Košice, Slovakia

Van der Waals heterostructures offer great potential for future device applications. Bilayer graphene on a transition-metal dichalcogenide (TMDC) experiences strong proximity spin-orbit coupling (SOC) [1], and record spin lifetime anisotropies are achievable [2]. Moreover, one can turn ON and OFF the SOC in bilayer graphene with a gate voltage [3], and realize a spin-orbit valve [1]. Similarly, one can have on-demand proximity exchange in a bilayer graphene/ferromagnetic-insulator heterostructure [4],realizing an exchange valve. The logical

next step is to combine both proximity effects, exchange and SOC in bilayer graphene sandwiched between TMDC and ferromagnet-insulator. In this talk, we will present our results of a time-reversal field effect valve in doubly proximitized bilayer graphene.

This work was supported by DFG SPP 1666, SFB 1277, the EU Horizon 2020 research and innovation program under Grant No. 785219, and by the reintegration scheme MSVVaS SR 90/CVTISR/2018 and VVGS-2019-1227.

[1] Gmitra et al., Phys. Rev. Lett. 119, 146401 (2017). [2] Omar et al., Phys. Rev. B 100, 155415 (2019). [3] Island et al., Nature 571, 85 (2019). [4] Zollner et al., N. J. Phys. 20, 073007 (2018).

HL 21: 2D Materials II: Electronic Structure, Excitations, etc. (joint session O/CPP/HL)

Time: Monday 15:00–18:15 Location: WIL C107

HL 21.1 Mon 15:00 WIL C107

Unfolding and analysis of a defect band structure using doped $MoSe_2$ and MoS_2 — •Stefan Rost, Christoph Friedrich, Irene Aguilera, Beata Kardynal, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We investigate substitutional doping of chromium and phosphorus in $MoSe_2$ and MoS_2 monolayers, as they are promising candidates for single photon emission. The systems are characterized by density-functional-theory (DFT) studies of structural relaxation, projected density-of-states, and band structure, all calculated with the Jülich FLAPW code family (www.flapw.de). Different sizes of super-cells are necessary to calculate the doped system depending on the strength of interaction between the dopants. The super-cells contain between 3×3 and 5×5 monolayer unit cells. Compared to the pristine material, the band structure of the defect system is backfolded in **K**-space, which complicates a straightforward interpretation, in particular for low doping concentrations. We have implemented a method for unfolding the bands obtained from the super-cell calculation. The resulting band structure resembles the one of the pristine material, but it contains additional information about the defect system, which, in this sense, can be regarded as a perturbed host system. – The authors gratefully acknowledge the computing time granted through JARA-HPC on the supercomputer JURECA at Forschungszentrum Jülich, (project cjpgi10) as well as the support through „Integration of Molecular Components in Functional Macroscopic System“ initiative of VW Stiftung.

HL 21.2 Mon 15:15 WIL C107

Geometry, electronic structure, and bonding of single-domain h-BN on Pt(110) — •Marco Thaler[1], Dominik Steiner[1], Alexander Menzel[1], Florian Mittendorfer[2], and Erminald Bertel[1] — [1]Physikalische Chemie, Universität Innsbruck, Österreich — [2]Institut für Angewandte Physik, TU Wien, Österreich

Recently we reported single-domain growth of hexagonal Boron Nitride (h-BN) on Pt(110)[1]. This is a peculiar system, where the substrate adapts to the h-BN adlayer by forming a (1xn) missing-row reconstruction (n = 5 or 6). The bandstructure was investigated by angle-resolved UV photoemission (ARPES) and is very similar to that of a free-standing h-BN monolayer except for the appearance of umklapp bands reflecting the periodicity of the Moiré pattern and testifying for the perfect film quality. Binding energies agree with other h-BN/transition metal systems if referenced to the vacuum level. Additionally, we studied the local density of states (LDOS) for differently positioned atoms in the h-BN film by DFT calculations. For N atoms on top of Pt atoms a small LDOS maximum appears at the Fermi level, indicating a weak covalent contribution to the h-BN-Pt bonding. This, the mean h-BN-Pt(110) distance, and the workfunction change place the present system at the borderline between purely dispersive and chemisorptive bonding[2]

[1] Steiner, D., Mittendorfer, F., Bertel, E. ACS Nano 13, 7083-7090(2019)

[2] Bokdam, M., Brocks, G., Kelly, P. J. Phys. Rev. B 90, 085415(2014)

HL 21.3 Mon 15:30 WIL C107

Photoinduced band renormalization in the nodal-line semimetal ZrSiSe — •Gianmarco Gatti[1], Alberto Crepaldi[1], Nicolas Tancogne-Dejean[2], Michele Puppin[3], Angel Rubio[2], Majed Chergui[3], and Marco Grioni[1] — [1]Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland — [2]Max Planck Institute for the Structure and Dynamics of Matter and Center for Free-Electron Laser Science, Luruper Chaussee 149, 22761 Hamburg, Germany — [3]Laboratory of Ultrafast Spectroscopy, ISIC, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

ZrSiSe is a layered material that is classified as a nodal-line semimetal. Its low-energy bandstructure is composed by linearly dispersing surface and bulk bands whose crossing points creates a one-dimensional contour in the momentum space with vanishing density of states close to the Fermi level. We investigate its equilibrium and out-of-equilibrium electronic structure by the means of angle- and time-resolved photoemission spectroscopy and compare the results with ab initio calculations. Our analysis indicates that the dispersion of the Dirac quasiparticle can be correctly reproduced by density functional theory with the inclusion local and non-local electronic correlations. Moreover, we observe a transient renormalization of the bands velocity above the Fermi level under the photoexcitation produced by ultrashort infrared pulses. We associate the microscopic origin of this effect to the increased screening of the non-local Coulomb interaction due to the presence of high-energy and non-thermalized carriers.

HL 21.4 Mon 15:45 WIL C107

Micro-focus ARPES on a twisted graphene/hBN field-effect device — •Alfred Jones[1], Ryan Muzzio[2], Davide Curcio[1], Deepnarayan Biswas[1], Jill A. Miwa[1], Philip Hofmann[1], Simranjeet Singh[2], Chris Jozwiak[3], Eli Rotenberg[3], Aaron Bostwick[3], Roland J. Koch[3], Søren Ulstrup[1], and Jyoti Katoch[2] — [1]Aarhus University, Aarhus, Denmark — [2]Carnegie Mellon University, Pittsburgh, Pennsylvania, USA — [3]Advanced Light Source, E. O. Lawrence Berkeley National Laboratory, Berkeley, California, USA

Graphene/ hBN heterostructures are an ideal testing ground for functional 2D devices owing to the atomically smooth surface and weak screening offered by hBN. On top of the record mobilities this structure offers, controlling the twist angle between layers creates a superlattice effect from which exotic electronic properties can occur.

Here, I present a study of the ARPES spectrum of graphene integrated in a device architecture with a hBN dielectric and graphite gate electrode. Micron-scale ARPES based on an X-ray capillary was used to collect the Dirac spectrum at different gate-voltages. A clear, reversible doping effect up to $5 * 10^{12}$ cm^{-2} is observed, providing access to the doping dependent quasiparticle dynamics in graphene on hBN.

Simultaneous measurements of this gate-dependent Dirac cone dispersion and the electrical resistance of the device enables extraction of electronic mobility and lifetimes. Our approach thereby demonstrates the tantalizing prospect of combining electron transport measurements with a spectroscopic probe of the electronic structure.

HL 21.5 Mon 16:00 WIL C107

Final-State Effects in Photoemission from Black Phosphorus — •Charlotte E. Sanders[1], Irene Aguilera[2], Klara Volkaert[3], Deepnarayan Biswas[3], Marco Bianchi[3], and Philip Hofmann[3] — [1]Central Laser Facility, STFC Rutherford Appleton Laboratory, Harwell OX11 0QX, UK — [2]Institute of Energy Research - Photovoltaic, Forschungszentrum Jülich, D-52425 Jülich, Germany — [3]Department of Physics and Astronomy, Aarhus University, 8000-C Aarhus, Denmark

Intrinsically doped bulk black phosphorus, although a van der Waals layered crystal, has nontrivial interlayer interactions and out-of-plane dispersing (k_z) electronic states, with a direct bandgap at the Z point of the three-dimensional (3D) Brillouin zone. The material's 3D character is related to key properties such as the thickness dependence of the bandgap in thin films and the tunability of the bandgap by strain and electric field. Interestingly, studies from angle-resolved photoemission spectroscopy (ARPES) of the k_z dispersion reveal intensity modulations near the Fermi level that are difficult to interpret in terms of the valence band dispersion predicted by theory. They have been at-

tributed to surface-resonant states [1,2]. However, on the basis of density functional theory calculations and ARPES data acquired across a broad photon energy range, we suggest here an alternative interpretation based on final-state effects. The results call attention to the meaning of the free-electron-like final-state assumption and to the limits of its applicability. [1] *PRB* **90** (2014) 085101. [2] *PRB* **93** (2016) 075207.

Invited Talk HL 21.6 Mon 16:15 WIL C107

Atomic scale neural circuitry capable of self-adaptation — •Brian Kiraly — Radboud University, Nijmegen, The Netherlands

Driven by the rise of artificial intelligence and its potential for reduced energy consumption, there have been expanded efforts directed toward investigating materials which can perform pattern recognition directly in hardware. This requires a step away from physical systems which show simple bistability, toward complex, stochastic systems, which are inherently tunable. At the moment, however, the state of the art in neuromorphic computing still struggles with fundamental issues, such as scaling or adaptability, often referred to as on-chip learning. In this talk, I will show a ground-breaking example, in which as few as 7 cobalt dopants on the surface of anisotropic semiconducting black phosphorus [1,2] can be utilized for pattern recognition. For this demonstration, we illustrate that controlled coupling between Co atoms [3] leads to a stochastic system which is well described using the concept of a Boltzmann machine. Both probing and reading the system with a scanning tunneling microscope, I will demonstrate how we realize an atomic scale synaptic memory and how the stochastic dynamics adapt and learn, depending on the input stimulus. The main aspects of this work have been carried out in the Scanning Probe Microscopy department at Radboud University. [1] Kiraly, Knol, Volckaert, Biswas, Rudenko, et. al., Phys. Rev. Lett. 123, 216403 (2019). [2] Kiraly, Hauptmann, Rudenko, Katsnelson, Khajetoorians, Nano Lett. 17, 3607 (2017). [3] Kiraly, Rudenko, Weerdenburg, Wegner, Katsnelson, Khajetoorians, Nature Commun. 9, 3904, (2018).

HL 21.7 Mon 16:45 WIL C107

Diffusion of magnetic dopants in pristine and defected phosphorene — •Rohit Babar[1] and Mukul Kabir[1,2] — [1]Department of Physics, Indian Institute of Science Education and Research, Pune, India — [2]Centre for Energy Science, Indian Institute of Science Education and Research, Pune, India

The incorporation of transition metal atoms is a robust way to imprint magnetism in non-magnetic 2D materials. In this regard, phosphorene has emerged as a versatile host for spintronic applications. Combining first-principles calculations with kinetic Monte Carlo simulations, we study the binding, magnetism, and diffusion of TM (TM = Cr, Fe, Co) atoms in pristine and defected phosphorene. The TM migration is highly anisotropic and favorable along the zigzag axis due to the puckered structure of phosphorene. While TM adsorption on pristine surface induces a local moment, the TM diffusion is uncontrolled at room temperature. We further show that vacancy defects exert an attractive potential beyond 1 nm and act as trapping centers for magnetic dopants. Our findings will assist in overcoming the practical limitations of surface decoration in phosphorene.

HL 21.8 Mon 17:00 WIL C107

Ab-initio structural dynamics of laser-excited graphene — •Sergej Krylow[1], Felipe Valencia Hernandez[2], Bernd Bauerhenne[1], and Martin E. Garcia[1] — [1]University of Kassel, 34132 Kassel, Germany — [2]National University of Colombia, 111321 Bogota, Colombia

We calculate the response of graphene to an ultrafast laser pulse using ab initio density functional molecular dynamics simulations. Our results show a biexponential decay of the Bragg peak intenities of the (100) and (110) peaks. We are able to show that the fast decay is caused by the equilibration between the electrons and a few strongly coupled optical phonons (SCOPs). The slower decay can be attributed to the equilibration of the SCOPs to the other phonon modes. Furthermore, we analyze the decay pathways from the SCOPs to the other phonon modes.

HL 21.9 Mon 17:15 WIL C107

Tailoring the opto-electronic response of graphene nanoflakes by size and shape optimization — •Raquel Esteban-Puyuelo[1], Rajat Sonkar[2], Bhalchandra Pujari[2], Oscar Gråsäs[1], and Biplab Sanyal[1] — [1]Division of Materials Theory, Department of Physics and Astronomy, Uppsala University, Box-516, SE 75120, Sweden — [2]Centre for Modeling and Simulation, Savitribai Phule Pune University, Ganeshkhind, Pune 411007, India

The long spin-diffusion length, spin-lifetime and excellent optical absorption coefficient of graphene provide a promising platform for building opto-electronic devices as well as spin-based logic in the nanometer regime. We have used time-dependent density functional theory to study how the magnetic structure and optical properties of graphene nanoflakes depend on their size and shape. We optimize the magnetic ground state and the exchange coupling between the edges of the flakes to tailor the external fields needed to switch the magnetic ordering. Finally it's shown that the magnetic state alters the optical response of the flake leading to the possibility of opto-spintronic applications.

HL 21.10 Mon 17:30 WIL C107

Electronic and optical properties of two-dimensional magnets (CrI_3) and their effects on adjacent material (WSe_2/CrI_3) — •Marie-Christin Heissenbüttel, Michael Rohlfing, and Peter Krüger — Institut für Festkörpertheorie WWU, Münster, Deutschland

For the development of novel opto-electronic devices the access and manipulation of the spin degree of freedom is of fundamental importance. The recently discovered 2D magnets provide a great opportunity to study the delicate interplay of spin, orbital, charge and lattice degree of freedom and the manipulation of other non-magnetic 2D materials, as for example TMDCs, by proximity effects. In this talk I will demonstrate our results from ab-initio calculations for the magnetic monolayer of chromium triiodide (CrI_3). The electronic and optical properties are analyzed as well as the effects of magnetism on the optics of WSe_2 within the heterobilayer tungsten diselenide (WSe_2) on CrI_3 are shown. The investigation of CrI_3 by many body perturbation theory (MBPT) within the LDA+*GdW* approximation reveals a ferromagnetic and insulating behavior and the optical absorption obtained from the solution of the BSE shows large exciton binding energies up to 1.04 eV. Furthermore due to the impact of ferromagnetic proximity effects on the TMDC WSe_2 in the heterosystem WSe_2 / CrI_3 a lifting of the energy degeneracy in the K-valleys of WSe_2 is found. Both the electronic band gap at ±K as well as the corresponding excitons in WSe_2 are affected.

HL 21.11 Mon 17:45 WIL C107

Engineering intrinsic π-magnetism in nanographenes — •Shantanu Mishra[1], Doreen Beyer[2], Kristjan Eimre[1], Shawulienu Kezilebieke[3], Reinhard Berger[2], Oliver Gröning[1], Peter Liljeroth[3], Carlo Pignedoli[1], Xinliang Feng[2], Pascal Ruffieux[1], and Roman Fasel[1] — [1]Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland — [2]Technical University of Dresden, Dresden, Germany — [3]Aalto University, Espoo, Finland

Among the multitude of properties realized in organic compounds due to the chemical versatility of carbon, magnetism remains one of the most challenging. The electronic structure of polycyclic aromatic hydrocarbons (nanographenes) depends critically on the topology of the underlying π-electron network, which provides a tunable platform to realize all-carbon magnetism at the nanoscale.

Combining rational design principles with on-surface synthesis, we engineer and probe emergent magnetism in elusive magnetic nanographenes, namely, Clar's goblet [1] and extended triangulenes [2], and their covalently-bonded assemblies. Our experimental approach follows low-temperature scanning tunneling microscopy and inelastic electron tunneling spectroscopy, with further insights provided by mean-field and many-body perturbation theory calculations.

[1] S. Mishra et al., Nature Nanotech. (in press)
[2] S. Mishra et al., J. Am. Chem. Soc. 141, 10621 (2019)

HL 21.12 Mon 18:00 WIL C107

Theoretical study on the magnetic structure of few-layer TMPS3 — •Tae Yun Kim[1,2,3] and Cheol-Hwan Park[1,2,3] — [1]Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea — [2]Gwanak-Gu Hoam-Ro 519 101-1205 — [3]Center for Theoretical Physics, Seoul National University, Seoul 08826, Korea

Transition metal phosphorus sulfides (TMPS3) are a family of the layered magnetic materials. Due to the layered structure and the rich spectrum of the magnetic structure [1], TMPS3 has been thought to be a good playground for testing two-dimensional magnetism in real world experiments [2]. It was found that the antiferromagnetic order in FePS3 remains down to the monolayer limit [3, 4], which was soon

followed by the discovery of two-dimensional ferromagnetism in CrI3 [5] and Cr2Ge2Te6 [6]. More recently, the existence of the magnetic ordering in few-layer TMPS3 has been investigated in experiments [7, 8]. In this contribution, we present an in-depth investigation of the magnetic structure of few-layer TMPS3 based on the results of our first-principles calculations.

[1] R. Brec, Solid State Ionics 22, 3 (1986).
[2] K. S. Burch et al., Nature 563, 47-52 (2018).
[3] X. Wang et al., 2D Materials 3, 031009 (2016).
[4] J.-U. Lee et al., Nano Letters 16, 7433 (2016).
[5] B. Huang et al., Nature 546, 270-273 (2017).
[6] C. Gong et al., Nature 546, 265-269 (2017).
[7] K. Kim et al., Nature Communications 10, 345 (2019).
[8] K. Kim et al., 2D Materials 6, 041001 (2019).

HL 22: 2D Materials and their Heterostructures I (joint session DS/O/HL)

Time: Tuesday 9:30–11:30 Location: CHE 89

HL 22.1 Tue 9:30 CHE 89

Plasma-enhanced atomic layer deposition of AlN at 40°C for encapsulation and dielectric integration of 2D materials — •Michele Bissolo, Alex Henning, Theresa Grünleitner, and Ian D. Sharp — Walter Schottky Institute, 85748 Garching, Germany

To date, hexagonal boron nitride (h-BN) is the material of choice for the dielectric integration of 2D materials since it preserves the intrinsic photoluminescence yield, charge carrier mobility, and band gap of 2D semiconductors by reducing strain, effects of interfacial defects, and remote phonons. However, h-BN must be either mechanically transferred with a polymer stamp onto a bulk substrate, which introduces contamination, or grown by MBE at temperatures above 800°C, which is incompatible with BEOL, microlithography, and temperature-sensitive materials. Here, we demonstrate atomically flat aluminum nitride (AlN), grown by plasma-enhanced atomic layer deposition (PEALD) at 40°C, as a scalable alternative to h-BN. AlN has a similar band gap (E_g = ∼6 eV) and a larger dielectric constant (ϵ = ∼9) in comparison to h-BN. Because ALD is conformal, it enables the full enclosure of the 2D material. In this work, we test PEALD AlN as a substrate and encapsulation layer for mono- and few-layer MoS_2. Raman spectroscopy suggests a strain-free integration of MoS_2 with AlN and photoluminescence shows a relatively stronger emission from the A and B excitons without emission from defects. We demonstrate the improved field-effect mobility with MoS_2 field-effect transistors enclosed by an AlN dielectric layer. This work provides a scalable route to the dielectric integration of 2D materials critical for future optoelectronics.

HL 22.2 Tue 9:45 CHE 89

Spin-Sensitive Readout of Two-Dimensional Wigner Crystals in Transition-Metal Dichalcogenides — •Johannes Knörzer[1,2], Martin Schuetz[3], Geza Giedke[4,5], Dominik Wild[3], Kristiaan de Greve[3], Richard Schmidt[1,2], Mikhail Lukin[3], and Ignacio Cirac[1,2] — [1]Max-Planck-Institut für Quantenoptik, Garching, Germany — [2]Munich Center for Quantum Science and Technology, München, Germany — [3]Physics Department, Harvard University, Cambridge, USA — [4]Donostia International Physics Center, San Sebastián, Spain — [5]Ikerbasque Foundation for Science, Bilbao, Spain

Wigner crystals are prime candidates for the realization of regular electron lattices under minimal requirements on external control and electronics. However, technical challenges have prevented their detailed experimental investigation to date. Here we propose an implementation of two-dimensional electron lattices for quantum simulation based on self-assembled Wigner crystals in transition-metal dichalcogenides. We show that these semiconductors allow for minimally invasive all-optical detection schemes of charge ordering and total spin. For incident light with optimally chosen beam parameters and polarization, we predict a strong dependence of the transmitted and reflected signals on the underlying lattice periodicity, thus revealing the charge order inherent in Wigner crystals. At the same time, the selection rules in transition-metal dichalcogenides provide direct access to the spin degree of freedom via Faraday rotation measurements.

HL 22.3 Tue 10:00 CHE 89

Growth of ultra-thin large sized 2D WS_2 flakes in at air-liquid interface — •Talha Nisar[1], Torsten Balster[1], Ali Haider[2], and Veit Wagner[1] — [1]Department of Physics and Earth Science, Jacobs University Bremen, Campus Ring 1, 28759, Bremen, Germany — [2]Department of Life Sciences and Chemistry, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

2D tungsten disulfide (WS_2) flakes were obtained at the air-liquid interface by a technique recently developed [1]. For this purpose, aqueous solution of ammonium tetrathiotungstate (ATTW) is used as precursor. The process exhibit a clear temperature dependence. At the room temperature, no flakes are observed. When the aqueous solution of ATTW is kept at 80°C, formation of flakes is observed. These flakes can be transferred from the air-liquid interface to a silicon substrate by a controlled dip-coating process. Large flakes with lateral size of up to 100μm were obtained. Thicknesses ranging from bilayer WS_2 to 5 MLs as measured by atomic force microscopy. Various spectroscopic techniques (FTIR, Raman, UV-Vis and XPS) are applied to investigate the chemical reaction mechanism for the formation of the flakes. These results show that the initial flakes are made of WO_3. The obtained flakes are converted to WS_2 by a post annealing step at 500-900 °C with an additional sulfur source in Ar/H_2 environment. The successful conversion to WS_2 after annealing is confirmed by Raman and XPS. This non-expensive growth technique can be used to produce large WS_2 flakes for various applications. [1] X. Zeng, et al, Nanoscale, 2017, 9, 6575-6580

HL 22.4 Tue 10:15 CHE 89

Electrical Properties and Doping effects of Chemical Vapor Deposition Growth Layered MoS2 Transistor on Different Back gate oxide Substrates — •Ying-Chun Shen and Yu-Lun Chueh — Department of Materials Science and Engineering National Tsing-Hua University 101, Sec. 2, Kuang-Fu Road, Hsinchu 30013, Taiwan, R. O. C

Recently, there have been many research evolvements in the transition-metal dichalcogenides (TMDCs) materials, which are featured by exotic properties of single or a few layers derivative in terms of direct or indirect bandgap, mechanical or electrochemical behavior. In addition to the pristine properties, the chemical and physical features of TMDCs can be controllably tuned by either nano-structure or dopants. Due to the nature of the TMDCs, they have been the promising candidates of the next-generation semiconductor devices. In our study, we have demonstrated the chemical vapor deposition growth layered MoS2 transistors on different back gate oxide substrates, such as SiO2, HfO*2 and Al2O3. Among these three substrates, HfO2 based MoS2 transistor exhibits the best performance, e.g., higher drain current up to 10 mA, on-off ratio about 106, stable mobility around 20 cm2/ V* s. Furthermore, we performed the doping effect by adding metal ions, and investigate the ion influence on the MoS2 transistor. Moreover, we also compared the electrical performance of distinct metal ions and the number of ions. Here, we provide not only the properties of back gate oxide selection but also a roadmap of ion doping effect to boost the electrical characteristics of the MoS2 transistors.

HL 22.5 Tue 10:30 CHE 89

Optical properties of TMDC monolayers interfaced with 2D metals — •Katharina Nisi[1], Shruti Subramanian[2,3], Florian Sigger[1], Margaux Lassaunière[4], David O. Tiede[4], Hendrik Lambers[4], Alexander Holleitner[1], Joshua Robinson[2,3], and Ursula Wurstbauer[4] — [1]Walter Schottky Institute and Physics Department, Technical University of Munich, Garching, Germany — [2]Department of Materials Science and Engineering, The Pennsylvania State University, USA — [3]Center for 2-Dimensional and Layered Materials, The Pennsylvania State University, USA — [4]Institute of Physics, University of Münster, Münster, Germany

Two-dimensional metals such as 2D-Ga or 2D-In prepared by confinement epitaxy are an emerging class of materials with peculiar properties including superconductivity and strong plasmonic response [1]. The plasmon resonance of those 2D metals spectrally overlaps with the excitonic transition energies of semiconducting transition metal dichalcogenides. Hybrid structures of 2D metals with TMDCs are promising for enhancing the light matter interaction. We investigate

the optical response of 2D metal-TMDC hybrid structure by a combination of spectroscopic imaging ellipsometry, photoluminescence and Raman spectroscopy.

[1] B. Bersch et al. arXiv:1905.09938 (2019).

HL 22.6 Tue 10:45 CHE 89

Rigid Band Shifts in Two-Dimensional Semiconductors through External Dielectric Screening — •Malte Rösner[1], Lutz Waldecker[2,3], Archana Raja[4,5], Christina Steinke[6], Aaron Bostwick[4], Roland J. Koch[4], Chris Jozwiak[4], Takashi Taniguchi[7], Kenji Watanabe[7], Eli Rotenberg[4], Tim O. Wehling[6], and Tony F. Heinz[2,3] — [1]Institute for Molecules and Materials, Radboud University, Netherlands — [2]Department of Applied Physics, Stanford University, USA — [3]SLAC National Accelerator Laboratory, USA — [4]Lawrence Berkeley National Laboratory, USA — [5]Kavli Energy NanoScience Institute, University of California Berkeley, USA — [6]Institute for Theoretical Physics, University of Bremen, Germany — [7]National Institute for Materials Science, Japan

We investigate the effects of external dielectric screening on the electronic dispersion and the band gap in the atomically thin, quasi-two-dimensional (2D) semiconductor WS2 using angle-resolved photoemission and optical spectroscopies, along with first-principles calculations. We find the main effect of increased external dielectric screening to be a reduction of the quasiparticle band gap, with rigid shifts to the bands themselves. Specifically, the band gap of monolayer WS2 is decreased by about 140 meV on a graphite substrate as compared to a hexagonal boron nitride substrate, while the electronic dispersion of WS2 remains unchanged within our experimental precision of 17 meV. These essentially rigid shifts of the valence and conduction bands result from the special spatial structure of the changes in the Coulomb potential induced by the dielectric environment of the monolayer.

HL 22.7 Tue 11:00 CHE 89

Unveiling valley lifetimes of free charge carriers in monolayer WSe_2 — •Manfred Ersfeld[1], Frank Volmer[1], Lars Rathmann[1], Luca Kotewitz[1], Maximilian Heithoff[1], Mark Lohmann[2], Bowen Yang[3], Kenji Watanabe[4], Takashi Taniguchi[4], Ludwig Bartels[3], Jing Shi[2], Christoph Stampfer[1,5], and Bernd Beschoten[1] — [1]2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany — [2]Department of Physics and Astronomy, University of California, Riverside, California 92521, USA — [3]Department of Chemistry and Materials Science & Engineering Program, University of California, Riverside, California 92521, USA — [4]National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan — [5]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany

We report on nanosecond long, gate-dependent valley lifetimes of free charge carriers in WSe_2, unambiguously identified by the combination of time-resolved Kerr rotation (TRKR) and electrical transport measurements. While the valley polarization increases when tuning the Fermi level into the conduction or valence band, there is a strong decrease of the respective valley lifetime consistent with both electron-phonon and spin-orbit scattering. The longest lifetimes are seen for spin-polarized bound excitons in the band gap region. We explain our findings via two distinct, Fermi level-dependent scattering channels of optically excited, valley polarized bright trions either via dark or bound states.

HL 22.8 Tue 11:15 CHE 89

Superconducting Properties of MXene Monolayers — •Cem Sevik[1], Jonas Bekaert[2], and Milorad Milosevic[2] — [1]Department of Mechanical Engineering, Eskisehir Technical University, Ankara, Turkey — [2]Department of Physics, University of Antwerp, Antwerpen, Belgium

MXenes are a new class of two-dimensional materials, consisting of a carbon or nitrogen layer sandwiched in between two transition metal layers. Various experimental studies have demonstrated that these crystals have broad and growing areas of application, such as Li-ion batteries, super-capacitors, fuel-cells, and hydrogen storage. Since most of the MXene monolayers are metals, they could also host superconductivity, depending on their electronic and vibrational properties. Therefore, we have systematically investigated the superconducting properties of monolayer MXenes of stoichiometry M2X (M being the transition metal and X either C or N), with a first-principles approach to Eliashberg theory. Due to the presence of the transition metal, we found the choice of the type of exchange-correlation and inclusion of spin-orbit interactions to be crucial to describe the vibrational and superconducting properties of these monolayers. Cautiously considering these, we have identified five new superconducting monolayer MXenes, out of which three carbides (Mo2C, W2C, and Sc2C) and two nitrides (Mo2N and Ta2N). The highest predicted critical temperature (Tc) of 17 K is found for Mo2N. Our first principle-based systematic analysis clearly has opened up a whole new class of superconductors with sizeable Tc in the monolayer limit.

HL 23: Ultra-fast phenomena

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

HL 23.1 Tue 9:30 POT 112

Atomic disorder in electroninc materials revealed by decoherence — •Samuel Palato[1], Hélène Seiler[1], Patanjali Kambhampati[2], Parmeet Nijjar[3], and Oleg Prezhdo[3] — [1]Frits-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14169 Berlin — [2]Department of Chemistry, McGill University, 801 rue Sherbrooke O., Montréal, Qc, Canada H3A 0B8 — [3]Department of Chemistry, University of Southern California, Los Angeles, California 90089

Disorder in electronic materials is a challenge for both experimental studies and theoretical description. Coherent dynamics provide a sensitive spectroscopic probe of electronic disorder. We exploit recent advances in multidimensional spectroscopy to study coherent dynamics in the model system of CdSe nanocrystal quantum dot (QD). Coherence mapping in both amplitude and phase reveals the nature of the coherent dynamics as vibrational or electronic. According to the standard model for the electronic structure of semiconductor QDs, decoherence is dominated by inhomogeneity in the sizes of the nanocrystals. Predictons from this model are inconsistent with the observation. Instead, we show decoherence arises naturally when accounting for the individual atoms by performing *ab initio* molecular dynamics of a single QD. Accounting for atomic positions results in a complicated electronic manifold. This atomistic disorder is intrinsic to the QD, and is expected to be a general phenomenon in nanostructures.

HL 23.2 Tue 9:45 POT 112

Ultrafast Laser Excitation of ZnO: A First-Principles Study — •Xiao Chen and Silvana Botti — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Laser device miniaturization is a focused area of nano optics, and ZnO nanowire lasers are attracting large interest in this context. ZnO is a well studied gain medium, and the faceted cylindrical geometry of ZnO nanowires forms a waveguide cavity. Recent experiments [1] focused on the pumping phase, and more specifically the multi-photon absorption and tunneling regimes. In this presentation, we discuss first-principles calculations of electronic excitations in ZnO, driven by strong lasers. These simulations were realized using time-dependent density functional theory, implemented in the open source code Octopus [2].

[1] R. Hollinger et al. Nano Lett. **19**, 6, 3563 (2019).
[2] X. Andrade et al., Phys. Chem. Chem. Phys, **17** 31371 (2015)

HL 23.3 Tue 10:00 POT 112

Optical Vortex Core Switching in Polariton Condensates — •Matthias Pukrop[1], Stefan Schumacher[1,2], and Xuekai Ma[1] — [1]Department of Physics and CeOPP, Paderborn University, Paderborn, Germany — [2]College of Optical Sciences, University of Arizona, Tucson, AZ 85721, USA

Vortices are topological objects carrying quantized orbital angular momentum, also known as topological charge, and have been widely studied in many physical systems. In those with spin degree of freedom the elementary excitations are so called half-vortices (HVs), referring to a vortex state carrying a topological charge in only one circular polarization component. Here we demonstrate the existence of localized

half-vortices in spinor polariton condensates, non-resonantly excited by a linearly polarized ring-shaped pump [1,2]. In the core region of the half-vortex the condensate is circularly polarized, while it is linearly polarized elsewhere. With TE-TM splitting, the pseudospin structure of the condensate gives rise to solutions with broken cylindrical symmetry. The attractive cross-interaction between different spin components can be used to realize optical vortex core switching between left- and right-circularly polarized HV states [1]. This switching process reverses the circular polarization in the HV core. It can be easily detected by measuring the polarization resolved intensity in the vortex core region. The same method can also be applied to higher order states, enabling multi-level switching configurations.

[1] M. Pukrop et al., arXiv:1907.10974 (2019).
[2] X. Ma et al., Physical Review Letters 121, 227404 (2018).

HL 23.4 Tue 10:15 POT 112

Comparison of atomic pathways during nonthermal melting in the isostructural elements germanium and silicon — •Tobias Zier and Martin Garcia — Theoretische Physik, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

Intense femtosecond-laser pulses can induce extreme non-equilibrium conditions in solids. As a consequence the crystalline structure of the solid exhibits nonthermal effects, like, coherent phonons, thermal phonon squeezing, or nonthermal melting. In the latter case the interatomic bonding is broken by the laser pulse, which excites a large amount of electrons from bonding into antibonding states. The ensuing atomic forces, that raise because of the change in the interatomic bonding, accelerate the atoms away from their initial positions. In a recent publication we could resolve the atomic motions and pathways during nonthermal melting in silicon by performing molecular dynamics simulations using our own electronic-temperature density-functional theory code CHIVES.[1] Here, we study the atomic motion during nonthermal melting in the isostructural element germanium, which has almost the same lattice parameter than silicon but less strong interatomic bonding. We will identify the most important melting directions and compare them to the results found in silicon, in order to find similarities and/or differences in the underlying melting mechanism. Our findings will help to find a general theory that describes the atomic pathways during nonthermal melting.

[1] T. Zier, E. S. Zijlstra, M. E. Garcia, Phys. Rev. Lett. **116**, 153901 (2016).

HL 23.5 Tue 10:30 POT 112

Structural Dynamics in Nanostructured Systems Probed by Ultrafast Transmission Electron Microscopy — •Nora Bach[1], Armin Feist[2], Marcel Möller[2], Claus Ropers[2], and Sascha Schäfer[1] — [1]Institute for Physics, University of Oldenburg, Germany — [2]4th Physical Institute - Solids and Nanostructures, University of Göttingen, Germany

A successful approach to investigate ultrafast nanoscale structural dynamics and to disentangle different excitation mechanisms in spatially inhomogeneous systems is based on local diffractive probing with nanofocussed femtosecond electron pulses in an ultrafast transmission electron microscope (UTEM).

Employing the advanced electron pulse properties of the Göttingen UTEM [1,2] in ultrafast convergent electron beam diffraction (U-CBED) mode [3], we study local dynamics in a multi-component model system consisting of a metal-/semiconductor hybrid structure. Ultrashort optical excitation of platinum stripes on a silicon membrane results in the generation of hot electrons and their subsequent coupling with the underlying silicon substrate. Pronounced lattice distortions are quantitatively tracked by U-CBED, and experimental results are compared to finite element simulations in order to provide deeper insights into local couplings and the efficiency of electronic and phononic transport channels across interfaces.

[1] A. Feist, N. Bach, et al., Ultramicroscopy 176, 63 (2017).
[2] N. Bach et al., Structural Dynamics 6, 014301 (2019).
[3] A. Feist et al., Structural Dynamics 5, 014302 (2018).

30 min. break

HL 23.6 Tue 11:15 POT 112

Femtosecond laser-induced electron emission from nanodiamond-coated tungsten needle tips — •Alexander Tafel, Stefan Meier, Jürgen Ristein, and Peter Hommelhoff — Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen

We present femtosecond electron emission from a tip-shaped metal-semiconductor heterostructure. By coating tungsten needle tips with thin nanodiamond (50-200 nm), we combine the high electron beam quality of tip-shaped emitters with the robustness and the negative electron affinity of diamond.

Due to the high peak intensity of femtosecond laser pulses, electrons can be photoexcited for wavelengths from the infrared (1932 nm) to the ultraviolet (235 nm) because multiphoton excitation becomes efficient over the entire spectral range. Depending on the laser wavelength, we find different dominant emission channels identified by the number of photons needed to emit electrons. Based on the band alignment between tungsten and nanodiamond, the relevant emission channels can be identified as specific transitions in diamond and its graphitic boundaries. Emission is stable at all wavelenths and bunch charges tested (up to 400 electrons per pulse). We infer a normalized emittance of less than 0.20 nm rad and a normalized peak brightness higher than $1.2 \cdot 10^{12}\mathrm{Am}^{-2}\mathrm{sr}^{-1}$.

Reference: A. Tafel et al., Phys. Rev. Lett. 123, 146902, **2019**.

HL 23.7 Tue 11:30 POT 112

Femtosecond electron diffuse scattering probes momentum-resolved phonon dynamics in black phosphorus — •Hélène Seiler[1], Daniela Zahn[1], Marios Zacharias[1], Patrick Hildebrandt[1], Thomas Vasileiadis[1], Will Windsor[1], YingPeng Qi[1], Maciej Dendzik[1], Christian Carbogno[1], Claudia Draxl[2], Fabio Caruso[2], and Ralph Ernstorfer[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany. — [2]Department of Physics, Humboldt-Universität zu Berlin, Brook-Taylor-Straße 6, 12489 Berlin, Germany

We employ femtosecond electron diffuse scattering in combination with first principle calculations to reveal the consequences of atomic and electronic structure anisotropy on phonon dynamics in prototypical anisotropic semiconductor black phosphorus. We show the presence of two dominant channels for electron-phonon scattering, namely intravalley scattering within the Gamma valley and intervalley scattering towards the Y valley. Phonons subsequently build up along the Gamma-X path over tens of picoseconds, as a result of phonon-phonon coupling. These measurements provide insights into the origin of anisotropic non-equilibrium properties with unprecedented level of detail. Our work provides direct experimental evidence that a transient nonthermal phonon distribution exists for tens of picoseconds in black phosphorus and highlights the key role of phonon-phonon scattering in phonon thermalization. That thermalization in black phosphorus is limited by phonon-phonon scattering is expected to have consequences on heat and electrical transport properties.

HL 23.8 Tue 11:45 POT 112

Photoelectron spectroscopy combining an ultrashort infrared field with an attosecond pulse pair — •Jan Vogelsang, Sara Mikaelsson, Chen Guo, Cord L. Arnold, Mathieu Gisselbrecht, Anders Mikkelsen, and Anne L'Huillier — Department of Physics, Lund University, 221 00 Lund, Sweden

We perform photoelectron spectroscopy in helium gas and at a zinc oxide (ZnO) surface using two attosecond pulses with a fixed delay and a 7-fs short infrared laser pulse. The experiments are enabled by a 200-kHz repetition rate OPCPA laser system, generating pairs of attosecond pulses in a high pressure gas jet. The measured photoelectron kinetic energy spectra are strongly modulated due to the interference of the electron matter waves emitted by the pair of attosecond pulses, showing the well-known odd-order harmonics. Additionally, the infrared dressing field leads to a periodic modulation of the spectra when we change the temporal delay, very much like in an attosecond streaking experiment, but with the spectral resolution of the harmonic frequency comb.

HL 23.9 Tue 12:00 POT 112

Non-perturbative subcycle nonlinearities of ultrastrong light-matter coupling — •Joshua Mornhinweg[1], Maike Halbhuber[1], Cristiano Ciuti[2], Dominique Bougeard[1], Rupert Huber[1], and Christoph Lange[1] — [1]University of Regensburg, Germany — [2]Université de Paris, France

In the ultrastrong-coupling regime, the rate of energy exchange between the light field of an optical resonator and an electronic excitation - the vacuum Rabi frequency, Ω_R - is comparable to the carrier frequency of light, ω_c, and anti-resonant interaction terms govern the dynamics. In this setting, novel quantum effects including the vacuum Bloch-Siegert shift, modified electronic transport, or light-induced su-

perconductivity have been explored. Yet, little is known about the nonlinearities of this extreme regime of light-matter interaction. Here, we investigate extreme subcycle nonlinearities of Landau cavity polaritons with a coupling strength of $\Omega_R/\omega_c = 0.6$. Two-dimensional terahertz (THz) spectroscopy probes the response with amplitude and phase resolution, on a subcycle scale. In a strong-field setting of multiple THz photons per Landau electron, the dynamics include pump-probe as well as four and six-wave mixing processing observed for each of the polaritons. Most importantly, we observe off-diagonal contributions, which our Liouville path analysis links to nonlinear interactions between the individual polariton states and to a collapse of the normal-mode approximation. Our quantitative microscopic theory links the nonlinearities to coherent Coulomb correlations resulting from non-perturbative excitation of the Landau system.

HL 23.10 Tue 12:15 POT 112

Ultrafast long-range energy transport via light-matter coupling in organic semiconductor films — •Raj Pandya and Akshay Rao — Cavendish Laboratory, JJ Thomson Avenue, CB3 0HE, Cambridge, United Kingdom

Efficient energy transport over macroscopic length scales is highly desirable in organic semiconductors. Here, we show this can be achieved at room temperature in a range of chemically diverse, organic semiconductor thin films through strong light-matter coupling to form exciton-polaritons, despite the absence of an external cavity. We directly visualize energy transport via femtosecond transient absorption microscopy with sub-10 fs temporal and sub-10 nm spatial precision and find energy transport lengths of up to ~270 nm at effective velocities of up to ~5 x106 m s-1. We find additional evidence of strong light-matter coupling via peak splittings in the reflectivity spectra and emission from collective polariton states. These results and the design rules that follow will enable a new generation of organic optoelectronic and light harvesting devices based on robust cavity-free exciton-polaritons.

HL 24: Functional semiconductors for renewable energy solutions I (joint session HL/CPP)

Time: Tuesday 9:30–12:00 Location: POT 151

Invited Talk HL 24.1 Tue 9:30 POT 151

Ionic Defects in Hybrid Perovskite Solar Cells — •Carsten Deibel[1], Sebastian Reichert[1], Qingzhi An[2], and Yana Vaynzof[2] — [1]Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany — [2]Technische Universität Dresden, Institut für Angewandte Physik and Centre for Advancing Electronics Dresden (cfaed), Nöthnitzer Straße 61, 01069 Dresden

Hybrid perovskite semiconductors are an interesting material system to build low-cost solar cells with high efficiency. However, processing them can be challenging: minimal and unintentional sample-to-sample variations during the fabrication process affect the ionic defects and thus the device performance. Here, I will present a joint study on the defect properties in perovskite solar cells consisting of methylammonium lead iodide ($MAPbI_3$) in dependence of the precursor solution stoichiometry. We applied impedance spectroscopy and deep-level transient spectroscopy. Our results show different ion species, and each of them features a distribution of the diffusion coefficients. The ion migration activation energies vary systematically with stoichiometry, which might explain the wide range of activation energies in the literature. I will show that the ionic defect properties we observed can be categorised using the Meyer–Neldel rule.

HL 24.2 Tue 10:00 POT 151

Ferroelectric Materials for Photocatalytic Water Splitting - Strained Mixed Anion Perovskites — •Nathalie Vonrüti and Ulrich Aschauer — University of Bern, Switzerland

Polarity, for example in ferroelectric materials, can significantly increase a catalyst's performance by improving charge-carrier separation. However, polar distortions also increase the band gap as shown for epitaxially strained SrTiO3 (1). While this band-gap increase is small for oxides, our density functional theory calculations show a much larger increase for oxynitrides: The enhanced covalency due to reduced electronegativity of nitrogen compared to oxygen results in larger strain-induced polar distortions and therefore more strongly increased band gaps by up to 1.5 eV. The reduced electronegativity, which leads to a higher valence band in oxynitrides and therefore a band gap in the visible that is attractive for photocatalysis, thus also has a detrimental effect on photo absorption when polar distortions are present. This results in a trade-off between small band gaps and polarity. We will discuss different strategies on how to overcome this trade-off with mixed anion perovskite compounds, which have not yet been considered for photocatalytic water-splitting. (1) RF Berger et al. PRL 107.14(2011):146804

Funding Acknowledgement: Swiss National Science Foundation PP00P2_157615

HL 24.3 Tue 10:15 POT 151

Preparation of $Mg_xZn_{1-x}O$ Photoanodes for Increased Photovoltage in Dye-sensitized Solar Cells — •Andreas Ringleb[1], Tsukasa Yoshida[2], and Derck Schlettwein[1] — [1]Justus Liebig University Gießen, Institute of Applied Physics — [2]Yamagata University (Yonezawa, Japan), Graduate School of Science and Engineering

ZnO is an n-type semiconductor and a promising candidate for applications in various types of optoelectronic devices due to its wide direct bandgap of about 3.3 eV and a high electron mobility. The targeted substitution of Zn with magnesium enables a tunable band gap of $Mg_xZn_{1-x}O$ in the ZnO wurtzite structure between 3.3 and 4.0 eV through control of the Mg-content. The tunability of the bandgap can be used to minimize losses during electron injection in dye-sensitized solar cells (DSCs). $Mg_xZn_{1-x}O$ nanoparticles have been prepared from acetate precursors in ethanol through a wet chemical route. Thin films have been deposited on quartz and FTO-coated glass substrates by screen-printing of pastes and subsequent annealing. SEM has been used to study the morphology of these films, while XRD was used to detect changes in the crystal lattice caused by Mg. The modulation of the band gap has been confirmed by UV-Vis spectroscopy. A focus has been put on the homogeneity and porosity of the resulting films. DSCs were prepared and analyzed to investigate the effect of the shifted band edge on the solar cell characteristics.

15 min. break.

HL 24.4 Tue 11:00 POT 151

Reactive sputtering of tantalum nitride for photoelectrochemical energy conversion — •Laura Wagner, Chang-Ming Jiang, and Ian Sharp — Walter Schottky Institut, Technische Universität München

Nitride semiconductors have gained increasing attention for photoelectrochemical (PEC) energy conversion. Traditionally, oxides have been widely investigated as photoelectrodes due to their chemical stability and versatile synthesis pathways; however oxide materials that simultaneously fulfill the efficiency and stability requirements have yet to be found. Many nitrides compounds are theoretically predicted to be semiconducting, though only a small fraction of these materials have been synthesized. Given their higher covalency compared to oxides, these nitrides may be promising candidates for PEC applications. Among transition metal nitrides, Ta3N5 has 2.1 eV bandgap and suitable valence band position for driving the water oxidation. While most studies perform nitridation on Ta or TaOx in order to obtain Ta3N5 thin films, we prepare Ta3N5 on various substrates by reactive magnetron sputtering deposition, which allows a wide range of control of chemical composition, crystallinity, and defect concentration. Additional to Ta3N5, this work also obtained a rarely reported Ta2N3 phase that adopts the Bixbyite structure. Detail characterization of structural, optical, and electrical properties of Ta2N3 are reported. Optimization of PEC performances of Ta3N5 and Ta2N3 thin films as photoanodes is achieved by adjusting deposition parameters. Improvement strategies for these emerging nitrides will also be discussed.

HL 24.5 Tue 11:15 POT 151

Atomic-Layer-Deposited TiO_2 protection layers for InP photocathodes — •Matthias Kuhl[1], Oliver Bienek[1], Alex Henning[1], Agnieszka Paszuk[2], Thomas Hannappel[2] und Ian D. Sharp[1] — [1]Walter Schottky Institut, Technische Universität München — [2]Institut für Physik, Technische Universität Ilmenau

InP has gained increased interest as a photocathode for solar fuels generation due to its suitable band gap of 1.34 eV, a conduction band edge slightly above the water reduction potential and a high incident photon to charge conversion efficiency (IPCE). While it has been found that a TiO_2 passivation layer, grown by atomic layer deposition (ALD), improve the InP/TiO_2 photocathode stability, the influence of the TiO_2 optoelectronic properties on surface reactions and interfacial charge transfer is not yet understood.

Here we investigate the role of ultrathin TiO_2 (<10nm), grown by plasma-enhanced ALD, its phase, as well as defect type and concentration for the photoelectrochemical (PEC) performance of InP/TiO_2 photocathodes. Tetrakis(dimethylamino)titanium (TDMAT) and titanium isopropoxide (TTIP) as precursors as well as H_2O and O_2-Plasma as oxidants are used to grow ALD TiO_2 films with different oxidation states and defect levels. X-Ray photoelectron spectroscopy of TiO_2 grown by PE-ALD revealed only trace amounts of impurities and stoichiometric TiO_2 consistent with a lower defect density measured by photothermal deflection spectroscopy. This work provides insights into how electronic properties of photocathode protection layers affect interfacial charge injection.

HL 24.6 Tue 11:30 POT 151

Photoanode protection by atomic-layer-deposited TiO_2 thin films — •Oliver Bienek, David Silva, and Ian D. Sharp — Technische Universität München, Walter Schottky Institut, Germany

In the development of artificial photosystems, significant effort has been devoted to preventing the degradation of photoanodes under harsh electrochemical reaction environments. A promising solution is the deposition of highly conformal protective coatings by atomic layer deposition (ALD). While the application of TiO_2 protection layers to improve the stability of photoanodes has been demonstrated successfully, questions remain regarding the mechanisms of charge carrier transport across the interface and the critical role of defects on performance characteristics. In this work, TiO_2 thin films are fabricated by plasma-enhanced ALD using different precursors and oxidizing agents on n-type Si substrates to vary both defect concentration and crystallinity of the films. In addition, the defect concentration, which is typically dominated by oxygen vacancies, is manipulated by post-annealing treatments in oxidizing atmosphere. The successful removal of defects is confirmed by analysis of sub-bandgap absorption using photothermal deflection spectroscopy. Grazing incidence X-ray diffractometry and Raman spectroscopy further prove changes in the film structure from amorphous to anatase phase upon annealing. Supplementing the optical and structural characteristics, the role of film structure and defect concentration on charge injection across the interface into the electrolyte during water oxidation is investigated using photoelectrochemical methods.

HL 24.7 Tue 11:45 POT 151

Pseudo-dreidimensionales schwerioneninduziertes Single-Event-Effect Mapping an Hochvolt Silizium Super-Junction-MOSFETs (SJ-MOS) — •Marcel Gerold[1], Michael Rüb[1], Günther Dollinger[2], Judith Reindl[2], Matthias Sammer[2] und Andreas Bergmaier[2] — [1]Ernst-Abbe-Hochschule Jena, SciTec, Carl-Zeiss-Promenade 2, 07747 Jena — [2]Universität der Bundeswehr München, LRT 2, Werner-Heisenberg-Weg 39, 85577 Neubiberg

Vertikale SJ-MOS sind weit verbreitete Halbleiterbauelemente, die in der Energiewandlung eingesetzt werden. SJ-MOS zeichnen sich durch eine komplexe drei dimensionale innere Struktur aus, welche einen niedrigen Einschaltwiderstand bei gleichzeitig hoher Spannungsfestigkeit ermöglichen. Dabei zeigt sich durch eine breite Driftzone, eine Empfindlichkeit gegenüber Partikelstrahlung. Bereits die Wirkung eines einzigen Partikels kann zu Single Event Burnout führen. Wir berichten über Ergebnisse zur Analyse der Empfindlichkeit von SJ-MOS auf Höhenstrahlung durch orts- und tiefenaufgelöste Bestrahlung mit hochenergetischen Kohlenstoffionen (E<=55 MeV, Mikrostrahlanlage "SNAKE", Maier-Leibnitz-Laboratorium, Garching). Während der Bestrahlung wird eine definierte Sperrspannung eingestellt und die Bauelementreaktion erfasst. Es werden Ladungs-Positions-Maps mit einer Auflösung von ca. 1 μm erstellt. Es zeigen sich charakteristische, mit dem Bauelementlayout korrelierbare Bereiche unterschiedlicher Sensitivität. Diese Arbeit demonstriert die Abbildung sensibler Volumina auf mikroskopischer Skala, mit dem Ziel das Verständnis von Ausfallsmechanismen bei Single-Event-Effekten zu verbessern.

HL 25: Perovskite and photovoltaics I (joint session HL/CPP)

Time: Tuesday 9:30–12:30 Location: POT 251

HL 25.1 Tue 9:30 POT 251

Properties of In_2S_3:V epitaxially grown on *p*-Si for Intermediate Band Solar Cell Applications — •Tanja Jawinski[1], Michael Lorenz[1], Roland Scheer[2], Marius Grundmann[1], and Holger von Wenckstern[1] — [1]Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Germany — [2]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, Germany

The Shockley Queisser limit of single junction solar cells can be overcome by introducing an intermediate band (IB) in wide band gap materials. Thus thermalization losses can be reduced [1]. Furthermore sub-bandgap photons can be absorped by valence band to IB and IB to conduction band transitions. According to theoretical calculations In_2S_3 hyper-doped with vanadium is a suitable candidate to realize such an IB solar cell [2].

Undoped and V-doped In_2S_3 layers are epitaxially grown by physical co-evaporation of the elements on *p*-type Si wafers. Using a combinatorial approach, we can cover a wide range of doping concentrations of up to 14 at-% V. Heterostructure *pin* solar cells are completed using *n*-ZnO:Al grown by pulsed laser deposition as transparent top electrode. Improved structural properties can be attributed to the epitaxial growth mechanism even for V-doped samples. We compare diode and solar cell parameters of undoped and V-doped sample by analyzing dark and illuminated current-voltage characteristics. Furthermore we use thermal admittance spectroscopy to investigate defect states, that are induced by V-doping. [1] Luque and Martí, *Phys. Rev. Lett.*, 1997, **78**, 5014. [2] Palacios *et al.*, *Phys. Rev. Lett.*, 2008, **101**, 046403.

HL 25.2 Tue 9:45 POT 251

Time resolved spin dynamics in lead halide hybrid organic perovskite $Fa_{0.9}Cs_{0.1}PbI_{2.8}Br_{0.2}$ — •Erik Kirstein[1], Eiko Evers[1], Vasilli V. Belykh[1,2], Evgeny A. Zhukov[1], Dennis Kudlacik[1], Ina V. Kalitukha[3], Olga Nazarenko[4], Maxim V. Kovalenko[4,5], Dmtri R. Yakovlev[1,3], and Manfred Bayer[1,3] — [1]Experimentelle Physik 2, Technische Universität Dortmund, D-44227 Dortmund, Germany — [2]P.N. Lebedev Physical Institute, Russian Academy of Sciences, 119991 Moscow, Russia — [3]Ioffe Institute, Russian Academy of Sciences,194021 St. Petersburg, Russia — [4]Laboratory of Inorganic Chemistry, ETH Zürich, CH-8093 Zürich, Switzerland — [5]Laboratory for Thin Films and Photovoltaics, Empa-Swiss Federal Laboratories for Materials Science and Technology, CH-8600 Dübendorf, Switzerland

Lead halide hybrid organic perovskites attract increased attention due their promising applications, related to high quantum efficiency and easy synthesis. Spin dynamics in perovskite materials is not studied in detail so far, but shows promising results. The studied $Fa_{0.9}Cs_{0.1}PbI_{2.8}Br_{0.2}$ bulk sample was grown out of solution of respective ions in polar solvents. Its bandgap of 1.51 eV makes this material well-suited for the resonant excitation with Ti:Sapphire laser. We study the coherent spin dynamics of electrons and holes by means of time-resolved pump-probe Kerr rotation technique at cryogenic temperatures and magnetic fields up to 6 T. We measure longitudinal spin relaxation times T_1, transverse dephasing times T_2^*, g-factor values and their spread Δg.

HL 25.3 Tue 10:00 POT 251

Ultrafast Charge Carrier Relaxation in Inorganic Halide Perovskite Single Crystals Probed by Two-Dimensional Electronic Spectroscopy — Xuan Trung Nguyen[1], •Daniel Timmer[1], Yevgeny Rakita[2], David Cahen[2], Alexander Steinhoff[3], Frank Jahnke[3], Christoph Lienau[1], and Antonietta De Sio[1] — [1]Institut für Physik, Carl von Ossietzky Universität, Germany — [2]Weizmann Institute of Science, Israel — [3]Institut für Theoretische Physik, Universität Bremen, Germany

In recent years, halide perovskites have become one of the most intensely studied semiconductors for the development of optoelectronic

devices. Regardless, the fundamental understanding of their optical and electronic properties still remains limited. To investigate the ultrafast dynamics of optical excitations we performed pump-probe and two-dimensional electronic spectroscopy (2DES) on CsPbBr3 single crystals with 10 fs time resolution [1]. While pump-probe spectra show a single bleaching feature near the band edge at 2.4 eV, 2DES maps reveal a more rich structure. In addition to a diagonal exciton bleaching peak, free carrier signatures in form of an elongated cross peak along the excitation axis appear. The separation of exciton and free carrier contributions allows to derive a rapid cooling rate of ¯3 meV/fs, indicating a strong electron-phonon coupling. The experimental findings are supported by theoretical simulations based on semiconductor Bloch equations. Our results suggest that strong electron-phonon couplings may substantially contribute to the unusual optoelectronic properties of perovskites. [1] Nguyen, X.T., et al., JPCL, 10, p. 5414-5421, 2019.

HL 25.4 Tue 10:15 POT 251

Two-Dimensional Perovskite Solar Cells with 14.1% Power Conversion Efficiency and 0.68% External Radiative Efficiency — •Weifei Fu[1,2], Alex K.-Y Jen[1], and Michael Saliba[2] — [1]University of Washington, Seattle, Washington 98195, United States — [2]Technical University of Darmstadt, Darmstadt, Germany

Quasi-2D perovskites are attractive due to their improved stability compared to 3D counterparts but they suffer from reduced performance. Here we report an efficient quasi-2D perovskite (PEA)2(MA)4Pb5I16 based optoelectronic device processed with NH4SCN and NH4Cl additives, showing a stabilized photovoltaic power conversion efficiency as high as 14.1 % (average value 12.9+_0.8 %), among the highest performing quasi-2D perovskite solar cells. These additives increase the perovskite crystallinity and induce a preferred orientation with the (0k0) planes perpendicular to the substrate, resulting in improved transport properties hence increased short-circuit current density. Furthermore, the NH4Cl treatment enriches the Cl-concentration near the PEDOT:PSS/perovskite interface, which passivates the electron traps leading to an enhanced electroluminescence external quantum efficiency (0.68% at +2.5 V bias). As a result, high open-circuit voltages of 1.21+_0.01 V with a record-low non-radiative VOC loss of only ¯ 0.16 V could be achieved for the quasi-2D perovskite system.

HL 25.5 Tue 10:30 POT 251

Structural Influence on the Exciton Fine Structure of Cesium Lead Halide Quantum Dots — •Torben Steenbock and Gabriel Bester — Institute of Physical Chemistry, University of Hamburg, Grindelallee 117, 20146 Hamburg, Germany.

Cesium lead halide quantum dots (QDs) show a bright emission, which makes them interesting for applications in optoelectronics. The origin of the bright emission is still under debate. One suggestion [1] is based on a theoretical effective mass model assuming a very strong Rashba effect, which would leads to an unusual bright exciton ground state. Another explanation is based on the idea of a phonon bottleneneck, wich leads to an efficient emission from the higher-energy bright state [2] without dark ground state.

We calculate the exciton fine structure splitting (FSS) based on ab-initio density functional theory combined with a screened configuration interaction approach for small $CsPbX_3$ (X=Cl,Br,I) QDs. We find that the bright-dark splitting for Cl, Br, and I $CsPbX_3$ perovskites amount to 17, 12 and 5 meV, respectively, with only small changes due to the symmetry (cubic, tetragonal, orthorhombic) so that we always obtain a dark ground state. The FSS (splitting between the bright states) is sensitive to the symmetry with splittings of up to 5 meV for the lowest symmetry orthorhombic structures.

[1] P.C. Sercel *et al.*, *Nano Lett.* **2019**, *19*, 4068–4077.
[2] P. Tamarat *et al.*, *Nat. Mater.* **2019**, *18*, 717–724.

30 min. break

HL 25.6 Tue 11:15 POT 251

Understanding the Role of Antisolvent Quenching in Film Formation, Device Performance, and Reproducibility of Triple Cation Perovskite Solar Cells — •Alexander Taylor[1,2], Qing Sun[1,2], Katelyn Goetz[1,2], Maximillian Litterst[1,2], Fabian Paulus[1,2], and Yana Vaynzof[1,2] — [1]Integrated Center for Applied Physics and Photonics, TU Dresden — [2]cfaed, TU Dresden

Organic-inorganic perovskite materials are promising candidates for high-efficiency solar cells, quickly approaching the performance of current state-of-the-art materials. However, irreproducibility between devices made by different research labs, even world leading labs, continue to plague the field. The causes of this issue seem to be related to small, hard to control details, such as stoichiometry variations of fractions of a percent. Herein, we seek to further the understanding of the irreproducibility in cutting edge "triple cation" perovskite solar cells by examining the minute technical differences exhibited by different researchers. We reveal that subtle differences during the crucial antisolvent step dramatically affect the resulting film microstructure, and therefore the final PV performance. By simulating this device-to-device variation, we can reliably produce devices with widely disparate power conversion efficiencies * as low as 15% and as high as 21%. Crucially, these devices would currently be reported in the literature with the exact same recipe. These results challenge some of the prevailing beliefs currently held by the research community, regarding not only what the highest performing antisolvents are, but also the general role of the antisolvent in fabricating high performance perovskite solar cells.

HL 25.7 Tue 11:30 POT 251

Efficient and Stable Hybrid Triple-Cation Perovskite/PbS Quantum Dot Solar Cells — •Miguel Albaladejo-Siguan[1], David Becker-Koch[1], Alex Taylor[1], Qing Sun[2], Vincent Lami[2], Pola Goldberg-Oppenheimer[3], Fabian Paulus[1], and Yana Vaynzof[1] — [1]Integrated Centre for Applied Physics and Photonic Materials and cfaed, Technical University Dresden — [2]Kirchhoff Institute for Physics, Heidelberg University — [3]School of Biochemical Engineering, University of Birmingham, United Kingdom

Solution-processed quantum dots (QDs) are promising for fabricating flexible, low cost and large-scale solar cells. Researchers have shown that QD devices employing a single monovalent cation perovskite shell exhibit an increased PCE when compared to standard ligand passivation. Herein we demonstrate that the use of a triple cation Cs_0.05(MA_0.17FA_0.83)_0.95Pb(I_0.9Br_0.1)_3 perovskite composition for surface passivation of the QDs results in highly efficient solar cells, which maintain 96 % of their initial performance after 1200h shelf storage. We trace the perovskite shell formation around the core by a range of spectroscopic techniques as well as high-resolution TEM. We find that the triple cation shell results in a favorable energetic alignment to the core of the dot, resulting in reduced recombination due to charge confinement without limiting transport in the active layer. Consequently, photovoltaic devices reached a maximum AM1.5G power conversion efficiency of 11.3 % surpassing previous reports of PbS solar cells employing perovskite passivation.

HL 25.8 Tue 11:45 POT 251

Microscopic Insights into the Ionic Defect Migration in Metal Halide Perovskites — •Nga Phung[1], Amran Al-Ashouri[1], Simone Meloni[2], Alessandro Mattoni[3], Steve Albrecht[1], Eva L. Unger[1], Aboma Merdasa[1], and Nga Phung[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Kekuléstr. 5, Berlin D-12489, Germany — [2]Dipartimento di Scienze Chimiche e Farmaceutiche (DipSCF), Università degli Studi di Ferrara (Unife), Via Luigi Borsari 46, I-44121, Ferrara, Italy — [3]Consiglio Nazionale delle Ricerche, Istituto Officina dei Materiali, CNR-IOM, Cagliari, Cittadella Universitaria, Monserrato 09042-I (CA), Italy

Halide perovskites are emerging as revolutionary materials for optoelectronics. Their ionic nature and the presence of mobile ionic defects have a dramatic influence on the operation of thin-film optoelectronics. This study combines photoluminescence (PL) experiments and molecular dynamics simulations to demonstrate that the grain boundaries within a perovskite film inhibit the movement of ions. Based on experimental observation and theoretical calculation, we find that the diffusion of ions is inhibited by grain boundaries, at the same time, the simultaneous removal of methylammonium and iodine causes a blue-shift of the PL spectrum. This blue-shift is reproduced by simulations, revealing that it is caused by a structural distortion of the perovskite*s Pb-I octahedral network induced by an increased concentration of ionic defects. These findings provide critical information for modeling and explaining the dynamic behavior of perovskite-based optoelectronics.

HL 25.9 Tue 12:00 POT 251

Highly stable perovskite nanocrystals in polymer micelles — •Juri G. Crimmann, Carola Lampe, and Alexander S. Urban — Nanospectroscopy Group, Nano-Institute Munich, Department of Physics, Ludwig-Maximilians-Universität München, Königinstraße 10, 80539 Munich, Germany

Halide perovskite nanocrystals (NCs) have been synthesized through many approaches. Comprising a variety of geometrical shapes, these NCs exhibit excellent optoelectronic qualities, such as near-unity quantum yields and tunable photoluminescence emission. However, perovskite nanocrystals suffer from stability problems as well as extremely mobile halide ions, both resulting in shifts of the photoluminescence emission and instant degradation in water. By using a polymer-templated synthesis we massively improve the stability and suppress halide ion migration by encapsulating NCs individually instead of entire devices. During our synthesis perovskite NCs are formed inside diblock copolymer micelles. The micelles act not only as nanoreactors, but also encapsulate and passivate the NCs, protecting them from the environment. The stability against water degradation increases significantly. Accordingly, even after 75 days of complete submersion in water, characteristic photoluminescence is observable. Furthermore, we have shown that halide ion migration through the polymer shell is nonexistent. We explore the extension of this synthesis to other perovskite compositions, comparing efficiencies and stability. And finally, we explore strategies for incorporating these highly stable NCs into working optoelectronic devices, such as light-emitting diodes (LEDs).

HL 25.10 Tue 12:15 POT 251

Optical Printing of Single Perovskite Nanoparticles — •Andreas Niklas Rank, Carola Lampe, Moritz Gramlich, and Alexander Urban — Nanospectroscopy Group, Nano-Institute Munich, Department of Physics, Ludwig-Maximilians-Universität München, Königinstraße 10, 80539 Munich, Germany

The investigation of single perovskite nanocrystals in different temperature regimes can reveal the fundamental optical properties of the individual nanocrystals and enable further improvement for optical applications. Spin-coating diluted dispersions is the typical approach to obtain films with single, separated nanocrystals. Another versatile method is optical printing, an already established approach for gold, silver and silicon nanoparticles. In this method, the optical forces of a focused laser beam are utilized to localize nanoparticles at specific positions on a substrate. A specific surface coating prevents unwanted binding of other nanoparticles. The remaining solution can be washed away, leaving only the printed nanoparticles bound to the substrate via Van der Waals forces. Here, we investigate the applicability of this method to perovskite nanocrystals. We look into different nanocrystal morphologies and compositions as well as important laser parameters and substrate materials. Adapting this method to perovskite nanocrystals would not only unlock facilitate the investigation of single perovskite nanocrystals but could also lead to complex, nanostructured substrates.

HL 26: Focus Session: Integrated Quantum Photonics I

The huge impact of semiconductor-based technologies on modern society has resulted from the ability to integrate small functional units or building blocks into integrated circuits with macroscopic functionality. In a similar way, integrated nanophotonic quantum circuits are believed to enable real-world quantum technologies with applications in secure communication, information processing, metrology and sensing.

Organizers: Kai Müller (TU Munich) and Tobias Heindel (TU Berlin)

Time: Tuesday 9:30–11:45 Location: POT 51

Invited Talk HL 26.1 Tue 9:30 POT 51

Nanophotonic quantum technology on silicon chips — •Carsten Schuck — Institute of Physics, University of Münster, Germany — CeNTech - Center for NanoTechnology, Münster, Germany — SoN - Center for Soft Nanoscience, Münster, Germany

Integrated quantum photonics holds great promise for increasing the complexity and system size of quantum communication, sensing and computation schemes through leveraging modern nanofabrication processes for replicating nanoscale devices with high reproducibility. The implementation of such integrated quantum technology requires single-photon sources, linear optic circuit components and single-photon detectors connected via a network of optical waveguides. Here we show how solid-state quantum emitters, nanophotonic devices and superconducting nanowire single-photon detectors can be efficiently interfaced to realize a versatile quantum technology platform on a silicon chip. We generate single-photons from defect centers in diamond as well as single molecules, which are efficiently coupled to optical waveguides. We realize nanophotonic circuit components that combine optical, electrical and mechanical functionality in novel material systems such as tantalum pentoxide-on-insulator and employ non-traditional computational design approaches. Waveguide-coupled superconducting nanowire single-photon detectors integrate seamlessly with such nanophotonic circuitry and offer high detection efficiency, low noise and excellent timing performance. We present progress towards integrating sources, circuits and detectors on-chip to match the demands of future large-scale implementations of quantum technologies.

Invited Talk HL 26.2 Tue 10:00 POT 51

Resonant excitation and coherent manipulation of quantum dots for quantum information experiments — •Ana Predojevic — Stockholm University, Stockholm, Sweden

Single self-assembled quantum dots are established emitters of single photons and entangled photon pairs. To be used in quantum information experiments quantum dots need to be excited resonantly and coherently. The use of resonant excitation makes this system well suitable for generation of photon pairs with near-unity efficiency and high purity and also for entangling schemes such as time-bin entanglement. The entanglement of photons generated by quantum dot systems can be employed in free space-and fibre-based quantum communication. In addition to this, the versatility of entanglement can be more optimally used and explored if the photons are entangled simultaneously in more than one degree of freedom - hyperentangled, which was also recently shown to be possible using quantum dots. However, the achievable degree of entanglement and readiness of the source for use in quantum communication protocols, depend on several additional functionalities such as high collection efficiency and coherence of the emitted photon pairs. Here, we will address engineered photonic systems that promise a more efficient and better performing sources of entangled photon pairs.

15 min. break.

HL 26.3 Tue 10:45 POT 51

Cavity-QED effects in dissipative resonators using coupled quasinormal modes — •Sebastian Franke[1], Stephen Hughes[2], Juanjuan Ren[2], Andreas Knorr[1], and Marten Richter[1] — [1]Technische Universität Berlin, Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Hardenbergstraße 36, 10623 Berlin, Germany — [2]Department of Physics, Engineering Physics and Astronomy, Queen's University, Kingston, Ontario, Canada K7L 3N6

Open cavity systems are of high interest in quantum optics and plasmonics and offer a variety of applications, including lasing/spasing and non-classical light generation. In many cavity-QED platforms, photons are usually described by lossless normal modes, e.g., in the Jaynes-Cummings model. However, for metallic or open cavities, the so-called quasinormal modes [1] (QNMs) with complex eigenfrequencies are more appropriate, and are the natural modes to quantize.

Using a recent developed quantization scheme [2] for three-dimensional open resonators on the basis of these QNMs, we explore the multi-photon regime in a plasmonic-photonic crystal cavity coupled to a two-level atom. On the basis of a generalized input-output theory for QNMs [3], we derive quantum correlations of the output fields using the QNM Lindblad master equation and compare the results to the phenomenological dissipative Jaynes-Cummings models.

[1] P. T. Leung *et al.*, *Phys. Rev. A* **49**, 3057, 1994
[2] S. Franke *et al.*, *Phys. Rev. Lett.* **122**, 213901, 2019
[3] S. Hughes *et al.*, *ACS Photonics* **6**, 8, 2168-2180, 2019

HL 26.4 Tue 11:00 POT 51

Optimized designs for telecom-wavelength quantum light sources based on hybrid circular Bragg gratings — •Lucas Rickert, Johannes Schall, Timm Kupko, Sven Rodt, Stephan Reitzenstein, and Tobias Heindel — Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany

We present finite-element simulations of optimized designs for hybrid circular Bragg grating devices operating at telecom O-band wavelengths [1]. The designs show Purcell factors up to 30 and photon extraction efficiencies exceeding 95%. We discuss how the optical properties are affected by the variation of structural parameters and investigate the designs' performance if possible fabrication-related structural imperfections are introduced, including imperfect side-wall etching and non-ideal positioning of the emitter inside the device. For the latter, we show that the devices are robust against emitter displacements well within reported deterministic fabrication uncertainties for structures with embedded semiconductor quantum dots. Additionally, we present simulations showing the CBG devices' compatibility to optical single mode fibers and obtain up to 80% fiber coupling efficiency with off-the-shelf fibers. We further investigate on how to improve the fiber coupling to close to unity by the use of specialty fibers and address C-band compatible CBG designs.

[1] Rickert *et al.*, Optics Express, arXiv.1908.08408, in press (2019)

Invited Talk HL 26.5 Tue 11:15 POT 51

Fully on-chip single-photon Hanbury-Brown and Twiss experiment integrating semiconductors and superconductors — •Simone Luca Portalupi[1], Mario Schwartz[1], Ekkehart Schmidt[2], Ulrich Rengstl[1], Florian Hornung[1], Stefan Hepp[1], Konstantin Ilin[2], Michael Jetter[1], Michael Siegel[2], and Peter Michler[1] — [1]IHFG-University of Stuttgart, IQST and SCoPE, Stuttgart, Germany — [2]IMS, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Stability and scalability of quantum computation and quantum simulation implementations will largely benefit from a platform capable to realize usual tabletop functionalities on a single chip. Although to fulfill this need, only few building blocks are absolutely necessary, demonstrating their successful simultaneous implementation remained elusive for long time. Here we will discuss the realization of a fully on-chip Hanbury-Brown and Twiss experiment, realizing on the same chip a non-classical light source, a basic photonic logic and two single photon detectors [1]. GaAs single-mode waveguides embedding semiconductor quantum dots are used in combination with superconducting material to realize a beamsplitter with two superconducting nanowire detectors at the output ports. To further increase the coupling of the quantum dot photons into the waveguide, the realization of waveguide-coupled Bragg grating cavities will also be discussed [2]. These results open the way to implement complex on-chip quantum photonics.

[1] M. Schwartz, et al., Nano Lett. 18, 6892 (2018).
[2] S. Hepp, et al., Opt. Express 26, 30614 (2018).

HL 27: 2D semiconductors and van der Waals heterostructures III (joint session HL/DS)

Time: Tuesday 9:30–13:00 Location: POT 81

Invited Talk HL 27.1 Tue 9:30 POT 81

Radiative Lifetime and Fine Structure of Excitons in Transition Metal Dichalcogenide Monolayers — •Xavier Marie — Université de Toulouse, LPCNO, INSA-CNRS-UPS, Toulouse, France

Optical properties of atomically thin transition metal dichalcogenides are controlled by robust excitons characterized by a very large oscillator strength [1,2,3]. Encapsulation of monolayers such as MoSe2 in hexagonal boron nitride (hBN) yields narrow optical transitions approaching the homogeneous exciton linewidth [4,5]. We demonstrate that the exciton radiative rate in these van der Waals heterostructures can be tailored by a simple change of the hBN encapsulation layer thickness as a consequence of the Purcell effect [6].

The time-resolved photoluminescence measurements together with cw reflectivity and photoluminescence experiments show that the neutral exciton spontaneous emission time can be tuned by one order of magnitude depending on the thickness of the surrounding hBN layers.

I will also discuss recent results on the fine structure of excitons in MoSe2 and MoS2 monolayers.

[1] G. Wang et al, Rev. Mod. Phys. 90, 021001 (2018) [2] D. Lagarde et al, PRL 112, 047401 (2014) [3] C. Robert et al, PRB 93, 205423 (2016) [4] F. Cadiz et al, PRX 7, 021026 (2017) [5] G. Wang et al, PRL 119, 047401 (2017) [6] H.H. Fang et al, PRL 123, 067401 (2019)

HL 27.2 Tue 10:00 POT 81

Control of Excitons in Monolayer Transitionmetal Dichalcogenides via Extrinsic Dielectric Screening — •Frederik Otto, Philip Klement, and Sangam Chatterjee — Institute of Experimental Physics I, Justus-Liebig-University Giessen, Heinrich-Buff-Ring 16, D-35392 Giessen, Germany

Electric field lines between charges in freestanding monolayers of transition metal dichalcogenides (TMDs) can extend freely outside the material's perimeters due to the absence of screening carriers on top and on the bottom of the sample. Similarly, field lines extending into a close dielectric, *e.g.*, the substrate, are subject to extrinsic screening effects. This effectively weakens the Coulomb interaction of charge carriers and therefore, iduces changes to the exciton binding energy and electrical band gap.

In order to obtain knowledge about the interaction range and the effect of the static dielectric constant of the surrounding dielectric environment on A and B-excitons of the K-point, we investigated monolayer samples WSe_2 supported on either TiO_2 (high static dielectric constant) or SiO_2 (low static dielectric constant) and samples encapsulated between the two substrate materials.

HL 27.3 Tue 10:15 POT 81

Revealing the quantum nature of excitons in encapsulated monolayers by optical dispersion measurements — •Lorenz Maximilian Schneider[1], Shanece S. Esdaille[2], Daniel A. Rhodes[2], Katayun Barmak[3], James C. Hone[2], and Arash Rahimi-Iman[1] — [1]Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, Marburg, 35032, Germany — [2]Department of Mechanical Engineering, Columbia University, New York, NY 10027, USA — [3]Department of Applied Physics and Applied Mathematics, Columbia University, New York, NY 10027

The dispersion of excitons in TMDC monolayers has been a topic of several recent theoretical studies and is the base of a true understanding of the physics of such systems. Nonetheless, the theoretical papers have contradicting predictions ranging from the formation of Dirac cones or the formation of a second linear exciton branch around zero in-plane momentum to calculations that just expect ordinary degeneracy-lifted parabolic dispersions. Here, we employ Fourier-space spectroscopy to directly measure the dispersion of the A-exciton in a high-quality h-BN encapsulated monolayer system. A remarkably strong dispersion with 2 meV shifts in within the light cone, respectively an effective mass of 7E-4 m_e can be deduced. Models based on exchange interaction and exciton–polariton formation due to the large oscillator strength are discussed in order to understand the phenomenon clearly observed in PL and reflection spectra [1]. Futhermore, density and temperature dependent behaviour is presented.

[1] L.M. Schneider et al., Optics Express (in press)

HL 27.4 Tue 10:30 POT 81

Light-driven capacitive charge injection in 0D-2D hybrid nanostructures — •Ilka Kriegel[1], Michele Ghini[1], Liberato Manna[1], Nicholas J. Borys[2], and P. James Schuck[3] — [1]Department of Nanochemistry, Istituto Italiano di Tecnologia, Italy — [2]Department of Physics, Montana State University, Bozeman, MT, USA — [3]Department of Mechanical Engineering, Columbia University, New York, NY, USA

In this work we reveal that the coupling of indium tin oxide (ITO) nanocrystals to monolayer MoS2 results in a light-driven charge-injection scheme that quasi-permanently dopes monolayer MoS2 to extents competing with electrostatic doping. The cooperative electronic properties of such novel 0D 2D hybrids display efficient and permanent charge separation after light absorption. The electrons are stored in the nanocrystals, while the holes are transferred to the 2D

material accumulating in regions of initially enhanced n-type doping and preferentially along edges and grain boundaries. Charge separation over distances up to 40 μm away from the local (micron sized) optical excitation spot are observed. Notably, carrier injection follows a capacitor-like behavior with capacitance values in the femto Farad range leading to the photo-charging of a model capacitor. An average optically induced photodoping of each nanocrystal with more than 40 carriers is extracted. These studies present a foundational building block for next-generation light-driven energy storage devices. Additionally, the remote-control of local charge density opens prospects for contactless and optically driven 2D material electronics.

30 min. break

HL 27.5 Tue 11:15 POT 81

Broken adiabaticity induced by Lifshitz transition in MoS_2 and WS_2 single layers — •Dino Novko — Institute of Physics, Zagreb, Croatia — Donostia International Physics Center (DIPC), San Sebastián, Spain

The breakdown of the adiabatic Born-Oppenheimer approximation is striking dynamical phenomenon, however, it occurs only in a handful of layered materials. Here I show that adiabaticity breaks down in doped single-layer transition metal dichalcogenides in a quite intriguing manner. Namely, significant nonadiabatic coupling, which acts on frequencies of the Raman-active modes, is prompted by a Lifshitz transition due to depopulation and population of multiple valence and conduction valleys, respectively. The outset of the latter event is shown to be dictated by the interplay of highly non-local electron-electron interaction and spin-orbit coupling. In addition, intense electron-hole pair scatterings due to electron-phonon coupling are inducing phonon linewidth modifications as a function of doping. Comprehending these intricate dynamical effects turns out to be a key for mastering characterization of electron doping in two-dimensional nano-devices by means of Raman spectroscopy.

HL 27.6 Tue 11:30 POT 81

Transient Valley Grating Spectroscopy on WSe_2 — •Julian Wagner, Henning Kuhn, Robin Bernhardt, Jingyi Zhu, and Paul van Loosdrecht — Universität zu Köln, II. Physikalisches Institut, D-50937 Köln, Germany

The absence of space inversion symmetry combined with strong spin-orbit interactions and time-reversal in monolayer transition metal dichalcogenides lead to the emergence of a new quantum degree of freedom, the valley pseudospin. This valley degree of freedom can be manipulated making use of the selection rules for light matter interaction, i.e. one can for instance create pure pseudospin up or down states. These states, however, will decay due to intervalley scattering of the excitonic states involved. The mechanisms leading to intervalley scattering are currently intensely debated, partially due to the lack of experiments directly addressing this.

A direct technique to address the intervalley scattering is Transient Valley Grating Spectroscopy, which is a novel 4-wave mixing approach similar to spin grating techniques. Using this approach, we investigated the valley pseudospin dynamics in monolayer WSe_2. This allows for a direct determination of the intervalley scattering rate. Its temperature dependence shows that the dominant valley depolarization process is optical-phonon mediated intervalley scattering.

HL 27.7 Tue 11:45 POT 81

Exciton diffusion in WS_2 monolayers with suppressed disorder — •Koloman Wagner[1], Jonas Zipfel[1], Marvin Kulig[1], Raül Perea-Causín[2], Samuel Brem[2], Jonas D. Ziegler[1], Roberto Rosati[2], Takashi Taniguchi[3], Kenji Watanabe[3], Mikhail M. Glazov[4], Ermin Malic[2], and Alexey Chernikov[1] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]Department of Physics, Chalmers University of Technology, Gothenburg, Sweden — [3]National Institute for Materials Science, Tsukuba, Ibaraki, Japan — [4]Ioffe Institute, St. Petersburg, Russia

Excitons are known to dominate optical properties of semiconducting transition metal dichalcogenides (TMDCs) both for monolayers and heterostructures. While excitons can also propagate across large distances due to the two-dimensional nature of the system, their behavior remains highly sensitive to local environmental inhomogeneities. In our work, we take advantage of material encapsulation in high-quality hexagonal boron nitride to study inherent exciton propagation unobscured by disorder. Using spatially- and time-resolved photoluminescence microscopy we find highly efficient linear diffusion and pronounced non-linear phenomena. In order to explain our findings we employ a combination of numerical and analytical approaches, discuss the role of dark states as well as non-radiative exciton-exciton scattering and present a mechanism for rapid diffusion facilitated by free electron-hole plasma.

HL 27.8 Tue 12:00 POT 81

Chemical Trend of Transition-Metal Doping in WSe_2 — •Dan Han[1,2,3], Shiyou Chen[1], and Mao-Hua Du[2] — [1]East China Normal University, Shanghai, China — [2]Oak Ridge National Laboratory, Oak Ridge, USA — [3]Ludwig-Maximilians-Universität München, Munich, Germany

Transition-metal dichalcogenides (TMDs) are promising nanoscale materials with a wide range of applications. Chemical doping is a powerful tool for tailoring the physical and chemical properties of TMDs for targeted functionalities. As an important TMD, WSe_2 has great potential for applications in FET and CMOS technologies. However, precise control over the type and density of free carriers remains challenging. We performed first-principles calculations to study intrinsic defects and transition-metal (TM) dopants in WSe_2. Our results show that TM doping can effectively control the Fermi level in WSe_2 with no significant compensation by intrinsic defects. Nb and Ta are effective p-type dopants capable of generating a high free hole density in WSe_2. While n-type doping is possible by Re and Cu, the doping efficiency is reduced due to the lower attainable dopant concentration and higher ionization energies. The chemical trend in the attainable concentration of various substitutional TM dopants in WSe_2 is largely determined by the competition between the dopant incorporation in WSe_2 and the formation of the secondary phase $TMSe_2$. Such a competition is strongly affected by the different crystal environments of the TM ion in $TMSe_2$ and WSe_2.

HL 27.9 Tue 12:15 POT 81

Interlayer excitons in pristine bilayer MoS2 with strong oscillator strength — •Etienne Lorchat[1], Maximilian Waldherr[1], Sefaattin Tongay[2], Takashi Taniguchi[3], Kenji Watanabe[3], Christian Schneider[1], and Sven Höfling[1] — [1]Technische Physik and Wilhelm Conrad RöntgenResearch Center for Complex Material Systems, Physikalisches Institut, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]School for Engineering of Matter, Transport and Energy, Arizona State University, Tempe, Arizona 85287, United States — [3]National Institute for Materials Science, Tsukuba, Ibaraki 305-0044, Japan

In the high density limit, the interaction between electrons in a 2D electron gas (2DEG) and excitons in Transition Metal Dichalcogenide (TMD) are predicted to yield a new, unconventional superconductive phase via excitonic cooper pairing. However, this interaction only gets notable if exciton aquires an out of plane dipole to interact with the 2DEG as well as an in-plane dipole to be easily excited with light. The commonly studied excitons in TMD monolayers or heterobilayers present solely one type of the dipole. Among the various approach, we will present here the hybrid interlayer exciton in MoS2. Using field-dependent photoluminescence spectroscopy as well as reflectivity we will demonstrate the emergence of an excitonic resonance, which combines a static dipole moment with a significant oscillator strength.

HL 27.10 Tue 12:30 POT 81

Optoelectronic transport in van der Waals heterostructures of Weyl semimetal $MoTe_2$ — •Maanwinder Partap Singh[1,2], Jonas Kiemle[1,2], Alexander Holleitner[1,2], and Christoph Kastl[1,2] — [1]Walter Schottky Institut, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstraße 4, D-80799 Munich, Germany

Unlike topological insulators which are topologically protected by the bulk band gap, Weyl semimetal's topological protection comes from the fact that their 3D Weyl nodes are separated in momentum space. $MoTe_2$ belongs to the family of transition metal dichalcogenides, and it crystallizes in several structures. At room temperature, it exists as either hexagonal (2H, a semiconducting phase) or monoclinic (1T', a metallic phase) structure. Upon cooling, the monoclinic phase undergoes a transition at 240 K into an orthorhombic phase known as T_d phase, which breaks inversion symmetry and results in a type II Weyl semimetal phase. Here, we study the optoelectronic properties of $MoTe_2$ as function of temperature and layer number using photocurrent and photoconductance spectroscopy. In particular, we in-

vestigate the ultrafast electron dynamics using an on-chip Terahertz spectroscopy to disentangle hot electron currents and photogalvanic effects.

HL 27.11 Tue 12:45 POT 81

Surface Ripplocations in van der Waals materials: Structural & Electronic Properties — •James McHugh[1], Pavlos Mouratidis[1], Kenny Jolley[1], and Patrick Briddon[2] — [1]Dept. of Chemistry, Loughborough University — [2]School of Engineering, Newcastle University

Ripplocations are a new class of defect, unique to layered solids, which are characterised by the accommodation of extra material at sharp, localised folds. Dislocations in three-dimensional materials arise from the balance of strain and disregistry. In contrast, anisotropic van der Waals materials may completely alleviate strain through out-of-plane buckling.

We have conducted first-principles and analytical investigation of the properties of surface ripplocations on van der Waals layers. Analytical expressions for the formation energy, height and width of ripplocations are derived and compared to ab-initio simulations, showing that surface ripplocations readily form epitaxially on van der Waals materials.

The accommodation of extra material across a ripple is considered in terms of a Frenkel-Kontorova model, where it is found that ripplocations exhibit a "double kink" structure owing to the interplay of curvature and disregistry across the defect. Additionally, it is found that ripplocations induce a reduction in the band gap of layered semiconductors, with PDOS simulations identifying this change with the transition metal atoms across the curved regions. In combination with their high mobility this suggests the possibility of using ripplocations as a defect engineering platform.

HL 28: Focus: Exploitation of Anisotropy in Organic Semiconductors I (joint session CPP/HL)

Molecular glasses and semi-crystalline thin films play a key role in organic semiconductor devices, particularly organic light-emitting diodes and solar cells. Surprisingly, some of these materials exhibit considerable anisotropies regarding their molecular orientation which leads to non-isotropic electronic properties. In spite of the importance for optoelectronic devices, however, this phenomenon is not fully understood yet. This focus session will bring together concepts from the physics of glasses, structure formation in soft matter as well as applications of such anisotropic molecular solids in organic electronics. Organized by: Wolfgang Brütting (University Augsburg), Sebastian Reineke (TU Dresden); Wolfgang Wenzel (Karlsruher Institut für Technologie).

Time: Tuesday 10:00–12:30 Location: ZEU 222

Invited Talk HL 28.1 Tue 10:00 ZEU 222

Anisotropic packing in vapor-deposited glasses — •Mark Ediger — University of Wisconsin-Madison, USA

Glasses are generally regarded as highly disordered and the idea of controlling molecular packing in glasses is reasonably met with skepticism. However, as glasses are non-equilibrium materials, a vast array of amorphous structures are possible in principle, even for a single component system. Physical vapor deposition (PVD) allows a surprising amount of control over anisotropic molecular packing in glasses. For organic semiconductors, glasses can be prepared in which the molecules have a substantial tendency to stand-up or lie-down relative to the substrate, and molecular layering can also be achieved. The high density and anisotropic packing of PVD glasses can be explained by a mechanism that is "anti-epitaxial" as structure is templated by the top surface rather than by the underlying substrate. This mechanism implies that similar structures can be prepared by increasing substrate temperature and by decreasing deposition rate, and this has recently been experimentally verified.

HL 28.2 Tue 10:30 ZEU 222

Clarifying the orientation mechanism of homoleptic Iridium-carbene complexes — •Markus Schmid[1], Kristoffer Harms[2], Thomas Morgenstern[1], Alexander Hofmann[1], Hans-Hermann Johannes[2], Wolfgang Kowalsky[2], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Institute for high frequency technology, TU Braunschweig, 38106 Braunschweig, Germany

Horizontal orientation of the emitting species is one of the most promising techniques to increase the efficiency of state of the art organic light emitting diodes. Especially metal-organic compounds have attracted great attention. While the alignment has been observed and explained for many heteroleptic Iridium complexes, there has been less progress for their homoleptic counterparts. Only few homoleptic compounds have been reported to show a beneficial morphology in guest-host systems. In this study, we investigated multiple derivatives and isomers of the sky-blue dye tris(N-dibenzofuranyl-N'-methylimidazole)iridium(III) ($Ir(dbfmi)_3$) doped in the hosts Bis[2-(diphenylphosphino)phenyl]ether oxide (DPEPO) and 3,6-bis(diphenylphosphoryl)-9-phenylcarbazole (PO9). By a combination of optical techniques to probe the transition dipole orientation and electrical measurements to access the permanent dipole moment, we revealed that this homoleptic complex is significantly aligned in both matrices. From our insights into the film morphology we postulate that an anisotropic interaction is responsible for the orientation and even identified the region of the molecule that causes this behavior.

HL 28.3 Tue 10:45 ZEU 222

Application of polar molecules to electret for vibrational energy generator: Improvement of device productivity and output power by utilizing spontaneous orientation polarization — •Yuya Tanaka[1,2], Noritaka Matsuura[1], and Hisao Ishii[1] — [1]Chiba University, Chiba, Japan — [2]Japan Science and Technology Agency, PRESTO, Saitama, Japan

Electret-based vibrational energy generator (E-VEGs) have attracted much attention because they can generate electrical power from ambient vibrations. The challenges for E-VEGs are to: (i) simplify charging process for making electret and (ii) enhance output power (P) of the device. Recently, we developed polar molecules (PM), such as Alq3 and TPBi, based VEGs that do not require any charging process by utilizing spontaneous orientation of the molecules. To increase P of the device, enhancement of surface potential (SP), namely, order parameter of the molecule, is required. In this study, we prepared PM films with various deposition rate (r). We found that the SP becomes larger in the case of high r, suggesting that molecular orientation can be controlled by r. Further, the estimated surface charge density was comparable to conventional polymer-based electret after charging (typically, 2 mC/m2). We believe that the realization of PM-VEGs will open up the novel ways for supplying electrical energy to the various devices.

HL 28.4 Tue 11:00 ZEU 222

Post processing temperature dependence of the emitter molecule orientation in organic thin films — •Christian Hänisch, Simone Lenk, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, Germany

One of the main loss channels reducing the efficiency of organic light-emitting diodes is optical trapping of already generated photons due to total internal reflection and coupling to plasmonic modes. Aligning the transition dipole moment of the emitter molecules parallel to the interface planes of the stratified device structure can drastically decrease the unusable power fraction.

In this work, the long term, post processing stability of the molecular orientation of two well-known phosphorescent emitters is investigated for different storage temperatures up to 95% of the glass transition temperature (Tg) of the host material. Both, photoluminescent samples and electroluminescent devices are analyzed. In the first case, the

emission layers are embedded between two layers of higher Tg in order to avoid crystalization of bare emission layers.

It is shown that the orientation keeps unchanged for several months as long as Tg is not exceeded but changes immediately as soon as the samples are exposed to temperatures above Tg for only a few minutes. The latter is demonstrated exemplarily for selected samples after the long term storage period.

15 min. break

Invited Talk HL 28.5 Tue 11:30 ZEU 222

Influence of stability and molecular orientation on the properties of stable glasses — •Javier Rodríguez-Viejo — Physics department, Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain

Stable glasses have attracted great interest since their discovery in 2007. Their superior behavior, compared to liquid-cooled glasses, includes higher kinetic and thermodynamic stability, higher density, sound velocity and elastic moduli or the modification of the low-temperature properties. The origin of the high thermodynamic and kinetic stability of these vapor-deposited glasses is related to the high mobility of surface molecules that enables them to settle into energetic favorable positions during the deposition process. Besides, depending on the molecular shape PVD glasses exhibit packing anisotropies that depend on the deposition temperature. Although molecular orientation does not seem to play a substantial role in the observed stability enhancement, it can have a significant impact in many properties of vapor-deposited glasses. For instance, we have previously shown that molecular orientation may induce variations of the growth front velocity during the heterogeneous transformation of a glass into the supercooled liquid state. In addition, molecular anisotropy plays a key role in charge and thermal transport. We will describe the impact of the deposition process and the molecular orientation on the thermal properties and on electronic and heat propagation. We also explore the benefits of using stable glasses grown at temperatures around 85% Tg to increase device efficiency and operational stability of OLEDs.

HL 28.6 Tue 12:00 ZEU 222

Infrared organic light-emitting diodes with horizontally oriented carbon nanotube emitters — •Caroline Murawski[1,3], Arko Graf[2,3], Jana Zaumseil[2], and Malte C. Gather[3] — [1]Kurt-Schwabe-Institut Meinsberg — [2]Universität Heidelberg — [3]University of St Andrews, UK

Semiconducting single-walled carbon nanotubes (SWCNT) have shown great potential as electrodes and transport layers in organic light-emitting diodes (OLEDs) and field-effect transistors. Here, we incorporate polymer-wrapped SWCNTs as emitter into OLEDs and achieve narrowband pure infrared emission between 1000 and 1200 nm. Due to the 1D nature of CNTs, the transition dipoles exhibit strong horizontal orientation, which results in an exceptionally high outcoupling efficiency of 49%.

HL 28.7 Tue 12:15 ZEU 222

Polarized blue photoluminescence of mesoscopically ordered electrospun non-conjugated polyacrylonitrile nanofibers — Xiaojian Liao[1], •Frank-Julian Kahle[2], Bin Liu[3,4], Heinz Bässler[2], Xinghong Zhang[3], Seema Agarwal[1], Anna Köhler[2], and Andreas Greiner[1] — [1]Macromolecular Chemistry II, U Bayreuth, Germany — [2]Softmatter Optoelectronics, U Bayreuth, Germany — [3]MOE Key Laboratory of Macromolecular Synthesis and Functionalization, Zhejiang University, P. R. China — [4]School of Energy and Power Engineering, North University of China, China

We demonstrate the fabrication of electrospun fibers from the non-conjugated polymer polyacrylonitrile (PAN) that can be aligned by a simple heat-stretching process. Upon excitation at 340 nm ribbons made from the nanofibres show polarized deep blue luminescence with an anisotropy of 0.37 and a quantum yield of about 0.31. Furthermore, they exhibit room temperature green phosphorescences with a lifetime of about 200 ms as well as a delayed deep blue fluorescence resulting from triplet-triplet annihilation (non-coherent photon upconversion). Wide and small angle X-ray scattering experiments show that the stretched electrospun nanofibers are highly aligned with nearly perfect uniaxial orientation within the fabricated ribbons. This results in mechanical robustness and flexibility, with a high specific tensile strength (534 ± 28) $MPa \cdot cm^3/g$ and toughness (79 ± 7) J/g. The combination of efficient polarized deep blue luminescence, room temperature phosphorescence, TTA, mechanical robustness and flexibility of these fibers opens up new avenues for applications.

HL 29: 2D Materials III: Growth and Heterostructures (joint session O/HL)

Time: Tuesday 10:30–13:45 Location: GER 38

HL 29.1 Tue 10:30 GER 38

High structural and optical quality of transition metal dichalcogenides grown by chemical vapor deposition — •Antony George[1], Shivangi Shree[2], Tibor Lehnert[3], Christof Neumann[1], Meryam Benelajla[2], Cedric Robert[2], Xavier Marie[2], Kenji Watanabe[4], Takashi Taniguchi[4], Ute Kaiser[3], Bernhard Urbaszek[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, 07743 Jena, Germany — [2]Université de Toulouse, INSA-CNRS-UPS, LPCNO, 135 Avenue Rangueil, 31077 Toulouse, France — [3]Ulm University, Central Facility of Materials Science Electron Microscopy, D-89081 Ulm, Germany — [4]National Institute for Materials Science, Tsukuba, Ibaraki 305-0044, Japan

We have achieved highly reproducible large area growth of high-quality monolayer transition metal dichalcogenides (TMDs) by our modified chemical vapor deposition (CVD) process. We correlate the structure of our CVD grown MoS2 monolayers studied by high-resolution transmission electron microscopy (HRTEM) with the optical quality revealed in temperature dependent optical spectroscopy. We determine a defect concentration of the order of 10^{13} cm^{-2} for our samples with HRTEM. We show optical transition linewidth of 5 meV at low temperature (T = 4 K) for the free excitons in emission and absorption after encapsulation in hBN. This is comparable to the best monolayer samples obtained by mechanical exfoliation of bulk material.

HL 29.2 Tue 10:45 GER 38

Analysis of Airborne Contamination on Transition Metal Dichalcogenides with Atomic Force Microscopy Revealing That Sulfur Is the Preferred Chalcogen Atom for Devices Made in Ambient Conditions — Korbinian Pürckhauer, •Dominik Kirpal, Alfred J. Weymouth, and Franz J. Giessibl — University of Regensburg, Germany

The fabrication of devices incorporating transition metal dichalcogenides (TMDCs) is mostly done in ambient conditions, and thus the investigation of TMDCs cleanliness in air at the nanoscale is important. We imaged MoS_2, WS_2, $MoSe_2$, and WSe_2 using atomic force microscopy. Mechanical exfoliation of the TMDCs provided clean terraces on sulfides MoS_2 and WS_2. In contrast, the selenides appeared to be contaminated directly after cleavage in most cases. Long-term measurements on $MoSe_2$ revealed that these unwanted adsorbates are mobile on the surface. In situ cleavage and imaging of WSe_2 in ultra-high vacuum shows clean surfaces, proving the airborne character of the adsorbed particles.

[1] K. Pürckhauer et al., ACS Appl. Nano Mater. 2(5), 2593 (2019)

HL 29.3 Tue 11:00 GER 38

Capturing the Carpet Growth of 2D-Silica Films — •Leonard Gura, Adrian Leandro Lewandowski, Zechao Yang, Heinz Junkes, Markus Heyde, Wolf-Dieter Schneider, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Silica films represent a new class of two dimensional (2D) network formers with interesting material properties. To understand the growth process of these van der Waals bound films, we need to understand their mesoscopic structure.

Exfoliation experiments and low energy electron microscopy (LEEM) studies emphasize a smooth and continuous growth of the silica films across single metal crystals [1,2].

In this study, we use scanning tunneling microscopy (STM) to resolve the ring structure of an amorphous silica bilayer film across

Ru(0001) step edges. The structural analysis verifies areas of the film with an intact and closed network structure over step edges. The ring sizes are determined with a program for semi-automated ring detection. In this program, we perform a segmentation of the STM image and build a region adjacency graph (RAG) based on the detected ring center coordinates.

We observed areas with carpet growth characteristics in the amorphous 2D-silica film. In future we hope to apply these tools for the detection of structural dynamics as a function of time and temperature.

[1] DOI: 10.1016/B978-0-12-409547-2.14171-X
[2] DOI: 10.1002/anie.201802000

HL 29.4 Tue 11:15 GER 38

Where the MoS_2 bilayer grows: An *in situ* LEEM study — •Moritz Ewert[1,2], Lars Buss[1,2], Francesca Genuzio[3], Tevfik Onur Menteş[3], Andrea Locatelli[3], Jens Falta[2], and Jan Ingo Flege[1,2] — [1]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany — [2]Institute of Solid State Physics, University of Bremen, Germany — [3]Elettra-Sincrotrone Trieste S.C.p.A., Basovizza, Trieste 34012, Italy

Molybdenum disulfide (MoS_2) is well-known for changing from an indirect to a direct semiconductor when its thickness is reduced to a single layer, rendering a high degree of growth control a necessity for optoelectronic applications. An extensively investigated model system is MoS_2 on Au(111), which using molecular beam epitaxy typically grows as clusters. Here, we present an in-situ low-energy electron microscopy (LEEM) study of the extended growth of MoS_2 at 700°C and 750°C. These conditions lead to the formation of micron-sized single-layer MoS_2 islands. The single-domain character of these islands is demonstrated by employing dark-field imaging and micro-diffraction (LEED), which allow quantifying the relative coverage of the two mirror domains. Furthermore, selected area angle-resolved photoelectron spectroscopy of these domains directly confirms their threefold symmetric electronic bandstructure. Interestingly, under certain conditions subsequent structural characterization by I(V)-LEEM clearly identifies regions where a bilayer of MoS_2 has nucleated. Parameters influencing the bilayer growth as well as its electronic properties will be discussed.

HL 29.5 Tue 11:30 GER 38

Growth of Hexagonal Boron Nitride and Borophene on Ir(111) via Thermal Catalytic Decomposition of Borazine (B3H6N3) — •Karim Omambac[1], Marko Kriegel[1], Christian Brand[1], Pascal Dreher[1], David Janoschka[1], Ulrich Hagemann[2], Nils Hartmann[2], Frank-Joachim Meyer zu Heringdor[1,2], and Michael Horn-von Hoegen[1] — [1]University of Duisburg-Essen, Germany — [2]Interdisciplinary Center for the Analytics on the Nanoscale (ICAN), Germany

Preparation of borophene has been performed by deposition from an e-beam heated high-purity boron rod via molecular beam epitaxy (MBE) [1]. However, the MBE technique is very expensive with low yield and most of all, epitaxially grown borophene islands are found small sized. Here we report on the first successful growth of large area borophene via the thermal catalytic decomposition of borazine (B3H6N3) on a Ir(111) substrate at high temperatures using conventional CVD technique. The observed growth mode is describe to be similar with boron dissolving into the bulk at high temperatures and segregating to the surface forming large borophene sheets as the sample is cooled [1]. The surface morphology and structure determination has been performed in-situ by real-time growth observation via low energy electron microscopy (LEEM) and high-resolution spot profile analyzing-LEED (SPA-LEED). The chemical composition has been determined ex-situ by X-ray photoemission spectroscopy (XPS) and time-of-flight secondary ion mass spectroscopy (ToF-SIMS) measurements. [1] ACS Nano 13, 3816-3822 (2019)

HL 29.6 Tue 11:45 GER 38

Electronic properties of coherently attached nanocrystals measured by scanning tunneling spectroscopy — •Pierre Capiod[1], Maaike van der Sluijs[1], Jeroen de Boer[1], Christophe Delerue[2], Ingmar Swart[1], and Daniel Vanmaekelbergh[1] — [1]Debye Institute for Nanomaterials Science, Utrecht University, PO Box 80 000, 3508 TA Utrecht, the Netherlands — [2]Université Lille, CNRS, Centrale Lille, ISEN, Université Valenciennes, UMR 8520 - IEMN, F-59000 Lille, France

2D systems have attracted considerable interest in recent years. The first 2D material was graphene which displays a rich band structure. While it is not possible to create a 2D honeycomb structure with any element we want, artificial lattices emerge as new field to explore. It was shown that it is possible to create superlattices based on semiconductor nanocrystals (PbSe, CdSe) as building blocks in a square and honeycomb geometry. It is of high interest to combine the large scale self-assembly of such superlattices with the possibility of optical and electrical switching. Theoretical works have been initiated based on tight-binding calculations. Those calculations have shown that the atomic crystalline structure of the nanocrystals combined with the square or honeycomb geometry determine the band structure of the system where Dirac-cones and non-trivial flat bands appear. Until now, the density of states of those structures has not been resolved. In this presentation, I will describe the synthesis and the preparation of the samples and present the measurements of the density of states on PbSe square superlattices by scanning tunneling spectroscopy

HL 29.7 Tue 12:00 GER 38

Deconfinement in van der Waals Stacks: Turning Mott Localized Electrons into Dirac Fermions — •Jose Pizarro[1,2], Severino Adler[3], Karim Zantout[4], Thomas Mertz[4], Paolo Barone[5], Roser Valentí[4], Giorgio Sangiovanni[3], and Tim Wehling[1,2] — [1]University of Bremen — [2]Bremen Center for Computational Material Sciences — [3]University of Würzburg — [4]Goethe University Frankfurt am Main — [5]CNR-SPIN, Italy

The interplay of topology and electronic correlations forms a rich ground for the realization of exotic states of quantum matter, with an increased importance in emergent flat bands systems in superlattices. Here, we show how strongly correlated spin-orbit coupled Dirac fermions emerge in bilayers of 1T-TaSe2 and related group V transition metal dichalcogenides. These materials realize the so-called Star-of-David (SoD) charge density wave (CDW) patterns in each layer, where the stacking of the CDW centers defines the symmetry of the resulting superlattice. When the CDW centers are arranged in a honeycomb pattern, the system realizes a generalized Kane-Mele model with a sizable on-site Hubbard interaction U. The isoelectronic series of 1T-TaSe2, TaS2, and NbSe2 traverses a region of the electronic phase diagram where weakly-to-strongly correlated Dirac semimetallic, Mott antiferromagnetic insulating and quantum spin Hall states compete. We show that stacking and relative rotations between the layers as well as perpendicular electric fields affect the emergent correlated Dirac fermions as effective gauge and mass fields, and control their creation, annihiliation and topology.

HL 29.8 Tue 12:15 GER 38

Proximity-induced superconducting gap in the quantum spin Hall edge state of monolayer WTe_2 — •Felix Lüpke[1], Dacen Waters[1], Sergio C. de la Barrera[1], Michael Widom[1], David G. Mandrus[2,3,4], Jiaqiang Yan[2], Randall M. Feenstra[1], and Benjamin M. Hunt[1] — [1]Department of Physics, Carnegie Mellon University, Pittsburgh, PA 15213, USA — [2]Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA — [3]Department of Materials Science and Engineering, University of Tennessee, Knoxville, TN 37996, USA — [4]Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996, USA

Van der Waals (vdW) heterostructures allow the combination of different material properties, e.g. non-trivial topology and superconductivity in order to create a topological superconducting state. We demonstrate a novel dry-transfer flip technique which we use to place atomically-thin layers of WTe_2, a quantum spin Hall (QSH) system, on $NbSe_2$, a vdW superconductor, while maintaining atomically clean surfaces and interfaces. Using scanning tunneling microscopy and spectroscopy (STM/STS), we demonstrate the presence of a proximity-induced superconducting gap in the WTe_2 for thicknesses from a monolayer up to 7 crystalline layers. At the edge of the WTe_2 monolayer, we show that the superconducting gap coexists with the characteristic spectroscopic signature of the QSH edge state [1].

[1] F. Lüpke *et al.*, arXiv:1903.00493 (2019)

HL 29.9 Tue 12:30 GER 38

MoSe2-WSe2 lateral heterostructures grown by chemical vapour deposition — •Emad Najafidehaghani[1], Antony George[1], Ziyang Gan[1], Tibor Lehnert[2], Christof Neumann[1], Xingcheng Li[1], Ute Kaiser[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, D-07743 Jena, Germany — [2]Ulm University, Central Facility of Materials Science Electron Microscopy, D-89081 Ulm, Germany

Recently two-dimensional (2D) transition metal dichalcogenides

(TMDs) such as MoS2, WS2, WSe2, MoSe2 etc. attracted great research interest due to their superior electronic and optical properties. They are identified as promising candidates for applications such as ultrathin, transparent and flexible electronics, optoelectronics and sensing. In order to realize advanced device architectures such as p-n junctions, complementary logic devices, ultrathin photovoltaics, etc. it is essential to develop efficient growth strategies for combining dissimilar monolayer TMDs to form lateral heterostructures. Here we show large area growth of monolayer MoSe2 -WSe2 lateral heterostructures by our modified chemical vapour deposition (CVD) technique which uses Knudsen type effusion cells for controlled delivery of precursors [1]. The grown monolayer MoSe2-WSe2 lateral heterostructures were characterized using complementary microscopic and spectroscopic techniques such as optical microscopy, Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), atomic force microscopy (AFM), Kelvin probe microscopy and high-resolution transmission electron microscopy (HRTEM) to reveal their structural and chemical quality.

HL 29.10 Tue 12:45 GER 38

Two-dimensional metal phases and non-stoichiometric phases of transition metal dichalcogenides — •Thomas Joseph, Mahdi Ghorbani-Asl, and Arkady Krasheninnikov — Helmholtz-Zentrum Dresden Rossendorf, Bautzner Landstraße 400, Dresden

Changing the stoichiometry of a material in a controllable manner is a powerful tool to tailor the structure and the properties of a compound solid. For example, new morphologies, such as inversion domains with the associated mirror twin boundaries [1] can be produced in 2D transition metal dichaclogenides by sputtering chalcogen atoms using electron beam [1]. Moreover, suspended monolayer Mo membranes were recently fabricated from monolayer $MoSe_2$ sheets via complete sputtering of Se atoms in a scanning transmission electron microscope [2]. Motivated by these results, we performed first-principles calculations to understand the energetics of 2D phases of binary compounds which can be referred to as strongly non-stoichiometric transition-metal dichalcogenides. We found that other intermediate metallic non-stoichiometric phases, which are energetically more favourable than pure 2D metals [3], can also exist.

[1] Komsa, H.-P. et al.; Native Defects in Bulk and Monolayer MoS 2 from First Principles. Phys. Rev. B 2015, 91 (12), 125304.
[2] X. Zhao et al.; Atom-by-Atom Fabrication of Monolayer Molybdenum Membranes. Advanced Materials 2018, 30 (23), 1707281.
[3] T. Joseph et al.; Nonstoichiometric Phases of Two-Dimensional Transition-Metal Dichalcogenides: From Chalcogen Vacancies to Pure Metal Membranes. J. Phys. Chem. Lett. 2019, 10 (21), 6492.

HL 29.11 Tue 13:00 GER 38

Visualization of multifractal superconductivity in a two-dimensional transition metal dichalcogenide in the weak-disorder regime — Carmen Rubio-Verdú[1], Antonio M. García-García[2], Hyejin Ryu[3], Deung-Jang Choi[1], Javier Zaldívar[1], Shujie Tang[3], Bo Fan[2], Zhi-Xun Shen[4], Sung-Kwan Mo[3], José Ignacio Pascual[1], and •Miguel M. Ugeda[5] — [1]CIC nanoGUNE, 20018 Donostia-San Sebastián, Spain. — [2]Shanghai Center for Complex Physics, Department of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai 200240, China. — [3]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA. — [4]Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA. — [5]Donostia International Physics Center (DIPC), 20018 San Sebastián, Spain.

Here we investigate the impact of multifractality on the superconducting state of a weakly disordered single-layer of NbSe2 by LT-STM/STS. The SC gap (width, depth and coherence peaks amplitude) shows characteristic spatial single-wavelength modulation coincident with the periodicity of the QPI pattern observed at EF. Spatial inhomogeneity of the SC gap width, which is proportional to the order parameter in the weak-disorder regime, shows a characteristic log-normal statistical distribution as well as a power-law decay of the two-point correlation function, in agreement with our theoretical model. This novel state is universal and governs the properties of even weakly disordered 2D superconductors with SOC.

HL 29.12 Tue 13:15 GER 38

Role of dark trions in the optical response of doped atomically thin semiconductors — •Ashish Arora[1], Nils Kolja Wessling[1], Thorsten Deilmann[1], Till Reichenauer[1], Paul Steeger[1], Piotr Kossacki[2], Marek Potemski[2,3], Steffen Michaelis de Vasconcellos[1], Michael Rohlfing[1], and Rudolf Bratschitsch[1] — [1]University of Münster, Germany — [2]University of Warsaw, Poland — [3]Laboratoire National des Champs Magnétiques Intenses, Grenoble, France

We perform absorption and photoluminescence spectroscopy of intravalley and intervalley trions in transition metal dichalcogenide (TMDC) monolayers encapsulated in hBN, depending on temperature [1]. We find that an interplay between the thermal distribution of bright and dark trions, and their oscillator strengths gives rise to the unique optical response of each monolayer material. The observed trends in our experiments are excellently reproduced using a model based on the Fermi-Dirac distribution of bright and dark trions. Our analysis yields that there is a dark trion 19 meV *below* the lowest energy bright trion in WSe_2 and WS_2. However, in $MoSe_2$, the dark trion lies 6 meV *above* the bright trion, while it almost coincides in energy with the bright trion in MoS_2. These results are in excellent agreement with our *GW*-BSE *ab-initio* calculations of trions for these materials. Our observations provide a quantitative understanding of the temperature-dependent optical response of TMDCs. [1] Preprint at https://arxiv.org/abs/1911.06252

HL 29.13 Tue 13:30 GER 38

Excited-State Trions in Monolayer WS_2 — •Thorsten Deilmann[1], Ashish Arora[2], Till Reichenauer[2], Johannes Kern[2], Steffen Michaelis de Vasconcellos[2], Michael Rohlfing[1], and Rudolf Bratschitsch[2] — [1]Institute of Solid State Theory, University of Münster, Germany — [2]Institute of Physics and Center for Nanotechnology, University of Münster, Germany

We discover an excited bound three-particle state, the 2s trion, appearing energetically below the 2s exciton in monolayer WS_2, using absorption spectroscopy and ab initio *GW* and Bethe-Salpeter equation calculations [1]. The measured binding energy of the 2s trion (22 meV) is smaller compared to the 1s intravalley and intervalley trions (37 and 31 meV). Our discovery underlines the importance of trions for the entire excitation spectrum of two-dimensional semiconductors. [1] *Phys. Rev. Lett.* **123**, 167401 (2019)

HL 30: Poster I

This poster session includes contributions from the following topics:

- Nitrides: Devices - Nitrides: Preparation and characterization - Focus Session: Functional Metal Oxides for Novel Applications and Devices - Oxide semiconductors - THz and MIR physics in semiconductors - Heterostructures, interfaces and surfaces - Quantum transport and quantum Hall effects - Transport properties

Please put up your poster at the beginning of the session and remove the poster immediately after the session. The person peresenting the poster should attend it for at least half of the session duration and indicate the time when to find him/her at the poster.

Time: Tuesday 13:30–15:45 Location: P3

HL 30.1 Tue 13:30 P3

Towards Sustainable, Flexible Electronics from Abundant Elements: Integrated Circuits Comprising TFTs Based on Amorphous Room-Temperature-Fabricated Zinc-Tin-Oxide

— •Oliver Lahr, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Linnéstraße 5, 04103 Leipzig, Germany

During the last decade, amorphous oxide semiconductors have advanced into a thriving research area for transparent and flexible electronics and since then, the field has grown rapidly towards, for instance, next-generation flat-panel displays. The widely commercially deployed and by far most mature representative indium-gallium-zinc-oxide, however, consists of rare elements such as indium and gallium that innovative research is attempting to substitute by materials containing abundant cations only.
Amorphous zinc-tin-oxide (ZTO) turns out to be a suitable candidate for sustainable, flexible and transparent electronics since it consists of abundant, non-toxic elements and exhibits promising performance even in case of room temperature fabricated circuits comprising MESFETs and JFETs [1,2]. Since previously reported TFTs relied on high-temperature processed ZTO channels, we report the first ZTO-based TFTs that neither require deposition at elevated temperature nor additional annealing in order to maintain compatibility with flexible substrates, while still representing current state-of-the-art devices.
[1] Lahr, IEEE Trans. Electron Devices, **66**, 8, 2019.
[2] Lahr, Adv. Electron. Mater., 1900548, 2019.

HL 30.2 Tue 13:30 P3

Effect of plasma treatment on electronic devices based on In_2O_3 — •Fabian Schöppach, Daniel Splith, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix Bloch Institute for Solid State Physics, Linnéstraße 5, 04103 Leipzig, Germany

Indium oxide (In_2O_3) has promising physical properties such as high conductivity and transparency in the visible. However, In_2O_3 is not used in active devices such as diodes or transistors yet. This is due to its tendency to form an electron accumulation layer on its surface which is reported to be caused by surface near oxygen vacancies [1]. Compensating Mg doping and plasma treatment are reported to reduce this effect and enable the resulting device operation [2,3].

In this work, the performance of first prototype metal-semiconductor field-effect transistors (MESFETs) based on In_2O_3 thin films was improved by an initial plasma treatment of the channel material. The thin films were grown via pulsed laser deposition and were treated afterwards with a pure oxygen plasma. For source and drain contacts gold was deposited via inert ambient sputtering. Schottky gate diodes were fabricated in a reactive sputter process, which is a requirement for obtaining rectifying contacts to In_2O_3 [5,6].

[1] King, et al. Physical Review B 80.8, 081201 (2009)
[2] Schmidt, et al. physica status solidi (b) 252.10, 2304-2308 (2015)
[3] Michel, et al. ACS Appl. Mater. Interf. 11, 27073-27087 (2019)
[4] von Wenckstern, et al. APL Materials 2.4, 046104 (2014)
[5] Schultz, et al. Phys. Rev. Appl. 9, 064001 (2018)

HL 30.3 Tue 13:30 P3

Investigation of charge carrier transport mechanism in amorphous ZnON and ZnSnO thin films by temperature dependent Hall effect measurements — Antonia Welk, Holger von Wenckstern, and •Marius Grundmann — Felix-Bloch-Institut für Festkörperphysik, Universität Leipzig, Linnéstraße 5, 04103 Leipzig, Germany

Amorphous semiconductors as zinc oxynitride (a-ZnON) or zinc tin oxide (a-ZTO) with Hall mobilities up to $100\,cm^2V^{-1}s^{-1}$ [1,2] or $13\,cm^2V^{-1}s^{-1}$ [3] are promising low-temperature deposition channel materials for thin film transistors (TFTs). For the enhancement of device performance it is necessary to gain a profound understanding of the charge carrier transport mechanism.
In this work we performed temperature dependent Hall effect measurements on magnetron sputtered ZnON and PLD grown ZnSnO thin films. We compared our experimental results to the theoretical description of percolation transport in the random band edge model [4,5]. That way we were able to validate the theoretical description for two further amorphous oxides aside of InGaZnO [5] and determined the band edge disorder parameter δ and the conduction mobility μ_0.

[1] A. Reinhardt *et al.*, Phys. Status Solidi A 213 (7), 1767 (2016)
[2] H. Kim *et al.*: *Sci. Rep.* **3**, 1459 (2013)
[3] P. Schlupp *et al.*, MRS Proceedings 1633, 101-104 (2014)
[4] I.I. Fishchuk *et al.*, Phys. Rev. B 93 (19), 195204 (2016)
[5] A.V. Nenashev *et al.*, Phys. Rev. B 100 (12), 125202 (2019)

HL 30.4 Tue 13:30 P3

Growth of transparent, p-conductive γ-CuI by PLD — •Philipp Storm, Michael Bar, Chang Yang, Daniel Splith, Holger von Wenckstern, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Felix-Bloch Institut für Festkörperphysik

Transparent semi-conductive materials (TSM) are typically unipolar such that heterostructures are required for pn-diodes. So far, n-type TSMs like ZnO or Ga_2O_3 typically have high electron mobility while p-TSMs suffer very low hole mobilities. CuI is currently one of the most promising p-type TSM due its wide band gap, high hole mobility and density as well as high exciton binding energy [1]. However, the physical vapor deposition (for example sputtering or thermal evaporation) of CuI turned out to be difficult to obtain smooth thin films [2,3] and therefore impeding progress towards uniform multilayered device structures. In this work, the growth of CuI by pulsed laser deposition (PLD) is presented. The morphological, structural and optical properties of the obtained thin films suggest a high potential of PLD-grown CuI for thin-film device applications.
[1] M. Grundmann *et al.* : Phys. Status Solidi A 210, 9, 1671 (2013)
[2] C. Yang *et al.* : Sci. Rep. 6, 21937 (2016)
[3] C. Moditswe *et al.* : Ceramics International 43, 6, 5121 (2017)

HL 30.5 Tue 13:30 P3

Electrical properties of all amorphous ZnMgON/$ZnCo_2O_4$ bipolar heterojunction diodes — •Arne Jörns, Antonia Welk, Anna Reinhardt, Holger von Wenckstern, and Marius Grundmann — Felix-Bloch-Institut für Festkörperphysik, Universität Leipzig, Linnéstraße 5, 04103 Leipzig, Germany

Amorphous zinc magnesium oxynitride (a-ZnMgON) is a promising low-temperature deposition material for flexible electronics. The incorporation of magnesium into amorphous ZnON, typically having free electron concentrations above $10^{18}\,cm^{-3}$ [1], leads to a reduction of the free carrier concentration and an absorption edge shift towards higher energies. By means of co-sputtering we were able to fabricate a-ZnMgON thin films with magnesium concentrations up to 5 at. %, free carrier concentrations in the range of 10^{16}-$10^{17}\,cm^{-3}$ and an absorption edge of 1.3 eV or higher.

In this study, we investigated all amorphous n-ZnMgON/p-$ZnCo_2O_4$ bipolar heterojunction diodes deposited on glass with rectification ratios in the range of 10^3-10^4. Modeling of the IV-characteristics yields a series resistance of 130-140 Ω, a parallel resistance in the range of 10^{10}-10^{11} Ω and an ideality factor of 2.8. In order to suppress leakage currents in the reverse bias regime, a thin insulating, highly resistive ZnMgON layer was introduced between ZnMgON and $ZnCo_2O_4$. Furthermore, the diodes were investigated by means of temperature dependent IV-measurements and capacitance voltage measurements.

[1] A. Reinhardt *et al.*, Phys. Status Solidi A 213 (7), 1767 (2016)

HL 30.6 Tue 13:30 P3

HyGlas - a novel approach for smart windows as energetically efficient hybrid double-skin facades using electrochromic WO_3 thin films. — •Florian Kuhl, Angelika Polity, and Peter J. Klar — Institute of Experimental Physics I and Center for Materials Research (ZfM/LaMa), Justus Liebig University Giessen, Heinrich-Buff-Ring 16, DE-35392 Giessen, Germany

Since about 40 % of the global energy demand and one third of CO_2 equivalent is consumed by buildings and for example their climate control, smart windows that are commercially available can be used to reduce this energy demand in the following years. However, as of 2050 the existing political concepts of the BRD and EU claim a completely climate-neutral building stock. In general there is a focus on minimizing the cooling load in summer and the heating demand in winter which can be put into practice by using the solar energy stored between the glazings of a facade. We introduce the idea of integrating differently switchable electrochromic smart windows combined with venting systems for the whole facade system in the Framework of the HyGlas project. A commercially available electrochromic smart window, whose transmittance can be switched in the visible range of the solar spectrum, will be extended by a second electrochromic multilayer system that can be modulated in the infrared region. For this purpose we investigate rf-sputtered WO_3 thin films in terms of their structural, stoichiometrical and compositional properties as well as in their electrochemical and optical behaviour, i.e. the modulation of the transmittance in the intended range of the solar spectrum.

HL 30.7 Tue 13:30 P3

Vertical field-effect transistors based on amorphous zinc-tin

oxide - simulation and fabrication — •Michael Bar, Daniel Splith, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Germany

Zinc-tin oxide (ZTO) is a wide gap semiconductor consisting of abundant, non-toxic elements. It unites transparency in the visible spectral range with high electron mobility in the amorphous state. Its deposition at room temperature has been proven successful for numerous device applications [1-3]. However, a greatly reduced channel length is needed for the fabrication of TFTs with high-frequency switching capabilities.
In this work a vertical device structure approach was used to fabricate vertical field-effect transistors (VFETs) with channel lengths of several hundred nanometers and without the use of submicrometer lithography equipment. Additionally, a finite element method has been used to simulate said devices. The static and dynamic properties obtained by transfer characteristics and drain-current modulation measurements were evaluated and compared to conventional lateral field-effect transistors. In this comparison the simulation of VFETs showed an increase in cut-off frequency of up to three orders of magnitude.

[1] S. Vogt *et al.*, Appl. Phys. Lett., **113**(13), 133501, (2018).
[2] O. Lahr *et al.*, IEEE Trans. Electron Devices, **66**(8), 3376, (2019).
[3] O. Lahr *et al.*, Adv. Electron. Mater., 1900548, (2019).

HL 30.8 Tue 13:30 P3

Electrical characterization of p-conductive transparent copper iodide thin films deposited by PLD — •Michael Bar, Philipp Storm, Holger von Wenckstern, Chang Yang, Michael Lorenz, and Marius Grundmann — Universtät Leipzig, Germany

Copper iodide (CuI) is a p-type, wide-bandgap semiconductor which unites transparency in the visible spectral range with exceptional hole conductivity. This makes CuI a viable candidate for various transparent electronic devices such as diodes and field-effect transistors. In recent years, sputtered CuI heterojunctions have been presented [1]. However, practical challenges regarding the growth of epitaxial films remain before CuI can be employed into TFTs.
In this contribution we present electrical properties of CuI thin films which were prepared by pulsed laser deposition. The electrical characterization of these films was performed using current-voltage and Hall measurements. Remarkable properties of these films are for example hole carrier densities in the order of $10^{17}\,\mathrm{cm}^{-3}$ and a hole mobility of $10\,\mathrm{cm}^2/\mathrm{Vs}$.

[1] C. Yang *et al.*, Sci. Rep., **6**(1), 21937, (2016).

HL 30.9 Tue 13:30 P3

Towards Thermal Conductivity measurements in β-Ga_2O_3 Thin Films — •Robin Ahrling[1], Martin Handwerg[1], Olivio Chiatti[1], Rüdiger Mitdank[1], Zbigniew Galazka[2], Günter Wagner[2], Andreas Popp[2], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Leibniz Institute for Crystal Growth, 12489 Berlin Germany

As a wide-band gap semiconductor with a high breakthrough field, gallium oxide (Ga_2O_3) has shown to be a promising material for applications in high power electronics. However, due to the materials low thermal conductivity [1,2] heat dissipation may pose a threat for future device applications. Therefore, the thermal transport in Ga_2O_3 films needs to be explored. Electrical measurements have shown, that in very thin films the scattering processes change drastically with decreasing film thickness. [3] In this work, we investigate the thermal conductivity in these thin films, using the 3-ω method.
A variation of the 3-ω method with sub μm heater widths, causing the heaters to be thinner than the thickness of the examined films, is used. The heaters are produced by electron beam lithography.
We investigate the thermal conductivity in dependence of temperature and the thickness of the Ga_2O_3 films with a special interest in changes in the the phonon transport machanisms in very thin films.

[1] M. Handwerg *et al.*, Semicond. Sci. Technol. **30** (2015) 024006
[2] M. Handwerg *et al.*, Semicond. Sci. Technol. **31** (2016) 125006
[3] R. Ahrling *et al.*, Sci. Rep. **9**, 13149 (2019).

HL 30.10 Tue 13:30 P3

Stabilization of single phase α-$(Al_xGa_{1-x})_2O_3$ by pulsed laser deposition — •Max Kneiss, Anna Hassa, Daniel Splith, Chris Sturm, Holger von Wenckstern, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik

The α-phase of Ga_2O_3 exhibits a bandgap of 5.3 eV, which is slightly larger than that of the thermodynamically stable β-phase, and crystallizes in the same rhombohedral crystal structure as α-Al_2O_3 (sapphire). The availability of cost-effective low-mismatch sapphire single crystal substrates and the possibility of heteroepitaxy without rotation domains as well as n-type doping [1] renders this phase highly promising for device applications. Bandgap engineering as well as heterostructure devices are possible by alloying with Al. However, reports on α-$(Al_xGa_{1-x})_2O_3$ are rather scarce. We present the expitaxial stabilization of α-$(Al_xGa_{1-x})_2O_3$ on sapphire substrates by PLD. Utilizing radially-segmented $(Al_xGa_{1-x})_2O_3/Ga_2O_3$ targets (VCCS-PLD [2]) we were able to grow thin films in the α-phase on a- and m-plane sapphire covering the complete composition range between α-Ga_2O_3 and α-Al_2O_3. In-plane as well as out-of-plane lattice constants were determined by reciprocal space map measurements and a linear dependence on x was found. Above a critical Al-content, pseudomorphic growth was confirmed on the a-sapphire substrates. Further, the composition-dependent bandgaps as well as surface morphologies will be presented. [1] Ahmadi *et al.*, J. Appl. Phys. **126**, 160901 (2019) [2] Kneiß *et al.*, ACS Comb. Sc. **20**, 643 (2018)

HL 30.11 Tue 13:30 P3

Rectifying contacts to κ-Ga_2O_3 — •Max Kneiss, Anna Hassa, Peter Schlupp, Daniel Splith, Holger von Wenckstern, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik

The orthorhombic κ-phase of Ga_2O_3 possesses a similarly high bandgap of 5 eV as the thermodynamically stable β-phase. Further, it is expected to exhibit a high spontaneous electrical polarization of $23\,\mu\mathrm{C/cm}^2$ [1] that can be utilized for polarization doping in heterostructures to localize a 2DEG by polarization differences at interfaces which then can serve as active layer in device applications. To employ κ-Ga_2O_3 in devices such as UV- or quantum-well infrared photodetectors, the realization of rectifying contacts is a prerequisite. However, reports on such contacts to κ-Ga_2O_3 are rare. In this talk, we present sputtered PtO_x/Pt and PdO_x/Pd Schottky contacts to κ-Ga_2O_3 as well as PLD grown NiO/κ-Ga_2O_3 and $ZnCo_2O_4$/κ-Ga_2O_3 pn-heterojunctions. The κ-Ga_2O_3 thin films were grown epitaxially by PLD from tin-containing targets [2] on ZnO/ZnO:Al growth templates on a-sapphire. The Al-doped ZnO layer is needed as highly conductive current-spreading backcontact since lateral transport is suppressed in our κ-Ga_3O_3 thin films due to the presence of rotation domains. A Ti/Al/Au layer stack was employed as ohmic contact. By IV-measurements, we found rectifying behavior for all investigated types of contacts with rectification ratios of up to 8 orders of magnitude. [1] Maccioni *et al.*, Appl. Phys. Expr. **9**, 041102 (2016) [2] Kneiß *et al.*, APL Materials **7**, 022516 (2019)

HL 30.12 Tue 13:30 P3

Material Investigations of Corundum-Structured Group-III-Sesquioxides by PLD on (00.1) Al_2O_3 — •C. Petersen, A. Hassa, M. Kneiss, H. Wenckstern, D. Splith, C. Sturm, and M. Grundmann — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Linnéstraße 5, 04103 Leipzig, Germany

Due to its outstanding material properties, recently much attention was drawn to the wide bandgap semiconductor gallium oxide for possible applications e.g. in high-power devices. Apart from the well-studied β-phase of Ga_2O_3, the corundum α-polymorph is in particular well suited for heterostructures, because it is isostructural to α-In_2O_3 and α-Al_2O_3. This, in principle, enables alloying the material system across the entire phase diagram and bandgap engineering over a considerable energy range ($E_{\mathrm{g,Ga_2O_3}} = 5.3\,\mathrm{eV}$, $E_{\mathrm{g,In_2O_3}} = 3.7\,\mathrm{eV}$ and $E_{\mathrm{g,Al_2O_3}} = 8.75\,\mathrm{eV}$ [1].
In this contribution we present material properties of binary α-Ga_2O_3 thin films as well as it's ternary alloys with In or Al. The thin films were grown by pulsed laser deposition with continuous composition spread [2] on (00.1) Al_2O_3. Resulting samples were investigated by means of X-ray diffraction, transmission, energy-dispersive X-ray spectroscopy, atomic force microscopy, and electrical transport measurements.

[1] S. Fujita *et al.*, Jpn. J. Appl. Phys., 1202A3 (2016).
[2] H. v. Wenckstern *et al.*, CrystEngComm 15, 10020 (2013).

HL 30.13 Tue 13:30 P3

The influence on defect states in Aluminium oxide on conductivity of a hydrogen-terminated diamond surface — •Dennis

Oing, Jens Kerski, Nicolas Wöhrl, Martin Geller, and Axel Lorke — Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

Hydrogen-terminated diamond shows a surface conductivity induced by transfer doping by acceptor states in adsorbate layers. Hence, the thermal and longtime stability of such devices is usually low. When covered with metal oxides, e.g. Al_2O_3 or MoO_3 a functionalized diamond surface show a higher thermal stability of reduced to $500°C$ due to not desorption of mentioned acceptor states.
In this study, defects in Al_2O_3-layers are used as acceptors on hydrogen-terminated diamond. These states are characterized using time-resolved charging and discharging of the defects by optical illumination using an UV-LED.
Temperature dependent Hall measurements show that the carrier density of the 2DHG induced by adsorbates from air is $1.3 \times 10^{-13}\,\mathrm{cm}^{-2}$, while it is $6.7 \times 10^{-12}\,\mathrm{cm}^{-2}$ with Al_2O_3 coverage. Carrier density is temperature independent in both cases. After illumination with an UV-LED, the conductivity of the 2DHG increases by 11 % at room temperature and 2.6 % at 200 K. The excitation shows 3 distinct time constants between 41 s and 40 min at room temperature. It is suggested that the transfer of electrons to the defect states is a three step process.

HL 30.14 Tue 13:30 P3

Modification of GaAs based Heterostructures by Laser Annealing — •Hans-Georg Babin, Julian Ritzmann, Marcel Schmidt, Arne Ludwig, and Andreas D. Wieck — Ruhr-Universität Bochum, D-44780 Bochum, Germany

Ex-situ thermal processing is a crucial step in semiconductor preparation. The applications range from the healing of crystal Damage[1], over the production of functional structures[2] up to the subsequent manipulation of material properties[3].

In addition to the obvious possibility of heating the sample in a furnace, high-intensity laser radiation can also be used for local heating of the semiconductor. This is called laser annealing.

This contribution deals with the realization of a Laser-Annealing-Setup for ex-situ modification of semiconductors. The construction and characterization will be discussed. In addition, the possibilities of laser annealing for the processing of GaAs heterostructures are estimated. The investigations include annealing of crystal damage, processing of insulating lines and alloying of ohmic contacts at GaAs/AlGaAs HEMTs. Finally, the change of the emission of quantum dots after Laser-Annealing is investigated.

1 S. D. Ferris et al.: AIP Conference Proceedings 50, 647, 1979
2 D. Bouwmeester et al.: Applied Physics Letters 95, 251104, 2009
3 L. Wang et al.: Applied Physics Letters 90, 073120, 2007

HL 30.15 Tue 13:30 P3

Molecular Beam Epitaxy growth and epitaxial lift off of (111)B-AlAs/GaAs heterostructures — •Tobias Henksmeier, Martin Eppinger, and Dirk Reuter — Department of Physics, Paderborn University, Warburgerstr. 100, 33098 Paderborn, Germany

In the recent years second harmonic generation (SHG) in nanoparticles has gained much interest as a platform for nonlinear optics. Thin (111)-GaAs films transferred to transparent substrates exhibit efficient forward directionality emission while for (100)-GaAs there is a strong pump pulse polarization dependence hindering efficient SHG emission perpendicular to the surface. We present the molecular beam epitaxy growth of $Al_xGa_{1-x}As$ heterostructures ($0<x<1$) on (111)B-GaAs substrates with a 1° miscut towards (211) and the fabrication of thin (111)B-GaAs films on arbitrary substrates via epitaxial lift off. We obtained similar growth rates on the (111)B surface as on the standard (100) surface. First, (111)B-$Al_xGa_{1-x}As$ ($x>0.7$) sacrificial layers were grown; then these layers were overgrown by a thin (111)B-GaAs layer. Surface roughness was investigated by atomic force microscopy (AFM). With optimized growth parameters a roughness <1 nm was obtained. 4×4 mm samples cleaved from the wafer were submerged in hydrofluoric acid to perform the epitaxial lift off of the GaAs layer. The etch rate of approximately 100μm/h is similar to those of (100)-$Al_xGa_{1-x}As$ ($0<x<1$) and will be discussed in detail. The released GaAs layer is bonded to a glass substrate. The film roughness <1 nm of the bonded GaAs was measured by AFM and the optical quality was checked by photoluminescence measurements.

HL 30.16 Tue 13:30 P3

Charge transport in graphene, encapsulated by hexagonal boron nitride, as a field effect transistor device — •Leo Schnitzspan[1], Alexander Tries[1,2,3], Marie-Luise Braatz[1,2], and Mathias Kläui[1,2] — [1]Institut für Physik, Johannes Gutenberg Universität Mainz — [2]Graduate School of Excellence Materials Science in Mainz — [3]Max Planck Institute for Polymer Research

Two dimensional van der Waals-materials with conducting, insulating or ferromagnetic properties attract attention due to their extraordinary charge- and spin-transport characteristics and their simple realization by stamping 2D layers one above the other. This can be accomplished by means of a dry transfer method [1]. This method was further developed in order to transfer hexagonal boron nitride (hBN) and graphene, to achieve a hBN/graphene/hBN heterostructure device. With electron beam-lithography (EBL), electrodes were patterned such that the temperature dependent charge transport and magnetoresistance could be measured. The data analysis showed a high charge carrier mobility and a non-negligible impact of the interface between electrode leads and graphene. In addition, Shubnikov-de Haas oscillations were observed at temperatures of 2 K, which allow the extraction of the carrier concentration in graphene.

[1] Zomer, P. J., et al., *Appl. Phys. Lett.* **105**, 013101 (2014).

HL 30.17 Tue 13:30 P3

Ab Initio investigations on the accuracy of the band offset in GaAs/AlGaAs heterojunction — •Felix Scholler[1], Jonas F. Schäfer-Richarz[1,2], Philipp Risius[1,2], and Christian Heiliger[1,2] — [1]Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen — [2]Zentrum für Materialforschung (LaMa), Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen

The prediction of materials properties for optimized material development requires an exact calculation of the band structure. A characteristic feature of the band structure of heterojunctions is the band offset. We want to assess the accuracy with which the Korringa Kohn Rostoker (KKR) method, which is a Green's functions based Density Functional Theory method, can predict the band offset of GaAs/AlGaAs heterojunctions. This system has been extensively studied experimentally, but theoretical treatment is challenging since a correct description of the alloy AlGaAs must be provided. Here, we treat AlGaAs with the Coherent Potential Approximation (CPA). Our results showcase the power of the KKR and the CPA for a simple materials system. Comparing the calculated values with experimental results allows us to assess the accuracy with which band offsets can be calculated not only for AlGaAs/GaAs heterojunctions, but also for other semiconductor junctions.

HL 30.18 Tue 13:30 P3

Do equidistant energy levels necessitate a harmonic potential? — •Fabian Teichert, Eduard Kuhn, and Angela Thränhardt — Institute of Physics, Technische Universität Chemnitz, 09107 Chemnitz, Germany

Experimental results from literature show energetically equidistant quantum well states in thin Bi films on surfaces, suggesting a harmonic oscillator description [1,2]. Yet is this conclusion imperative, especially considering that any measurement only yields energy levels in a finite range and with a nonzero uncertainty? Within this study we investigate whether equidistant energy levels actually necessitate a harmonic potential or whether alternative potential shapes with equidistant levels exist. First, we describe experimental results from literature by a harmonic oscillator model, obtaining a realistic size and depth of the resulting quantum well. Second, we use the shift-operator approach to calculate anharmonic non-polynomial potentials producing (partly) equidistant spectra. We discuss different potential types and interpret the possible modeling applications [3]. Finally, by applying nth order perturbation theory we show that exactly equidistant eigenenergies cannot be achieved by polynomial potentials, except by the harmonic oscillator potential.

[1] P. Kröger et al.: Physical Review B 97 (2018), 045403
[2] T. Hirahara et al.: Physical Review B 75 (2007), 035422
[3] F. Teichert et al.: arXiv:1910.12522 [quant-ph]

HL 30.19 Tue 13:30 P3

Focused ion beam implantation of rare-earth ions in semiconductor nanostructures — •Christian Düputell[1], Arne Ludwig[1], Jörg Debus[2], Manfred Bayer[2], and Andreas D. Wieck[1] — [1]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum — [2]Experimentelle Physik 2, Technische Universität Dortmund

We report on focused ion beam (FIB) implantation of rare-earth ions in semiconductor nanostructures. Semiconductor nanostructures have attracted a lot of attention due to their unique optical, electrical and mechanical properties. There is a huge potential for applications in many fields. To use nanostructures for a certain purpose, often very specific properties have to be achieved. An elegant method to tune the electrical and optical properties of semiconductor nanostructures is focused ion beam implantation. Using ion beams offers high-resolution lateral engineering, local band gap modulation due to ion-induced intermixing as well as local doping applications. To carry out implantation of rare-earth ions in semiconductor nanostructures we especially focus on the incorporation of Erbium ions into GaAs. Erbium and rare-earth ions, in general, are known for their huge magnetic moments, which exceed the Bohr magneton of at least a factor of 7. The dominant part of this magnetism originates from the $4f$ magnetic moments. Not only the f- but also d-states can participate in spin interactions so that we are going to obtain a rich spectrum of possible spin coupling processes in our studies. Therefore, we also examine the influence of annealing processes and the dependence on the ion fluence.

HL 30.20 Tue 13:30 P3

Correlation of optical properties and interface morphology in type-II semiconductor heterostructures — •Luise Rost, Milan Maradiya, Jannick Lehr, Wolfgang Stolz, and Wolfram Heimbrodt — Department of Physics and Materials Sciences Center, Philipps-Universität Marburg, Germany

The (Ga,In)As/GaAs/Ga(As,Sb) material system is used for lasers operating over a wide spectral range in the infrared. To further optimize the design of such heterostructures, it is important to have deep understanding of the influence of the interface morphology and the charge carrier dynamic through the interface. Here (Ga,In)As/GaAs/Ga(As,Sb) type-II double quantum well heterostructures and the inverted structure have been grown by metall-organic vapor phase epitaxy. A growth interruption procedure was used to intentionally modify the morphology of the internal interfaces. Here we show a furrow investigation of the influence of interface morphology and optical properties, for this 0s, 10s and 120s growth interruptions were introduced on different places of the heterostructure. With photoluminescence spectroscopy and atomic force microscopy we will illustrate this correlation and its importance for laser performance.

HL 30.21 Tue 13:30 P3

Atomic structure of $GaAs_xP_{1-x}$ surfaces during MOCVD-preparation — •Agnieszka Paszuk, Oliver Supplie, Jan Philipp Stöckmann, Harita Gordhanbhai Rupapara, Peter Kleinschmidt, and Thomas Hannappel — Institute of Physics, University of Technology Ilmenau, Germany

Low defect $GaAs_xP_{1-x}$ graded buffers grown on Si enable highly efficient III-V-on-Si multi-junction solar cells. The As/P content of individual GaAsP graded buffer layers can be quantified *in situ* during metalorganic chemical vapor phase deposition with reflection anisotropy spectroscopy (RAS) due to a characteristic spectral fingerprint of the GaAsP surfaces [1]: With increasing As supply, a peak close to the GaP E_1 critical point energy shifts towards GaAs E_1 at lower energy. Here, these RAS fingerprints are correlated with the surface reconstructions and chemical composition identified in UHV by LEED and XPS, respectively. We show that the surface structure of GaAsP buffers depends on the GaAsP stoichiometry and post-growth process route. GaAsP surfaces with low As content exhibit P-rich, (2x1) reconstructed surfaces. LEED patterns of GaAsP buffers with 50% of As in the bulk exhibit a mix of (2x1) reconstruction with additional spots present at third order. We find both P-P and As-As dimers present at this surface. The same buffers annealed additionally at 500°C exhibit As-rich (2x4) reconstructed surfaces, whereas annealing at 700°C leads to Ga-rich surfaces. Future studies are aimed to resolve the actual atomic structure of the complex surface unit cell. [1] O. Supplie et al., Proceedings 45th IEEE PVSC Conf. (2018) 3923.

HL 30.22 Tue 13:30 P3

Back-gated FET operation in 4H SiC for controlling transport in epitaxial graphene nanojunctions — •Maria T. Schlecht, Christian Ott, Stefan Malzer, and Heiko B. Weber — Lehrstuhl für Angewandte Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen, Germany

For many experiments with epitaxial graphene on Silicon carbide (SiC) it is essential to leave graphene accessible, therefore charge carrier control must be achieved by a backgate buried in the substrate. This can be realized by placing an implanted conductive layer in the substrate without losing its semi-insulating behaviour. This has been successfully established on 6H SiC due to the vanadium compensation of the semi-insulating material [1]. Implanting a working back-gate within the technologically more relevant polytype 4H SiC is more challenging as it is "intrinsically" semi-insulating. Here, we present a study on implanted bottom gates for quasi-freestanding bilayer graphene (QF-BLG) on 4H SiC using nitrogen as a dopant. Investigating various implantation profiles we found an optimum at an implantation concentration of $5{\cdot}10^{17}$ cm^{-3} and a depth of 1 μm. A reduction of the charge carrier concentration by $5{\cdot}10^{12}$ cm^{-2} at a gate voltage of 90 V was achieved. The back gate was proven to be working in the temperature range of interest from 30 K to 300 K and was only limited by leakage current. A local maximum of the leakage current at 120 K will be discussed taking into account defect levels within the SiC.[1] Waldmann et al, DOI: 10.1038/nmat2988 (2011)

HL 30.23 Tue 13:30 P3

Electronic properties of the GaP/Si(001) heterointerface studied by HAXPES — Oleksandr Romanyuk[1], •Jan P. Stöckmann[2], Agnieszka Paszuk[2], Oliver Supplie[2], Regan G. Wilks[3], Jakob Bombsch[3], Claudia Hartmann[3], Raül Garcia-Diez[3], Shigenori Ueda[4], Igor Bartoš[1], Ivan Gordeev[1], Jana Houdkova[1], Peter Kleinschmidt[2], Marcus Bär[3], Petr Jiříček[1], and Thomas Hannappel[2] — [1]Institute for Physics, Fundamentals of energy materials, University of Technology, Ilmenau, Germany — [2]Institute of Physics, Prague, Czech Republic — [3]Department Interface Design, Helmholtz-Zentrum Berlin, Germany — [4]SPring-8, National Institute for Materials Science (NIMS), Japan

For highly efficient III-V-on-Si optoelectronic devices it is crucial to prepare defect-free III-V/Si heterointerfaces with defined electronic properties. Defects known as antiphase boundaries in the III-V layer can be avoided by preparing the Si(100) surface with double-atomic steps. Here, GaP/Si(001) heterointerfaces prepared by MOCVD were investigated by hard X-ray photoelectron spectroscopy. Thin (4 - 50 nm) GaP films were grown on H- or As-terminated Si(001) surfaces. Preparation of double-atomic steps on Si surface was controlled by optical in situ spectroscopy. We observed core-level broadening and shifts of peak maxima positions depending on GaP thickness, Si wafer doping type and Si surface preparation. We were able to identify interface-related core level components and to deduce the valence band offsets at the heterostructures. These results are related to charge displacements at the interface.

HL 30.24 Tue 13:30 P3

Investigation of Poole-Frenkel-ionization in magnesium-doped AlGaN short period superlattices — •Emil Mickein[1], Anton Muhin[1], Norman Susilo[1], Luca Sulmoni[1], Martin Guttmann[1], Christian Kuhn[1], Tim Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics, Berlin, Germany — [2]Ferdinand-Braun-Institut, Leibnitz-Institut für Höchstfrequenztechnik, Berlin, Germany

UVC-transparent $Al_xGa_{1-x}N$:Mg/$Al_yGa_{1-y}N$:Mg short period superlattices (SPSL) with $x, y \geq 0.6$ are required for efficient light emitting diodes with emission wavelength below 280 nm. However, AlGaN:Mg layers with high aluminum mole fractions exhibit high acceptor ionization energies and consequently a poor electrical conductivity. Moreover, the electric properties of AlGaN:Mg-SPSL are not well established, especially for high Al mole fraction. In this paper the vertical conductivity (σ_V) of $Al_{0.71}Ga_{0.29}N$:Mg/$Al_{0.65}Ga_{0.35}N$:Mg-SPSLs will be investigated. By comparing LEDs with varing SPSL-thickness σ_V was extracted. The value of σ_V was found to be strongly field- and temperature-dependent and fits well to predictions made by 3D-Poole-Frenkel-effect (3D-PFE). An activation energy of 530 meV and an intertrap distance of 6 nm were extracted for the SPSL. When comparing a SPSL with an Al-content of 78 % and a SPSL with an Al-content of 65 % σ_V is increased by more than one order of magnitude, respectively.

HL 30.25 Tue 13:30 P3

Effect of Mg doping in the electron blocking layer on UVC-LED efficiency characterized by temperature–dependent electroluminescence spectroscopy — •Katharina Müller[1], Priti Gupta[1], Norman Susilo[1], Martin Guttmann[1], Tim Wernicke[1], Markus Weyers[2], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics, Berlin, Germany — [2]FBH, Berlin, Germany

The external quantum efficiency (EQE) of UVC emitters crucially depends on the Mg doping profile in the LED heterostructure. In this study, a series of flip-chip mounted AlGaN-based UVC-LEDs with different Mg doping in the electron blocking layer (EBL) is investigated using temperature–dependent (100 K - 330 K) electroluminescence spectroscopy. During the growth, the Cp_2Mg/group-III precursor ratio (x) in the EBL layer was varied with x = 0.155%, 1.0% and 1.5%. At 330 K and 10 mA, LEDs with x = 1.0% show higher EQE (up to 0.28%) compared to LEDs with x = 0.155% (EQE: 0.11%) and x = 1.5% (EQE: 0.15%). This difference between different doping levels becomes more pronounced with decreasing temperature. While the EQE increases with decreasing temperature for x = 1.0% with a maximum at around 210 K, the EQE for x = 0.155% and 1.5% continuously decreases or remains very low with lowering temperature. This indicates a higher injection efficiency in LEDs with x = 1%, in comparison to x = 0.155% and x = 1.5%. The optimal doping profile in the EBL was found to be at around x = 1.0%, leading to an improved carrier injection and thus higher EQE.

HL 30.26 Tue 13:30 P3

Simulation of Magnetoelectric Microbeams — Simeon Katzer[1], Bernd Hähnlein[1], •Maximilian Krey[2], Katja Tonisch[1], Stefan Krischok[1], and Hannes Toepfer[2] — [1]Technical Physics 1 Group, Technische Universität Ilmenau, Germany — [2]Advanced Electromagnetics Group, Technische Universität Ilmenau, Germany

Magnetic field sensors cover a wide field of applications, for example in bio-medicine, non-destructive testing or geo-exploration. In terms of sensitivity, super conductive quantum interference devices (SQUIDs) are state of the art, but with the disadvantage of the necessary liquid helium cooling in order to reach a super conductive state. Thus, our research efforts focus on the development of magnetic field sensors based on magnetoelectric resonant MEMS for room temperature operation. In beam-like structures a combination of piezoelectric and magnetostrictive materials is used to convert the magnetic field input in an electrically measurable output. The sensor principle is based on an eigenfrequency shift of the structure under the influence of a magnetic field. Simulations of this behavior require the consideration of aspects such as material science, mechanical vibrations, magnetism, electricity as well as mutual effects like piezoelectricity, magnetostriction and the Delta-E- effect. Due to the multi-physics problem many degrees of freedom arise, which can be used to optimize the structure for maximum output signal amplitude and frequency shift. We present an investigation targeting a simulative description of a magnetoelectric sensor based on scandium aluminum nitride with Comsol Multiphysics.

HL 30.27 Tue 13:30 P3

Highly reflective and conductive AlInN/GaN distributed Bragg reflectors realized by Ge-doping — •Cleophace Seneza, Christoph Berger, Hartmut Witte, Jürgen Bläsing, Anja Dempewolf, Armin Dadgar, Jürgen Christen, and André Strittmatter — Otto-von-Guericke-University Magdeburg, 39106 Magdeburg, Germany

Lattice-matched AlInN has been proven as well-suited material to realize highly reflective AlInN/GaN distributed Bragg reflectors (DBRs), which are mandatory for the fabrication of vertical-cavity surface-emitting lasers (VCSELs) using GaN-based material. In contrast to GaAs-VCSELs with highly conductive arsenide-based DBRs, AlInN/GaN-based DBRs usually exhibit high electrical resistance due to large polarization fields and a significant conduction band offset between GaN and AlInN. Therefore, intracavity contacts are employed for VCSELs to inject current into the active region. We demonstrate that Ge can be used as n-type donor to realize low-resistive lattice-matched AlInN/GaN DBRs. Various Ge-doping levels were utilized to study the vertical electrical conductivity and reflectance properties of lattice-matched AlInN/GaN DBRs grown by MOVPE. We will present the effect of Ge-doping on structural properties, electrical and optical properties of DBRs. With Ge-doping, lattice-matched AlInN/GaN DBRs exhibit ohmic behavior and high reflectivity. Such DBRs structures have a huge potential to improve the current-injection, lower the threshold-current density and will also help to simplify the fabrication processes for VCSELs.

HL 30.28 Tue 13:30 P3

A study of ultrathin c-plane GaInN/GaN quantum wells and discs grown by MBE — •André Schendel, Heiko Bremers, Uwe Rossow, and Andreas Hangleiter — Institut für Angewandte Physik, Technische Universität Braunschweig

In this contribution we present our study of ultrathin c-plane GaInN/GaN quantum wells (QWs) and incomplete quantum wells (discs) grown by molecular beam epitaxy (MBE) in terms of morphology and composition homogeneity. The ternary semiconductor GaInN offers many opportunities for applications as optoelectronic devices with its direct band gap tunable between 0.65 eV for InN and 3.42 eV for GaN. Nowadays, especially green emitting LED's are in the focus of research, because there is no high efficient green emitting LED available yet for any kind of material. Theoretically, GaInN should be able to close this gap, but in practice the In-content can hardly be increased above 30% if it is grown on GaN. Additionally, the emissivity in the green spectral range is very low due to increased defect formation which is caused by the increased lattice mismatch between the two material systems with increasing In-content. In this study, the growth process of GaInN with low and high In-content is investigated in terms of morphology and composition homogeneity by varying the growth parameters material fluxes and growth temperature to get a better understanding of the impact of the single parameters.

HL 30.29 Tue 13:30 P3

Structure and dielectric function tensor of (Al,Sc)N thin films — •Sascha Kürth, Rüdiger Schmidt-Grund, Stefan Krischok, and Katja Tonisch — Institut für Physik, Technische Universität Ilmenau, Weimarer Straße 32, 98693 Ilmenau, Germany

We present the dielectric function tensor of (Al,Sc)N thin films for the full composition range and derive material properties such as bandgap energies and refractive index dispersion. The thin films have been grown on silicon with conductive interlayers such as platinum and titanium nitride and on sapphire by reactive sputter deposition. Both, the structural as well as optical properties vary with Sc content and with the actualy used substrate. While excitonic enhancement is observed mainly for pristine aluminium nitride, the transition between the hexagonal and cubic crystal structure of ScAlN is observed by the transition between optic uniaxiality and isotropy. For increasing Sc content, we further observe a redshift of the optical absorption edge as well as an increase of the refractive index.

(Al,Sc)N is a very promising material system for piezoelectric applications as the piezoelectric coefficient gains values as big as d_{33} = 28 pm/V [1]. But only recently films of sufficient quality have been achieved, thus a comprehensive understanding of optical and electronic properties is still missing.

[1] T. Yanagitani, M. Suzuki, Appl. Phys. Lett. **105**, 122907 (2014).

HL 30.30 Tue 13:30 P3

Nonempirical dielectric-dependent hybrid functional for semiconductors and insulators — •Wei Chen[1], Giacomo Miceli[2], Gian-Marco Rignanese[1], and Alfredo Pasquarello[2] — [1]Institute of Condensed Matter and Nanoscicence (IMCN), Université catholique de Louvain, Louvain-la-Neuve 1348, Belgium — [2]Chaire de Simulation à l'Echelle Atomique (CSEA), Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

We present a general scheme of range-separated hybrid functionals in which the mixing parameters of Fock exchange are determined solely from the dielectric function and hence fully nonempirical. We show that the full dielectric dependence leads to an unscreened Fock exchange in the short range, while the Fock exchange is correctly screened by the macroscopic dielectric constant in the long range. The range separation is obtained by fitting to the calculated static dielectric function in the long-wavelength limit. The resulting dielectric-dependent hybrid functional (DD-CAM) accurately accounts for the band gaps of various semiconductors and insulators with a mean absolute error of 0.2 eV.

HL 30.31 Tue 13:30 P3

Theoretical investigation of the monoclinic and orthrombic phase of WO_3 — •Felix Bernhardt and Simone Sanna — Institut für Theoretische Physik and Center for Materials Research, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

Tungsten trioxide (WO_3) is a semiconductor which proved suitable for a wide variety of applications, due to its many temperature driven phase transitions, and an electronic band gap within the optical spectrum [1]. It is employed in a multitude of devices, ranging from smart windows [3] to gas sensors [5]. In this work, we concentrate on the equilibrium structures of the at room temperature stable monoclinic phase, as well as the orthrombic phase of WO_3. Within density func-

tional theory the lattice parameters, electronic band structure and phononic band structure are calculated. The phonon spectra are then used to describe the thermodynamic properties and the transition temperature. Our results are in excellent agreement to other theoretical investigations [1,4] as well as experiments [2]. [1] M. Mansouri, T. Mahmoodi, Turkish Journal of Physics 41, 238 (2017) [2] B. O. Loopstra, H. M. Rietveld, Acta Cryst., 25(1420) (1968) [3] L. Liang et al, Sci. Rep. 3, 1936 (2013) [4] F. Wang et al, Journal Of Physical Chemistry, 115(8345) (2011) [5] N. Yamazoe et al, Catalysis Surveys from Asia 7, 63-75 (2003)

HL 30.32 Tue 13:30 P3

Gating technologies for bilayer 2D carrier systems — •Jana Marie Meyer[1], Jan Scharnetzky[2], Simon Parolo[2], Christian Reichl[2], Werner Dietsche[2], Werner Wegscheider[2], Lars Tiemann[1], and Robert Blick[1] — [1]Center for Hybrid Nanostructures, University of Hamburg, 22761, Germany — [2]ETH Zürich, 8092 Zürich, Switzerland

Electrostatic gating is a versatile and crucial tool in nanotechnology and allows to change the intrinsic electron density of two-dimensional carrier systems, that is given by doping in the growth process. Bilayer systems like gallium arsenide double quantum wells can be electrically separated and the electron density of each layer can be tuned independently with a sophisticated system of patterned back gates and metallic top gates. To achieve a higher sample quality, the back gates are patterned via ion implantation before the overgrowth of the double layer system allowing also a low charge carrier concentration. This versatile technology is can be applied to generate confinement potentials, tune the carrier concentration and study a variety of quantum phenomena.

HL 30.33 Tue 13:30 P3

Quantum Hall Effect in Bulk-insulating Sn-doped $Bi_{1.1}Sb_{0.9}Te_2S$ Topological Insulators — •Dingxun Fan, Yongjian Wang, and Yoichi Ando — II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln, Deutschland

Realization of bulk-insulating materials is among the central tasks of the research efforts in the past decade in the field of topological insulators (TIs). To better address the intriguing properties of the topological surface states, it is desired to have a TI platform with a single Dirac cone well isolated from the bulk bands.

We have grown Sn-doped $Bi_{1.1}Sb_{0.9}Te_2S$ topological insulator single crystals by a modified Bridgman method. Transport characterization on these crystals shows large low temperature bulk resistivity, low bulk carrier density, and clear Shubnikov-de Haas oscillations from the surface state. We also observed the integer quantum Hall effect in dual-gated Hall bar devices fabricated from exfoliated thin flakes. Efforts of proximitizing the surface state by superconducting contacts will also be shown.

HL 30.34 Tue 13:30 P3

Anomalous and topological hall effect in magnetically-doped topological insulator thin films grown by molecular beam epitaxy — •Anjana Uday[1], Gertjan Lippertz[1,2], Andrea Bliesner[1], Alexey Taskin[1], and Yoichi Ando[1] — [1]Physics Institute II, University of Cologne, Germany — [2]Quantum Solid State Physics, KU Leuven, Belgium

There is an increasing demand for magnetic topological quantum materials in recent years as such materials offer a productive platform for the development of next-generation spintronic devices. When a topological insulator (TI) is magnetically doped, the breaking of time reversal symmetry (TRS) opens up an energy gap at the Dirac point of the surface states. Furthermore, a remarkable quantum phenomenon known as the quantum anomalous Hall effect (QAHE) is observed in such materials when their fermi level is tuned into this exchange gap. When the QAHE is realized, the spontaneous magnetization leads to a dissipationless spin-polarised edge channel, giving rise to a quantized Hall resistance of h/e^2. An additional topological Hall component has recently been observed in such samples, possibly originating from the formation of Skyrmions. Our observation of the anomalous and topological Hall effect in V- and Cr-doped $(Bi_xSb_(1-x))_2Te_3$ films grown by MBE show how a gradient in the Bi/Sb ratio along the growth direction leads to a broken inversion symmetry and the appearance of an additional topological Hall component near the coercive field while homogeneous samples exhibit the usual anomalous Hall effect close to the quantized Hall resistance of h/e^2.

HL 30.35 Tue 13:30 P3

Topological insulator nanowires grown selectively by molecular beam epitaxy — •Gertjan Lippertz[1,2], Andrea Bliesener[1], Anjana Uday[1], Gian-Luca Ansermetti[1], Oliver Breunig[1], Alexey Taskin[1], Lino Pereira[2], and Yoichi Ando[1] — [1]Physics Institute II, University of Cologne, Germany — [2]Quantum Solid State Physics, KU Leuven, Belgium

Inducing superconductivity into a topological insulator (TI) nanowire by proximitizing it with an s-wave superconductor is predicted to give rise to Majorana bound states. However, TI nanowires grown by the Vapor-Liquid-Solid (VLS) technique are difficult to integrate into scalable device structures. Therefore, we are pursuing an alternative route towards nanowire structures, selective-area growth (SAG) by molecular beam epitaxy (MBE). A Si_3N_4 layer is deposited on a sapphire substrate and patterned into nanowire devices using electron-beam lithography and reactive ion etching. Within a small parameter range, $(Bi_{1-x}Sb_x)_2Te_3$ can be selectively grown by MBE inside the trenches of the pre-patterned substrate. Control over the chemical potential of the nanowires is achieved by a side-gate fabricated in the same process, alleviating the need for additional fabrication steps after growth.

In this presentation, we show our first results towards growing bulk-insulating TI nanowires with a width below 100 nm. Such SAG-TI nanowires are expected to show non-equidistant resistance peaks as a function of the gate voltage, which was recently shown to be the unique signature of quantum-confined Dirac surface states.

HL 30.36 Tue 13:30 P3

Optical-pump/THz-probe spectrometer using mode-matching via field-enhancement — •Julia Lang, Michael Seidel, and Georg Herink — Experimental Physics VIII, University of Bayreuth, Germany

Optical-pump/THz-probe spectroscopy presents a powerful scheme for characterizing the transient carrier dynamics in electronic materials and devices. In order to improve the sample excitation and the probe signal strength, we introduce mode-matching between optical-pump and THz-probe. Specifically, this approach employs sub-diffraction Terahertz confinement in metallic microstructures to reduce the large mismatch between optical and THz foci. The setup, based on a compact high repetition rate mode-locked fiber laser, efficient frequency conversion and photoconductive detection, is demonstrated for transient spectroscopy of photo-induced charge carriers in semiconductors.

HL 30.37 Tue 13:30 P3

Switchable THz wavefront modulators made of thermocromic $V_xW_{1-x}O_2$ thin films — •Janine Lorenz[1], Florian Kuhl[1], Angelika Polity[1], Yan Zhang[2], and Peter J. Klar[1] — [1]Institute of Experimental Physics I and Center for Materials Research (ZfM/LaMa), Justus Liebig University Giessen, Heinrich-Buff-Ring 16, DE-35392 Giessen, Germany — [2]Beijing Key Lab for Metamaterials and Devices, Capital Normal University, Beijing, China

Due to the rapid progress in the reasearch field of terahertz generation and detection over the last years, terahertz applications have recently gained a lot of interest. Similar to VO_2 the insulator to metal transition (IMT) in thermochromic $V_xW_{1-x}O_2$ allows us to design thermally switchable THz optics.

Here we present microfabricated resonator structures in rf-sputtered $V_xW_{1-x}O_2$ thin films. The fabrication of the resonators is realised by photolithography and ion beam etching. Modulation properties of the resonators can be improved by depositing TiO_2 buffer layers onto the c-sapphire substrates used. In comparison to VO_2, the switching temperature of $V_xW_{1-x}O_2$ can be reduced and tuned by varying the concentration x of tungsten. Measurements on unstructured thin films show typical switching temperatures for VO_2 of about 55 °C and 35 °C for $V_xW_{1-x}O_2$ with x between 1 and 2 %. The modulating behavior of the resonator structures in the insulating and metallic phase was investigated by terahertz time-domain spectroscopy. Switchable devices are obtained since THz modulation only occurs in the metallic phase.

HL 30.38 Tue 13:30 P3

Creation of a shallow graphitic layer in diamond for field effect applications — •Dennis Oing, Martin Geller, Axel Lorke, and Nicolas Wöhrl — Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

Diamond is a promising wide band gap semiconductor with high hole and electron mobilities, high electric breakdown field and the highest thermal conductivity.

However, a field effect transistors based on the surface conductivity of the two-dimensional hole gas need a dielectric material, e.g. Al_2O_3, between the diamond surface and the gate. However, these materials have a lower electric breakdown field and lower thermal conductivity. Hence, transistors using these materials lack the potential that transistors solely made from diamond possess.
In this contribution, graphitic layers as bottom-gate below the two-dimensional hole gas were produced 100 nm below the diamond surface by ion implantation. Implantation was done on CVD-grown single crystal layers using ^{12}C-ions with a kinetic energy of 95 keV. The samples were subsequently annealed from 210° up to 650° to form the graphitic layers. The produced layers were characterized using Raman spectroscopy and measuring IV-characteristics.
Raman spectroscopy reveals that after implantation a small G-peak appears. Additionally, a D-peak can be observed after annealing. These peaks correspond to the formation of amorphous carbon layers. Our results suggest that the created structures can be used for field effect applications.

HL 30.39 Tue 13:30 P3

Deep level transient spectroscopy on thin rutile films — •Lukas Berg[1], Laurin Schnorr[1], Thomas Heinzel[1], Carlos Cesar Bof Bufon[2] und Leandro Merces[2] — [1]Heinrich Heine - Universität Düsseldorf — [2]Brazilian Center for Research, Campinas

Time resolved electro-optical admittance measurements were performed on mono-crystalline Rutile thin films through an optically transparent rolled-up gold gate. Excitation pulses of different wavelengths in the infrared band were applied to the structure as a function of the temperature and the electric field and the admittance transients were recorded. The analysis of the time evolution reveals a binding energy of 0.6 eV for a single prominent defect level. Furthermore, a temperature and light intensity dependent delayed trap response was observed and investigated under various conditions.

HL 30.40 Tue 13:30 P3

Thermoelectric properties of Bi-based core/shell nanowires — •Maximilian Kockert[1], Jeongmin Kim[2], Hongjae Moon[2], Danny Kojda[1], Mahni Müller[1], Rüdiger Mitdank[1], Anna Mogilatenko[3], S. Hoda Moosavi[4], Michael Kroener[4], Peter Woias[4], Wooyoung Lee[2], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Departement of Materials Science and Engineering, Yonsei University, 03722 Seoul, Republic of Korea — [3]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, 12489 Berlin, Germany — [4]Laboratory for Design of Microsystems (IMTEK), University of Freiburg, 79110 Freiburg, Germany

Bi-based core/shell nanowires are promising thermoelectric materials in order to improve the dimensionless figure of merit $ZT = \frac{\sigma S^2}{\lambda} T$, with the electrical conductivity σ, the Seebeck coefficient S, the thermal conductivity λ and the bath temperature T. The mismatch of the different lattice constants between the core (Bi) and the shell (Te or TiO_2) lead to a strain-induced reduction of the band overlap in the Bi-core [1].

However, the determination of σ, S, λ and structural properties of the same individual [2] core/shell nanowire remains an open issue. Here, we present a complete temperature-dependent thermoelectric and structural characterization of an individual Bi/Te and Bi/TiO_2 core/shell nanowire.

[1] J. Kim *et al.*, *Acta Materialia* **144**, 145 (2018).
[2] D. Kojda *et al.*, *Physical Review B* **91**, 024302 (2015).

HL 30.41 Tue 13:30 P3

Electroluminescence emission in a GaAsSb resonant tunneling diode with emitter prewell — •Edgar David Guarin Castro[1], Edson Cardozo de Oliveira[1], Andreas Pfenning[2], Fabian Hartmann[2], Lukas Worschech[2], Sven Höfling[2,3], Gilmar Marques[1], Marcio Daldin Teodoro[1], and Victor Lopez-Richard[1] — [1]Departamento de Física, Universidade Federal de São Carlos, 13565-905 São Carlos, SP, Brazil — [2]Technische Physik and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Physikalisches Institut, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [3]SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, KY16 9SS, United Kingdom

We study the electroluminescence (EL) emission of an n-type GaSb resonant tunneling diode with pseudomorphically grown ternary $GaAs_0.05Sb_0.95$ emitter prewell and quantum well. Emission peaks are observed along to the spectral range of 1.1 μm to 1.6 μm. We attribute the radiative recombination to the generation of holes via impact ionization processes. Comparing EL and photoluminescence (PL) emissions, we observe a high EL on-off-ratio which is one order of magnitude greater than the PL on-off-ratio. The larger EL on-off ratio correlates with the coherent current channel. To understand the carrier dynamics inside the quantum well, we characterize the carrier lifetimes using Time-resolved Photoluminescence spectroscopy. We demonstrate the existence of different carrier relaxation processes, unveiled under different current conditions.

HL 30.42 Tue 13:30 P3

Contactless Measurement of the Sheet Resistance of two-dimensional Electron Gases — •Timo A. Kurschat, Arne Ludwig, and Andreas D. Wieck — Angewandte Festkörperphysik, Ruhr-Universität Bochum, Universitätsstraße 150, D-44780 Bochum

The aim of this work is to measure the sheet resistance of two-dimensional electron gases in GaAs without the need for built-in contacts. Thus a characterization is possible without destroying the wafer. With this method quality and homogeneity can be evaluated before further processing.

The sheet resistance is measured by placing two electrodes (round metal plates) close to the sample. These electrodes form capacitances C with the conductive layer. With a high-frequency alternating voltage applied to one electrode, the transmitted power can be measured at the other one. The measured amplitude depends on the sample resistance and the impedance of the capacitance, which is proportional to $1/\omega C$.

The electrodes have a diameter of 3 mm and 6 mm center-to-center distance. For low surface resistances from 100 to over 1000 Ω/sq the amplitude was evaluated at a frequency of 10 GHz. At higher resistances up to some 10 kΩ/sq, a frequency sweep from 1 MHz to 400 MHz was performed, and the resistance was determined with a fit.

It is possible to create maps of complete wafers. The lateral resolution depends on the size of the electrodes, so we expect an effective footprint of around 5 mm diameter.

HL 30.43 Tue 13:30 P3

Schottky junctions on GeSn bottom-up grown nanowires by Nickel-stanogermanidation via flash-lamp annealing — •Shima Jazavandy Ghamsari, Artur Erbe, and Yordan M. Georgiev — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Bautzner Landstrasse 400, 01328 Dresden, Germany

Direct bandgap was achieved in Ge by introducing high contents of Sn (>6%) [1]. GeSn was also predicted to exhibit high carriers* mobilities, making it an ideal material for co-integration of optoelectronic and high-speed electronic devices. Moreover, GeSn nanowires can add the gate-all-around benefit in efficient electrostatic control of FET device channels. Beside the large body of data on GeSn thin films growth, the number of reports on growth of GeSn nanowires with significant Sn incorporation is very limited. Silicon and germanium metal alloys were widely studied for low-resistance contacts. For GeSn thin films, however, there are only few studies on Ni and NiPt stanogermanides (NiGeSn and NiPtGeSn). In this work, the benefits of flash-lamp annealing were used for producing Schottky junctions on GeSn bottom-up grown nanowires [2], to overcome the thermal budget limitations because of the low Sn melting point. [1] S. Gupta et al., J. Appl. Phys. 113, 073707 (2013). [2] S. Biswas et al. Nat Commun. 7, 11405 (2016).

HL 31: Complex Oxides: Surfaces and Interfaces (jointly with DS, HL, KFM, MA, O) (joint session TT/MA/HL)

Time: Tuesday 14:00–15:45 Location: HSZ 02

HL 31.1 Tue 14:00 HSZ 02

Ultradense tailored vortex pinning arrays in $YBa_2Cu_3O_{7-\delta}$ thin films created by He ion beam irradiation — •Max Karrer[1], Bernd Aichner[2], Benedikt Müller[1], Vyacheslav Misko[3], Kristijan L. Mletschnig[2], Meirzhan Dosmailov[4], Johannes D. Pedarnig[4], Franco Nori[3], Reinhold Kleiner[1], Wolfgang Lang[2], and Dieter Koelle[1] — [1]Physikalisches Institut and Center for Quantum Science (CQ) in LISA$^+$, Universität Tübingen, Germany — [2]Faculty of Physics, University of Vienna, Austria — [3]Theoretical Quantum Physics Group, RIKEN Cluster for Pioneering Research, Wako-shi, Saitama, Japan — [4]Institute of Applied Physics, Johannes Kepler University Linz, Austria

Magnetic fields penetrate a type II superconductor as magnetic vortices. In a clean superconductor they arrange in a hexagonal lattice; by addition of artificial pinning sites many other arrangements are possible. With a focused He ion beam, we fabricate periodic patterns of pinning sites with spacings down to 70 nm in $YBa_2Cu_3O_{7-\delta}$ thin films. In ultradense kagomé-like patterns, magnetic caging of vortices results in unconventional commensurability effects, yielding peaks in the critical current and minima in the resistance versus applied field up to ~ 0.4 T. The various vortex patterns at different magnetic fields are analyzed by molecular dynamics simulations of vortex motion, and the magnetic field dependence of the critical current is confirmed. These findings open the way for a controlled manipulation of vortices in cuprate superconductors by artificial sub-100 nm pinning landscapes.
[1] B. Aichner *et al.*, ACS Appl. Nano Mater. **2**, 5108–5115 (2019).

HL 31.2 Tue 14:15 HSZ 02

Strain-dependent electronic reconstruction in Sr_2CoIrO_6 double perovskite from DFT+U+SOC calculations — •Jiongyao Wu and Rossitza Pentcheva — Department of Physics and Center for Nanointegration (CENIDE) Universitat Duisburg-Essen, Duisburg, Germany

The double perovskite Sr_2CoIrO_6 (SCIO) can be regarded as a (111)-superlattice of alternating $SrIrO_3$ (SIO) and $SrCoO_3$ (SCO) layers. Here we explore the electronic and magnetic properties in the framework of density functional theory (DFT) including a Hubbard U term and spin-orbit coupling (SOC) with the PBEsol exchange correlation functional. While the end member SIO is metallic with a quenched spin and orbital moment and bulk SCO is a G-type antiferromagnetic (AFM) insulator with spin and orbtial moment of 2.7 and 0.26 μ_B, respectively, the double perovskite SCIO emerges as an AFM Mott insulator with a band gap of $\sim$ 500 - 600 meV. Additionally, Ir acquires a spin moment of 1.5 μ_B pointing towards a $j = 1/2$ Mott insulating state in SCIO, similar to other iridates. Analysis of the orbital occupation indicates substantial charge transfer from the Ir to the Co ion. Moreover, subtle changes in orbital occupation are observed as the strain is varied from compressive (a_{NdGaO_3}) to tensile (a_{SrTiO_3}).

We acknowledge funding by the German Science Foundation within CRC/TRR80, project G3.

HL 31.3 Tue 14:30 HSZ 02

Sensitivity of non-local fluctuations on surface effects in ultrathin $SrVO_3$ films — •Matthias Pickem, Jan M. Tomczak, and Karsten Held — Institute of Solid State Physics, TU Wien, Austria

Recent experiments show that strong electronic correlations cause the conventional Fermi-liquid state of bulk $SrVO_3$ to be destroyed in films below a critical thickness. However new experimental results challenge the current understanding of the details of this breakdown.

To this end we perform realistic density functional theory (DFT) + dynamical mean-field theory (DMFT) calculations of $SrVO_3$ on $SrTiO_3$ substrate. Depending on the simulated interface ($SrVO_3$ termination, surface reconstructions, or additional $SrTiO_3$ capping) we find that different mechanism cause this aforementioned break-down of the Fermi-liquid state.

Furthermore, calculations on the two-particle level (DMFT susceptibilities) reveal that the different interfaces result in vastly different instabilities.

HL 31.4 Tue 14:45 HSZ 02

Planar GHz resonators on $SrTiO_3$: Suppressed losses at temperatures below 1 K — Vincent T. Engl, Nikolaj G. Ebensperger, Lars Wendel, and •Marc Scheffler — 1. Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany

The complex dielectric constant $\hat{\epsilon} = \epsilon_1 + i\epsilon_2$ of $SrTiO_3$ reaches high values $\epsilon_1 \approx 2 * 10^4$ at cryogenic temperatures, while the dielectric losses (ϵ_2) are much stronger than for other crystalline dielectrics. $SrTiO_3$ is a common substrate for oxide thin films, like the superconducting $LaAlO_3/SrTiO_3$ system, but the large ϵ_1 and ϵ_2 restrict high-frequency quantum devices on $SrTiO_3$. Here we present superconducting coplanar Nb resonators on $SrTiO_3$, which we successfully operate in a distant-flip-chip geometry [1] at frequencies that exceed 1 GHz. We find a pronounced and unexpected increase in resonator quality factor Q at temperatures below 1 K, reaching up to $Q \approx 800$. We attribute this to substantial changes of the dielectric losses in $SrTiO_3$ at mK temperatures, and we also detect non-monotonous changes in the temperature-dependent ϵ_1. These findings [2] challenge our present understanding of the dielectric properties of $SrTiO_3$ and at the same time demonstrate that cryogenic high-frequency devices on $SrTiO_3$ are more feasible than previously assumed.
[1] L. Wendel *et al.* arXiv:1911.10518 [cond-mat.supr-con]
[2] V. T. Engl *et al.* arXiv:1911.11456 [cond-mat.supr-con]

HL 31.5 Tue 15:00 HSZ 02

Tuning superconductivity at the $Al_2O_3/SrTiO_3$-interface with light — •Daniel Arnold, Dirk Fuchs, and Roland Schäfer — Institute for Solid State Physics, Karlsruhe Institute of Technology, Karlsruhe, Germany

The 2-DEG at $SrTiO_3$-based interfaces is sensitive to illumination with visible light [1], which at low temperatures can be used to tune the transition temperature of the superconducting state in a nonvolatile manner [2]. We present studies on an $Al_2O_3/SrTiO_3$ sample with micro bridges running along different crystallographic directions at the interface. We are able to tune the low temperature conductance by illuminating the sample and reverse the altered state by thermal treatment at low temperatures ($T < 15$ K). Transport measurements in dependence of the magnetic field and temperature are conducted in different states, characterized by the tunable but time independent resistance at 1 K. The Berezinskii-Kosterlitz-Thouless transition in this system can be addressed by the current voltage behavior, which simultaneously gives further information on the inhomogeneous nature of the superconducting phase.
[1] M. Yazdi-Rizi et al., PRB 95 (2017)
[2] D. Arnold et al., APL 115 (2019)

HL 31.6 Tue 15:15 HSZ 02

Crystalline anisotropy of magnetoresistance in LAO/STO nanostructures — •Mithun Sheena Prasad[1] and Georg Schmidt[1,2] — [1].Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, D-06120 Halle, Germany — [2]Interdisziplinäres Zentrum für Meterialwissenschaften, Martin-Luther-Universität Halle-Wittenberg, Heinrich-Damerow-Straße 4, D-06120 Halle, Germany

The high-mobility two-dimensional electron gas (2DEG) confined at the interface $LaAlO_3$ (LAO) and $SrTiO_3$ (STO) provides new opportunities to explore Nano electronic devices. In our group we have developed an industry compatible Nano patterning technique [1] for the LAO/STO interface. Recent studies on this interface have revealed that at low temperature the current is confined to filaments which are linked to structural domain walls in the STO with drastic consequences for example for the temperature dependence of local transport properties. We have investigated magneto-transport in nanostructures having different orientation with respect to the lattice. Our experiments show that not only the resistance but also the magnetoresistance varies with orientation. The magnetoresistance can even change sign for different orientations and again this can change after a warm-up cool-down cycle strongly supporting the model of filamentary charge transport.
[1] M. Z. Minhas, H. H. Blaschek, F. Heyroth, and G. Schmidt, AIP Advances 6, 035002 (2016)

HL 31.7 Tue 15:30 HSZ 02

Study of 2D superconductivity at oxide interfaces by microwave resonators — •Edouard Lesne[1], Yildiz Saglam[1], Daniel Bothner[1], Felix Schmidt[1], Marc Gabay[2], Gary Steele[1], and Andrea Caviglia[1] — [1]Delft University of Technology — [2]Université Paris-Saclay

The emergent two-dimensional electron system (2DES) formed at the interface between LaAlO3 (LAO) and SrTiO3 (STO) insulating oxides has been a subject of great interest in condensed matter physics during the last decade. Recently, (111)-oriented LAO/STO interfaces have been shown to exhibit an electronic correlation driven reconstruction of its band structure and a two-dimensional superconducting (SC) ground state, both tunable by electrostatic field-effect.

Superconducting coplanar waveguide (SCPW) resonators are tools of exquisite sensitivity for probing low energy excitations in quantum materials, due to their intrinsic low ohmic losses and high quality factors, highly relevant to quantum technology platforms. Here, in order to study the superconducting state at the LAO/STO(111) interface, we designed embedded SCPW resonators whose microwave resonance frequency can be tuned by electrostatic gating, manifesting a change of the 2DES superfluid density through a large change of its kinetic inductance. This allows us to map the SC phase diagram in a detection scheme that goes beyond traditional resistive measurements. Our work highlights the potential of such an approach to the fundamental study of superconductivity in complex materials.

HL 32: Twisted Bilayer Graphene (jointly with DY, MA, HL, DS, O) (joint session TT/HL)

Time: Tuesday 14:00–15:45 Location: HSZ 201

HL 32.1 Tue 14:00 HSZ 201

Valley splitter and transverse valley focusing in twisted bilayer graphene — •Christophe De Beule[1], Peter Silvestrov[1], Ming-Hao Liu[2], and Patrik Recher[1,3] — [1]Institute for Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany — [2]Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan — [3]Laboratory for Emerging Nanometrology, 38106 Braunschweig, Germany

We study transport through electrostatic barriers in twisted bilayer graphene and show that for certain configurations, electrons from the K (K') valley are transmitted only to the top (bottom) layer, leading to valley-layer locked bulk currents. We show that such a valley splitter is obtained when the potential varies slowly on the Moiré scale and the Fermi energy in the barrier exceeds the kinematic barrier between Dirac electrons from the top and bottom layer. Furthermore, we show that for a given valley the current is transversely deflected, as time-reversal symmetry is broken in each valley separately, resulting in valley-selective transverse focusing at zero magnetic field.

HL 32.2 Tue 14:15 HSZ 201

Quantum capacitive coupling in large-angle twisted graphene layers — •Ming-Hao Liu — Department of Physics, National Cheng Kung University, Tainan, Taiwan

Magic-angle twisted bilayer graphene (tBLG) has revealed exotic physics of strong correlation in graphene systems and attracted enormous attention on twistronics of 2D materials. In the opposite extreme of large twist angles, relatively less attention has been paid. Due to the required large momentum change, scattering between different graphene layers of large-angle tBLG is forbidden. Through quantum capacitance of individual graphene layers, however, tBLG is electrostatically coupled, though electronically decoupled. Here, I introduce a self-consistent electrostatic model for carrier densities in decoupled tBLG systems and apply the model to perform quantum transport simulations for a recent experiment on a dual-gated large-angle tBLG device [1]. Good agreement between the experiment and theory confirms the electronic decoupling and indicates that the decoupled large-angle tBLG can be the thinnest parallel-plate capacitor in the world. The model can be further generalized to multi-layer systems composed of decoupled graphene sheets.
[1] P. Rickhaus *et al.*, arXiv:1907.00582 (2019).

HL 32.3 Tue 14:30 HSZ 201

Skyrmion lattices in twisted bilayer graphene — •Thomas Bömerich, Lukas Heinen, and Achim Rosch — Institute for Theoretical Physics, University of Cologne, Germany

We investigate the groundstate properties of magnetic skyrmions in anomalous Quantum Hall (AQH) systems. In these systems, the topological charge density, which characterizes the winding of a skyrmion, is directly proportional to the electric charge density. Therefore magnetic skyrmions are electrically charged excitations stabilized by Coulomb interactions between each other. At finite densities the skyrmions form regular lattices and can be controlled by external gate voltages. Our theory can be applied to twisted bilayer graphene as there is experimental evidence of ferromagnetic order and an AQH effect at specific fillings.

Starting from a free energy functional, we solve some limiting cases analytically and use micromagnetic simulations to study the lattice structure as a function of skyrmion density and skyrmion radius. From this we obtain a phase diagram with different skyrmion lattices. In particular we analyse the groundstate and its symmetries without external magnetic field. Additionally, we calculate the total magnetization as a function of skyrmion density, which can be used to detect experimental signatures of skyrmions in AQH systems.

HL 32.4 Tue 14:45 HSZ 201

Magnetism of magic-angle twisted bilayer graphene — •Javad Vahedi[1,2], Andreas Honecker[2], Robert Peters[3], and Guy Trambly de Laissardière[2] — [1]Institut für Mathematische Physik, Technische Universität Braunschweig, Germany — [2]Laboratoire de Physique Théorique et Modélisation, Université de Cergy-Pontoise, France — [3]Department of Physics, Kyoto University, Japan

Recently, correlated insulators and superconductivity have been discovered experimentally in twisted bilayer graphene (TBG) [1]. The Moiré pattern of the bilayers at so-called "magic angles" leads to localization of the low-energy electrons in the AA-stacking regions, reflected by very flat regions in the band structure [2]. This reduction of the kinetic energy enhances the relative importance of interactions and thus renders the bilayer systems much more susceptible to correlation effects than a single layer. We investigate the magnetic instabilities at half filling in TBG using a real-space Hartree-Fock and RPA analysis. We find that at charge neutrality an antiferromagnetic state localized in the AA region emerges for values of the Coulomb interaction U that are an order of magnitude smaller than what would be required to render an antiferromagnetic state in a single graphene sheet. Furthermore, doping of a few electrons per Moiré unit cell pushes the system into a ferromagnetic phase.
[1] Y. Cao *et al.*, Nature **556**, 80 (2018); Nature **556**, 43 (2018)
[2] G. Trambly de Laissardière *et al.*, Nano Letters **10**, 804 (2010)

HL 32.5 Tue 15:00 HSZ 201

Quantum diffusion in twisted bilayer graphene — •Guy Trambly de Laissardière[1], Omid Faizy Namarvar[2,3], Ahmed Missaoui[1], Javad Vahedi[1,4], Andreas Honecker[1], Laurence Magaud[2], and Didier Mayou[2] — [1]Laboratoire de Physique Théorique et Modélisation, CNRS (UMR 8089), Univ. de Cergy-Pontoise, France — [2]Institut Néel, CNRS, Univ. Grenoble Alpes, France — [3]XLIM, Univ. Limoges, CNRS (UMR 7252), Limoges, France — [4]Department of Physics and Earth Sciences, Jacobs University Bremen, Germany

It has been shown theoretically and experimentally that twisted bilayer graphenes (TBG), forming Moiré patterns, confine electrons in a tunable way as a function of the angle of rotation of one layer with respect to the other. Since 2018 the discovery of correlated insulators and superconductivity at so-called "magic angles" has stimulated an avalanche of experimental and theoretical activities. In the framework of the Kubo-Greenwood formula for the conductivity, we present tight-binding calculations of quantum diffusion properties in TBG at various angles including the first magic angle. We analyze in particular the effect of static defects, the effect of an electric bias and electron-electron interactions. One of the main results is the decisive role of inter-band transitions [1] in the conductivity of TBG at the magic angle.
[1] G. Trambly de Laissardière et al., Phys. Rev. B **93**, 235135 (2016).

HL 32.6 Tue 15:15 HSZ 201

Fractional quantum Hall states for Moiré superstructures in

the Hofstadter regime — •Bartholomew Andrews and Alexey Soluyanov — Department of Physics, University of Zurich, Winterthurerstrasse 190, 8057 Zurich, Switzerland

We apply a perpendicular magnetic field to the minimal effective two-orbital Fermi-Hubbard model based on a description of the low-energy physics of twisted bilayer graphene at the first magic angle. Through the use of a Peierl's substitution, we determine the Landau level splitting and study the structure of the resulting Chern bands for a range of magnetic flux per plaquette. We identify isolated, topological, and flat bands in the spectrum at low energies. We show that, with the inclusion of a nearest-neighbor density-density interaction, fractional quantum Hall states can be realized solely within these flat bands. Specifically, we characterize the $\nu = 1/3$ Laughlin state through the use of change pumping, spectral flow, entanglement scaling, and CFT edge state counting; and we analyze its dependence on orbital mixing. Ultimately, we comment on the applicability of this model for experiment.

HL 32.7 Tue 15:30 HSZ 201

Kernel Polynomial Method applied to Twisted Bilayer Graphene — Van-Nam Do[1], Duy Nguyen Van[1], Anh Le Hoang[1], and •Dario Bercioux[2,3] — [1]Phenikaa Institute for Advanced Study (PIAS), C1 Building, Phenikaa University, Hanoi 10000, Vietnam — [2]Donostia International Physics Center (DIPC), Paseo Manuel de Lardizbal 4, E-20018 San Sebastián, Spain — [3]IKERBASQUE, Basque Foundation of Science, 48011 Bilbao, Spain

We apply the Kernel Polynomial Method (KPM) [1] for investigating various spectral properties of twisted bilayer graphene. Contrary to standard methods based on Bloch's theorem, with the use of the KPM we can investigate twisted bilayer graphene with any twist angle, commensurate and incommensurate [2]. We show how within the KPM it is possible to study the evolution of a state, initially localized on one of the layers, to the other one. The resulting oscillating behaviour resembles Fabry-Pérot-like oscillations. We show that the characteristic transfer time between the two layers has a minimal dependence on the twist angle [3]. We further show how the chiral structure of twisted bilayer graphene allows for a finite transverse optical Hall conductivity even in the absence of external magnetic fields [4].

[1] Weiße *et al.*, Rev. Mod. Phys. **78**, 275 (2006).
[2] H. A. Le & V. N. Do, Phys. Rev. B **97**, 125136 (2018).
[3] H. Nam Do, H. Anh Le, & D. Bercioux, Phys. Rev. B **99**, 165127 (2019).
[4] V. Nam Do, H. Anh Le, V. Duy Nguyen, S. Ta Ho & D. Bercioux *in preparation.*

HL 33: Optical properties

Time: Tuesday 14:00–16:00 Location: POT 112

HL 33.1 Tue 14:00 POT 112

Influence of edge roughness on the optical properties of ZnSe-based microdisks — •Wilken Seemann[1], Alexander Kothe[1], Gesa Schmidt[2], Alexander Pawlis[2], and Jürgen Gutowski[1] — [1]Institute of Solid State Physics, Semiconductor Optics, University of Bremen, 28359 Bremen, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany

The considerable storage of light in whispering gallery modes (WGM) being favored in microdisk resonators is necessary to achieve low-threshold lasing [1]. It is furthermore an interesting aspect for the use of these resonators in several quantum optical applications where emission centers inside the disk act as single-photon sources or spin-qubits, like quantum memories [2].

We will show micro-photoluminescence (μPL) spectra of WGMs from ZnSe-based quantum well microdisks with diameters in the range of 2.5 to 4 μm and relate their optical properties to structural properties obtained from the analysis of scanning electron microscopy (SEM) images of the disks. We discuss that recutting the disks with a focused ion beam (FIB) can reduce the roughness of their edges and thus lead to better optical quality, i.e. increased light containment.

[1] L. He et al.: Laser & Photonics Reviews 7(1), 2013, 60.
[2] J.I. Cirac et al.: Physical Review Letters 78(16), 1997, 3221.

HL 33.2 Tue 14:15 POT 112

Quantifying Exciton Effects in Graphene Nanoribbons — •Alexander Tries[1,2,3], Paniz Soltani[3], Mischa Bonn[3], Hai I. Wang[3], and Mathias Kläui[1,2] — [1]Institute of Physics, Johannes Gutenberg-University Mainz — [2]Graduate School of Excellence Materials Science in Mainz — [3]Max Planck Institute for Polymer Research, Mainz

Owing to their massless nature, charge carriers in graphene can possess extremely high electron mobility. Yet, its gapless, semi-metallic nature can present a drawback for applications. Recent advances in bottom-up synthesis allows for the atomic control of graphene nanoribbons (GNRs)with well-defined bandgap and optical properties. [1,2]

In these structures, carrier confinement in the lateral dimension induces a bandgap corresponding to visible wavelengths. Owing to the strongly reduced charge screening effect in these atomically flat nanoribbons, strong exciton effects are expected and exciton binding energies in excess of ˜1 eV have been predicted. [3] We will present recent optical ultrafast conductivity studies on atomically precise GNRs using THz spectroscopy, which demonstrates and confirms the strong exciton and charged exciton effects [4]. Time-dependent photoconductivity measurements shed light on the sub- picosecond dynamics of the different quasi-particles.

[1] J. Cai et al., Nature 2010, 466, 470 [2] Z. Chen et al., J. Am.Chem. Soc. 2017, 139, 3635. [3] L. Yang et al., Nano Lett. 2007, 7 (10), 3112 [4] A. Tries et al.,ArXiv:1911.04431

HL 33.3 Tue 14:30 POT 112

Optical Tuning between the Trivial and Topological Regime of InAs/GaSb Quantum Wells — •Manuel Meyer[1], Sebastian Schmid[1], Gerald Bastard[2], Fabian Hartmann[1], and Sven Höfling[1] — [1]Technische Physik, Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Am Hubland 97074 Würzburg, Germany — [2]Département de Physique, Ecole Normale Supérieure de Paris, 75005 Paris, France

Topological Insulators (TI) are a state of matter characterized by an insulating bulk and gapless helical edge states which were first demonstrated on HgTe/CdTe heterostructures[1]. The proposed TI based on composite InAs/GaSb heterostructures are especially appealing due their rich phase diagram that can be accessed via controlling external electrical fields[2]. We present another tuning knob of the phase diagram in InAs/GaSb quantum wells via optical excitation. Under constant illumination the majority charge carrier type switches from electrons to holes. At an intermediate value of illumination time both carrier types are present, indicating electron-hole hybridization[3]. Magnetic fields applied parallel to the surface enable us to determine the topological insulating phase. The optical tuning is caused by the negative persistent photoconductivity of antimonides in combination with a persistent charge carrier accumulation. This paves the way to an optical control of the phase diagramm of InAs/GaSb heterostructures.

[1] M. König et al., Science 318, 766 (2007).
[2] F. Qu et al., Phys. Rev. Lett. 115, 036803 (2015).
[3] G. Knebl et al., Phys. Rev. B 98, 041301(R) (2018).

HL 33.4 Tue 14:45 POT 112

Selective emitters for thermophotovoltaics at 1400 °C — •Alexander Petrov[1,2], Manohar Chirumamilla[1], and Manfred Eich[1,3] — [1]Institute of Optical and Electronic Materials, Hamburg University of Technology, Hamburg, Germany — [2]ITMO University, St. Petersburg, Russia — [3]Institute of Materials Research, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany

In order to tailor thermophotovoltaic emitters to match specific photovoltaic receivers we demostrate spectrally selective emitters that have close to black body emission at short wavelengths and substantially reduced emission at long wavelengths. To emit significant power at the wavelengths usable for photovoltaic conversion (below 2 micron) the far-field emitter should be heated to high temperatures. The development of such thermally stable selective emitters requires strong cooperation between material science and optics, which was possible in the frame of the Hamburg based Collaborative Research Center SFB 986 "Tailor-made multiscale Materials Systems". We demonstrate selective band-edge emitters based on a W-HfO2 refractive metamaterial

and a yttria stabilized ZrO2 opal monolayer on tungsten both stable up to 1400°C. The metamaterial exhibits almost angle independent selective emission due to a topological transition of its isofrequency surface. The monolayer approach, on the other hand, allows keeping the tungsten unstructured and thus demonstrates exceptional emission suppression at longer wavelengths. The physics behind the selective emission of the demonstrated concepts and an outlook for further improvement and enhanced thermal stability will be presented.

HL 33.5 Tue 15:00 POT 112

Chirooptical activity of surface-functionalized CdS nanorods — •Ilka Vinçon, Aksana Svirydava, Simon Prins, Yiou Wang, Jacek Stolarczyk, and Jochen Feldmann — Chair for Photonics and Optoelectronics, Nano-Institute Munich and Department of Physics, Ludwig-Maximilians-Universität (LMU), Königinstr. 10, 80539 Munich, Germany

Excitonic transition and subsequent charge separation is a key component in photovoltaic studies, as well as in solar water splitting. Introducing chirooptical properties in semiconductor nanocrystals via surface functionalization with chiral molecules has emerged as a promising tool to generate a new class of polarization sensitive materials with potential applications for spintronics, enantioseparation and more. To achieve basic control of chirooptical properties, there is a need to fundamentally understand the mechanism of chirality transfer between a chiral ligand and a nanocrystal's surface. We have chosen CdS nanorods as a suitable material with well-defined excitonic transitions. Circular dichroism (CD) has been induced in the excitonic transitions via surface functionalization with chiral ligands. Since the binding motif seems to play a key role in the chirality transfer, ligands with different anchor groups were attached to the surface of the CdS nanorods. Their influence on optical properties was probed via absorption, photoluminescence and CD spectroscopy.

HL 33.6 Tue 15:15 POT 112

Spectroscopic investigation of the radiative efficiency of ordered GaAs/(In,Ga)As core/shell nanowire arrays — •Michał Góra, Miriam Oliva, Jesús Herranz, Manfred Ramsteiner, Lutz Geelhaar, and Oliver Brandt — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e. V., Hausvogteiplatz 5-7, 10117 Berlin, Germany

The vapor-liquid solid growth of GaAs nanowires on Si enables the integration of the III-As semiconductors on a Si platform for optoelectronic applications. In addition, GaAs/(In,Ga)As core/shell nanowires allow us to extend the emission wavelength toward the telecommunication range. An important question for actual applications of these structures is their internal quantum efficiency for longer emission wavelengths. In the present study, we utilize temperature- and power-dependent photoluminescence spectroscopy to investigate the radiative efficiency of ordered GaAs/(In,Ga)As core/shell nanowire arrays synthesized by molecular beam epitaxy. The shell consists of either (In,Ga)As quantum wells with different In content or an InAs/(In,Ga)As dot-in-a-well structure. The absolute efficiency is determined by comparison with GaAs/(Al,Ga)As core/shell nanowires with known internal quantum efficiency. Our results show that the internal quantum efficiency of the (In,Ga)As quantum well shell decreases strongly with increasing In content. However, InAs/(In,Ga)As dot-in-a-well shells are found to enable emission wavelengths in the telecommunication O band at 1.26 μm, while maintaining a comparatively high quantum efficiency up to room temperature.

HL 33.7 Tue 15:30 POT 112

Influence of Amino Acids on the Optical Properties of Cu2O-Amino-Acid Cocrystals — •Mariam Kurashvili[1], Iryna Polishchuk[2], Simone Strohmair[1], Boaz Pokroy[2], and Jochen Feldmann[1] — [1]Chair for Photonics and Optoelectronics, Nano-Institute Munich and Department of Physics, Ludwig-Maximilians-Universität (LMU), Königinstr. 10, 80539 Munich, Germany — [2]Department of Materials Science and Engineering and the Russell Berrie Nanotechnology Institute, Technion - Israel Institute of Technology, 32000 Haifa, Israel

Biomineral systems are composed of organic and inorganic compounds. These materials exhibit highly interesting properties. For example, it was found that hardness of calcite single crystals can be increased via embedding amino acids in its lattice [1]. Also optical properties can be altered by amino acid incorporation, as a recent study of our group showed for zinc oxide [2,3]. Copper oxide is a very versatile direct band gap semiconductor, having promising applications in photovoltaics and water splitting. In this context, we report the optical properties of a model biomineral system consisting of copper oxide-amino acid cocrystals. We use steady state and time resolved photoluminescence spectroscopy, along with scanning electron microscopy to elucidate the changes, which are induced by different concentrations of amino acids in copper oxide. Our study emphasizes the great impact of amino acids on the optical and thus intrinsic structural properties of copper oxide.

[1] Y. Kim. et al., Nature Mat. 15, 903 (2016)
[2] A. Madathumpady et al., J. Phys. Chem. C 122, 6348 (2018)
[3] A. Brif et. al. Adv. Mater., 26, 477–481 (2014)

HL 33.8 Tue 15:45 POT 112

Anomalous Raman Scattering in Lead salts — •Nimrod Benshalom[1], Olle Hellman[2], and Omer Yaffe[1] — [1]Weizmann Institute of Science, Rehovot, Israel — [2]Linköping University, Linköping, Sweden

I present experimental evidence for the violation of symmetry constraints in the Raman spectra of rock-salt Lead-Chalcogenides.

The theoretical framework describing Raman scattering relies almost entirely on the harmonic approximation. In the standard (harmonic) Raman picture an incident photon inelastically scatters by either absorbing or emitting a quantum of energy into a vibrational normal mode excitation, or phonon. The phonon itself is a construct of the harmonic approximation.

Given well-defined normal modes, group-theory translates symmetry considerations into selection rules for the kind of allowed light-matter scattering events. In some crystal structures, like rock-salt, symmetry forbids any single phonon Raman scattering.

Using polarization dependent measurements, we observe two new low-frequency modes consistent with a reduced effective symmetry. These modes persist across the Lead-Chalcogenides series, following a number of curious spectroscopic trends. I discuss this anomalous Raman activity as the result of anharmonic temperature activated symmetry breaking.

HL 34: Functional semiconductors for renewable energy solutions II (joint session HL/CPP)

Time: Tuesday 14:00–15:30 Location: POT 151

HL 34.1 Tue 14:00 POT 151

Small-polaron transport and the role of defects in $BiVO_4$ photoanodes for solar water splitting — •Tim F. Rieth, Viktoria F. Kunzelmann, and Ian D. Sharp — Walter Schottky Institute and Physics Department, TU Munich, Garching, Germany

Photoelectrodes can provide a route to a renewable energy supply by absorbing solar light and, thereby, drive an electrochemical reaction to produce chemical fuels. Bismuth vanadate ($BiVO_4$) exhibits the necessary properties for solar water splitting, namely visible light absorption, efficient charge carrier separation and well positioned band edges, and is the highest performing oxide photoanode to date [1]. Despite these advantages, the performance of $BiVO_4$ is inhibited by a low charge carrier mobility caused by small-polaron formation [2]. In our work, we investigate the limiting thermally activated hopping transport of small-polarons by the determination of the associated energy barrier E_h with temperature-dependent conductivity measurements on polycrystalline $BiVO_4$ thin films. Furthermore, we study how E_h is impacted by intentionally introduced defects such as vacancy defects and hydrogen impurities, which has been shown to greatly enhance the conductivity of $BiVO_4$ [3]. An improved understanding of charge carrier transport and its modification by defects can help to increase the performance of $BiVO_4$ and gives insights that aid in the development of new metal oxide photoelectrodes.

[1] I.D. Sharp et al., ACS Energy Lett. 2, 139 (2017)
[2] A.J.E. Rettie et al., Appl. Phys. lett. 106, 022106 (2015)
[3] J.K. Cooper et al., Chem. Mater. 28, 5761 (2016)

HL 34.2 Tue 14:15 POT 151

InP(100) surfaces for efficient photoelectrochemical water splitting — •Olfa Dani[1], Mario Kurniawan[2], Agnieszka Paszuk[1], Manali Nandy[1], Andreas Bund[2], and Thomas Hannappel[1] — [1]Institute of Physics, Technische Universitaet Ilmenau, Germany — [2]Institute of Materials Science and Engineering, Technische Universitaet Ilmenau, Germany

To date, III-V semiconductor device structures enable the highest solar-to-hydrogen efficiencies. In this approach, a detailed understanding of the reactions at the semiconductor-electrolyte interface is essential to design the semiconductor surface for efficient charge transfer [1]. In this work, we studied the atomic structure of InP(100)-based photocathode surfaces before and after exposure to an aqueous electrolyte. The preparation of P- or In-rich surfaces on p-type InP(100) wafers with metal organic vapor phase epitaxy (MOVPE) was monitored in situ with reflection anisotropy spectroscopy (RAS). After contamination-free transfer from an MOVPE reactor to ultra-high vacuum, the surface structures were characterized by photoelectron spectroscopy (PES) and low-energy electron diffraction (LEED). Subsequently, the samples were transferred under nitrogen gas to a sealed photoelectrochemical cell for photocurrent density-potential measurements. In order to resolve changes in the surface chemistry and structure after exposure to the electrolyte, the samples were analyzed again by RAS, PES and LEED. For comparison, the same measurements were performed on InP(100) wafers with a native oxide layer. [1] M. M. May et al., J. Phys. Chem. C 118 (2014) 19032.

HL 34.3 Tue 14:30 POT 151

Random structure search: Solving the kesterite-stannite puzzle in $(Cu,Ag)_2ZnSnSe_4$ solid solution — •Daniel Fritsch[1] and Susan Schorr[1,2] — [1]Department Structure and Dynamics of Energy Materials, Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Department of Geosciences, Freie Universität Berlin, Malteserstr. 74−100, 12249 Berlin, Germany

$Cu_2ZnSnSe_4$ and $Ag_2ZnSnSe_4$ are both crystallising in the kesterite structure with the structurally similar stannite structure being energetically slightly less favourable. In the solid solution, however, there is experimental evidence that for some intermediate concentrations the stannite structure is energetically favoured. This behaviour is so far not understood.

Here, we're using density functional theory calculations to shed some light into the structure-property relations in $(Cu,Ag)_2ZnSnSe_4$. In order to simulate the different concentrations within the solid solution, we're employing the supercell approach based on the respective end members in the kesterite and stannite structure. The Ag and Cu cations are distributed randomly within the supercell, thereby creating several structure models for the solid solutions for further analysis. All random structure models are geometry optimised employing the recently developed SCAN functional. In order to obtain more reliable electronic and optical properties, selected optimised structures are subjected to single-shot calculations employing the more accurate hybrid functional HSE06.

HL 34.4 Tue 14:45 POT 151

Photocatalytic performance of ALD-functionalized Nanoporous Anodic Alumina Photonic Crystals — •Carina Hedrich[1], Siew Yee Lim[2], Abel Santos[2], Robert H. Blick[1], and Robert Zierold[1] — [1]Center for Hybrid Nanostructures (CHyN), Universität Hamburg, 22761 Hamburg, Germany — [2]School of Chemical Engineering and Advanced Materials / Institute for Photonics and Advanced Sensing (IPAS) / ARC Centre of Excellence for Nanoscale BioPhotonics (CNBP), The University of Adelaide, South Australia 5005, Australia

Nanoporous anodic alumina (NAA) membranes feature self-organized, highly ordered pores with distinct geometrical characteristics. Modifying the electrochemical anodization parameters and applying pulse-like anodization profiles tailors the pore morphology from straight to modulated structures such as distributed Bragg reflectors or gradient index filters. The photocatalytic performances of these photonic crystals (PCs) can be enhanced by functionalizing the surface with photocatalytically active materials (e.g. TiO_2, ZnO, WO_3) or tuning the photonic stopband of the NAA by adapting the pore morphology. Herein, thickness-controlled surface modifications of NAA-PCs by atomic layer deposition (ALD) are conducted and the photocatalytic properties of these structures are investigated by studying the photodegradation of methylene blue. Optimizing and combining these different preparation strategies to further improve the photocatalytic efficiency and to tune the wavelength selectivity of NAA-PCs could expand their utilization as tailor-made photocatalysts.

HL 34.5 Tue 15:00 POT 151

Thermoelectric transport properties of mesoporous silicon and mesoporous silicon - poly(3,4-ethylenedioxythiophene) hybrids — •Haider Haseeb[1,2], Danny Kojda[1], Klaus Habicht[1,2], and Tommy Hofmann[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie Gmbh, Hahn-Meitner-Platz 1, 14109 Berlin — [2]Universität Potsdam - Institut für Physik, Karl-Liebknecht-Straße 32, 14476 Potsdam

This presentation studies thermoelectric transport in mesoporous silicon (pSi) and mesoporous silicon-poly(3,4-ethylenedioxythiophene) (pSi-PEDOT) hybrids. We comprehensively explain electrochemical etching of pSi and infiltration of PEDOT based polymer blends (PEDOT:PSS, PEDOT:Tos) into pSi by dip- and drop-casting and vapor-phase polymerization. Surface sensitive SEM and volume sensitive nitrogen sorption isotherms probe morphological features such as pore size distributions, specific surfaces and porosities of as-etched pSi and pSi-PEDOT hybrids. Macroscopic transport measurements determine electrical and thermal conductivity, Hall mobility, charge carrier concentration and Seebeck coefficient of pSi, PEDOT, and pSi-PEDOT hybrids. We compare the temperature dependent thermoelectric performance of pSi-PEDOT hybrids with the properties of the corresponding inorganic and organic bulk systems. Our quantitative data analysis of charge and heat transport focuses on effective medium models.

HL 34.6 Tue 15:15 POT 151

Impact of *p*-doping on the electronic and optical properties of copper iodide — •Michael Seifert, Claudia Rödl, and Silvana Botti — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

The lack of viable *p*-type transparent conductors represents a critical bottleneck for future transparent electronics. CuI, with its direct band gap of 3.1 eV and its demonstrated *p*-type conductivity, is a promising candidate for such a material. Recently, it has raised significant renewed interest due to the production of transparent conducting bipolar CuI/ZnO heterostructure diodes, its applications as hole collection layer in organic electronics, or as promising candidate for a flexible, transparent thermoelectric material.

The possibility to enhance and tune key properties of the material is a major step towards potential technological applications. One ansatz to achieve this is substitutional doping. In a recent study by Graužinytė *et al.*, PCCP **21**, 18839 (2019), the chalcogen elements have been identified as promising candidates for *p*-type doping of CuI, due to thermodynamically accessible transition levels to a hole-generating charge state ($q = -1$). Here, the effect of such *p*-doping on the electronic structure and absorption spectrum is explored in the framework of density-functional theory and the properties of the doped material are compared to those of pristine CuI.

HL 35: Perovskite and photovoltaics II (joint session HL/CPP)

Time: Tuesday 14:00–16:00 Location: POT 251

HL 35.1 Tue 14:00 POT 251

Temperature-dependent exciton-phonon coupling in CsPbBr3 crystal using ultrafast two-dimensional electronic spectroscopy — •Xuan Trung Nguyen[1], Daniel Timmer[1], Yevgeny Rakita[2], David Cahen[2], Alexander Steinhoff[3], Frank Jahnke[3], Christoph Lienau[1], and Antonietta De Sio[1] — [1]Institut für Physik, Carl von Ossietzky Universität, Germany — [2]Weizmann Institute of Science, Israel — [3]Institut für Theoretische Physik, Universität Bremen, Germany

Halide perovskites (HaPs) are promising semiconductor materials for developing efficient solar cells. It is, however, still debated how the un-

usual electron-lattice couplings in these materials affect their optical and electronic properties. Here, we investigate the temperature dependence of near band gap optical transitions in CsPbBr3 single crystals by 10fs-time-resolution two-dimensional electronic spectroscopy (2DES). At room temperature, the 2DES maps show rapid charge carrier relaxation within the continuum and the concurrent build-up of exciton screening by free carriers on a <30fs time scale [1]. At 70K, we detect large, persistent oscillations of both amplitude and resonance energy of the exciton peak with periods corresponding to the phonon modes of the lead-halide sublattice. Our results point to strong exciton-phonon couplings and to the importance of many-body interactions for the optical and transport properties in HaPs.

[1] Nguyen, X.T., et al., JPCL, 10, p. 5414-5421, 2019.

HL 35.2 Tue 14:15 POT 251

Solution-Processed Two-Dimensional Materials for Perovskite Optoelectronics — •Antonio Gaetano Ricciardulli[1,2], Paul Blom[2], and Michael Saliba[1] — [1]Technische Universität Darmstadt, Darmstadt, Germany — [2]Max-Planck-Institut für Polymerforschung, Mainz, Germany

The efficiency of perovskite based perovskite solar cells and light-emitting diodes (PSCs and PLEDs, respectively) is limited by hole injection/transport and high leakage current, generated by a high hole injection barrier and poor perovskite morphology, respectively. Black phosphorus (BP), a newly emerged 2D layered semiconductor, is endowed with thickness-dependent bandgap, which spans from 0.3 eV (bulk) to 2.0 eV (monolayer). Hence, by carefully selecting the appropriate thickness, BP can be used as interlayer to enhance charge transport and injection in either PLEDs or PSCs. As a proof of concept, we reported a feasible strategy to reduce both hole injection barrier and defects at the perovskite interface by introducing 2D BP as hole injection layer in a PeLED stack. A continuous film composed of high*quality, ultrathin, and large BP sheets on top of PEDOT:PSS simultaneously improves the hole injection and morphology of the green*emitting CsPbBr3. Inclusion of BP enhances over 4 times efficiency of CsPbBr3 based PeLEDs. Incorporating BP to enhance the hole injection from PEDOT:PSS might also be of interest to increase the open*circuit voltage of PSCs of which the perovskite absorber has deeper valence band. Currently, we are developing novel PSCs based on 2D materials with specific functionalities.

HL 35.3 Tue 14:30 POT 251

Ultrafast vibrational dynamics in lead halide perovskites — •Ajay Jha[1], Hong-Guang Duan[1], Vandana Tiwari[1], Golibjon Berdiyorov[2], Alexey Akimov[3], Pabitra Nayak[4], Zheng Li[1], Hernry Snaith[4], Michael Thorwart[5], Mohamed Madjet[2], and R. J. Dwayne Miller[1,6] — [1]MPSD, Hamburg — [2]Qatar Environment & Energy Research Institute, Doha — [3]Department of Chemistry, State University of New York — [4]Department of Physics, University of Oxford — [5]I. Institut für Theoretische Physik, University of Hamburg — [6]Departments of Chemistry and Physics, University of Tornoto

Hybrid organic-inorganic perovskites have gathered much attention owing to their unprecedented success in photovoltaics. To unravel the secrets to this success, we have studied the ultrafast dynamics of lead halide perovskites using heterodyne-detected transient grating and 2D spectroscopy in thin films for tetragonal (room temperature) and orthorhombic phases (T = 20 K). Our measurements capture the different ultrafast exciton dynamics in two phases of perovskite. In addition, we distinctly observe the ground and excited state vibrational modes corresponding to organic and inorganic sub-lattices in two phases. The interplay of strongly coupled dominant vibrational modes to ultrafast carrier generation process will be discussed. To rationalize our observations, we have employed density functional theory (DFT) predicting changes in the vibrational observations highlighting the importance of interaction between organic cation and inorganic sub-lattice in stabilization of charges upon photoexcitation.

HL 35.4 Tue 14:45 POT 251

Lead-free co-evaporated perovskites for photovoltaic applications. — •Tim Schramm, Martin Kroll, Frederik Nehm, Zongbao Zhang, Karl Leo, and Yana Vaynzof — Dresden Integrated Center for Applied Physics and Photonic Materials(IAPP), Technische Universität Dresden

The performance of lead-based perovskites has dramatically increased over the past decade reaching power conversion efficiencies of over 25%. Despite these remarkable advances, lead-based perovskite suffer from serious challenges, most notably lead related toxicity and poor stability, which remain significant obstacles for their integration into industrial applications.

One promising route to circumvent these issues is by turning to novel absorber material systems such as the lead-free double perovskites. Herein, we present our recent results on the formation of $Cs_2AgBiBr_6$ perovskites by thermal evaporation. In particular, we employ a triple-source co-evaporation of the precursor materials, followed by thermal annealing and characterize their microstructure, crystallinity and optical properties. We identify processing conditions that lead to high quality crystalline films with large domains and investigate their performance in photovoltaic devices. Our results pave the route for further development of double perovskites for optoelectronic applications.

HL 35.5 Tue 15:00 POT 251

Ion Migration Induced Modification of the Interfacial Energetics in Perovskite Solar Cells and its Effect on Device Performance — •Joshua Kress[1,3,4], Qingzhi An[1,3,4], Nir Tessler[2], and Yana Vaynzof[1,3,4] — [1]TU Dresden — [2]Technion, Haifa — [3]Integrated Center for Applied Physics and Photonics — [4]Center for Advancing Electronics Dresden

The migration of ions in perovskite materials has been linked to many negative phenomena such as hysteresis and device degradation. Herein, we demonstrate that, under certain conditions, the migration of ions may also lead to an improvement in device performance. Specifically, by performing ultra-violet photoemission spectroscopy depth profiling experiments, we show that upon the application of an electric field during PV characterization of MAPbI3 inverted architecture solar cells, the migration of iodine ions to the interface between the perovskite active layer and electron extraction layer results in the modification of the electronic structure at that interface. The increase in the density of iodine ions leads to a band bending, resembling the electronic structure of iodine-rich overstoichiometric MAPbI3 films. This change in the interfacial electronic structure results in a significant enhancement of the built-in potential and open-circuit voltage of the photovoltaic cells in subsequent measurements, commonly observed by researchers in the field. Finally, our results are corroborated by numerical device simulations which include the presence and migration of ions.

HL 35.6 Tue 15:15 POT 251

Reduction of s-shape formation induced by transparent top-contact sputter deposition in Perovskite solar cells — •Marlene Härtel[1,2], Ruslan Muydinov[1], Steve Albrecht[1,2], and Bernd Szyszka[1,2] — [1]Technische Universität, Berlin, Deutschland — [2]Helmholtz-Zentrum, Berlin, Deutschland

Depositing transparent top electrodes in Perovskite tandem solar cells without adequate buffer layers leads to damaging of the sensitive organic charge transport layers (CTL), due to harsh conditions during the sputter process. However, commonly used buffer layers utilize thermal atomic layer deposition, which is time consuming and could induce reactions with moisture. Therefore, direct sputter deposition is preferred, but sputter damage is mirrored in an s-shaped current-voltage characteristic, accompanied by a fill factor loss. In this contribution, the origin of the s-shape is analyzed by employing photoluminescence, and intensity and temperature dependent current-voltage measurement, and identified as an energetic barrier, which is formed at the CTL. The findings are supported by electrical simulations based on SCAPS. Moreover, two different sputter deposition techniques, namely radio-frequency magnetron and hollow cathode gas flow sputtering, are implemented and compared with regard to their application in damage-free sputter-deposition. By varying sputter process conditions, such as the power, or sample to target position, the s-shape in the solar cell devices can be reduced, thereby improving their electrical performance. Sputter damage-free TCO deposition allows for future enhancements in tandem device fabrication and their commercialization.

HL 35.7 Tue 15:30 POT 251

Structural and optical properties of defect-engineered organic-inorganic halide perovskites — •Chang-Ming Jiang[1], Wen-Yu Cheng[1], Michael Ehrenreich[2], Gregor Kieslich[2], and Ian Sharp[1] — [1]Walter Schottky Institut, Technische Universität München — [2]Fakultät für Chemie, Technische Universität München

Incorporating large organic cations into the ABX3 hybrid perovskite is known to yield the so-called 'hollowed perovskite' structure. To accommodate the oversized cation onto the A-site, certain concentrations of B2+ cation and X- anion vacancies form. The presence of these point defects and associated dangling bonds are expected to

affect the electronic properties, charge carrier dynamics, and phase stability. In the case of FASnI3, incorporation of ethylenediammonium (en2+) cations enlarges the optical bandgap and significantly improves the photovoltaic efficiency and stability. In this work, we aim at understanding the composition-dependent optical properties and relative phase stability in the defect-engineered (en)MAPbI3 system. Thin films with tunable bandgaps from 1.60-1.85 eV are fabricated, and the non-radiative recombination pathways associated with intentionally added point defects are studied by time-resolved PL techniques. Additionally, by measuring temperature dependence of PL, we find that both the orthorhombic-to-tetragonal and tetragonal-to-cubic phase transition temperatures are affected by the extent of large organic cation incorporation. This work sheds light on the interactions between organic cations and the inorganic lattice and provides insights into the defect tolerance in hybrid halide perovskite semiconductors.

HL 35.8 Tue 15:45 POT 251

Band Gap Engineering of Double Perovskite Halides $Cs_2AgBiCl_6$ through Different Sites Alloying — •Dan Han, Masako Ogura, Andreas Held, and Hubert Ebert — Department of chemistry, Ludwig-Maximilians-Universität München, Munich, Germany

Recently, double perovskite halides have been proposed as potential Pb-free photovoltaic materials. However, many experimentally or theoretically reported double perovskite halides have indirect and large band gaps, hindering efficient sunlight absorbing. Thus, tuning the band gap of double perovskite halides is required for their future photovoltaic application. Forming alloys is a practical way for band gap engineering. Here, we presented a systematic study of alloying on different sites for a representative double perovskite halide $Cs_2B'B"X_6$(B'=Ag, B"=Bi, X=Cl) using the fully relativistic Korringa-Kohn-Rostoker (KKR) Green function in combination with the coherent potential approximation (CPA) method. $Cs_2Na_xAg_{1-x}BiCl_6$, $Cs_2AgSb_xBi_{1-x}Cl_6$ and $Cs_2AgBi(Br_xCl_{1-x})_6$ (x=0.25, 0.5, 0.75) all show a band gap bowing behavior, i.e., a nonlinear band gap dependence on the chemical composition. Additionally, we evaluated the mixing thermodynamical stability of $Cs_2AgSb_xBi_{1-x}Cl_6$ and show $Cs_2AgSb_xBi_{1-x}Cl_6$ alloy is thermodynamically stable at room temperature. Bloch spectral functions of alloys with different compositions exhibit broadening due to CPA technique. Alloys at B' and B" sites could tune the finite lifetime of carrier more effectively than alloys at X site.

HL 36: Focus Session: Integrated Quantum Photonics II

The huge impact of semiconductor-based technologies on modern society has resulted from the ability to integrate small functional units or building blocks into integrated circuits with macroscopic functionality. In a similar way, integrated nanophotonic quantum circuits are believed to enable real-world quantum technologies with applications in secure communication, information processing, metrology and sensing.

Organizers: Kai Müller (TU Munich) and Tobias Heindel (TU Berlin)

Time: Tuesday 14:00–15:45 Location: POT 51

Invited Talk HL 36.1 Tue 14:00 POT 51

Towards One-way Quantum Repeaters with Spin Qubits in Nanophotonic Interfaces — •Tim Schröder — Institut für Physik, Humboldt-Universität zu Berlin — Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik

We show progress on theoretical concepts and experimental implementation of *One-Way* Quantum Repeaters. While to date *one-way* quantum repeater proposals rely on a relatively large number of resources, we introduce a scheme that requires only one single photon emitter and two ancilla qubits per communication node. We analyse achievable quantum communication rates and propose a physical implementation that is accessible with today*s technology [arXiv:1907.05101]. On the experimental side, we demonstrate coherent control of single InAs quantum dot electron spins in nanobeam waveguides and show that coherence times reach those of spins in bulk. We furthermore demonstrate nanobeam to fibre coupling efficiencies of 92%; together with waveguide*photon coupling of up to 0.95 this enables highly efficient photonic systems for the generation of multi-photon cluster states. Towards improving waveguide*photon coupling efficiencies beyond 0.95 we introduce a novel waveguide-integrated nanocavity and demonstrate a 30-fold quantum dot lifetime reduction. Finally, we demonstrate that quantum dot spin-photon interfaces in nanobeams are well suited for the demonstration of two-qubit gates, an important requirement for the generation of photonic cluster states. Towards this goal we show that a single waveguide-coupled quantum dot enables spin-state dependent transmission of single photon states.

HL 36.2 Tue 14:30 POT 51

Applications of a Wannier-Stark modulator in waveguide configuration for optical signal regeneration, memory operation and computing in the telecom wavelength range — •Heinz-Christoph Neitzert — Dept. of Industrial Engineering (DIIn), Salerno University, Via Giovanni Paolo II 132, 84084 Fisciano (SA), Italy

Based on an InGaAs/InP superlattice, a Wannier-Stark type EA-modulator has been operated around 1550 nm. A large transmission contrast with low applied voltage changes has been observed. Operating the modulator in a resistor based self-electrooptic effect configuration, a large tunability of the optical transfer function has been achieved by varying the electrical bias voltage and the feedback resistor value. As an example just the functionality of optical thresholding for the noise suppression in a digital optical transmission system and signal frequency multiplication will be shown. Simulation results demonstrate the feasibility to use this type of device for the realization of logic gate operations, like NOR and NAND. Due to the functional completeness theorem this means that in principal every logic functionality can be achieved. The critical parameters during optical computing operations are the optical bias stability and high frequency limitations due to the low-pass filter in the electrical feedback circuit. The waveguiding configuration ensures, however, a good stability and operation at low optical powers.

HL 36.3 Tue 14:45 POT 51

Deterministic integration of single quantum dots into on-chip waveguide devices using in-situ electron beam lithography — •Johannes Schall[1], Peter Schnauber[1], Samir Bounouar[1], Theresa Höhne[2], Anshuman Singh[3], Suk In Park[4], Geun-Hwan Ryu[4], Tobias Heindel[1], Sven Burger[2], Jin-Dong Song[4], Kartik Srinivasan[3], Sven Rodt[1], Marcelo Davanco[3], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, TU Berlin, Berlin, Germany — [2]Zuse Institut Berlin, FU Berlin, Berlin, Germany — [3]NIST, Gaithersburg, United States — [4]KIST, Seoul, Korea

The deterministic integration of quantum emitters into on-chip photonic elements is crucial for the implementation of scalable integrated quantum circuits. We report on the single step deterministic integration of QDs into on-chip WGs using in-situ EBL. We realize multimode interference (MMI) splitters acting as 50/50 coupling elements and demonstrate the functionality by μPL spectroscopy and photon cross-correlation [1]. Furthermore, we integrate InAs QDs as single-photon sources in SiN WGs. Our deterministic fabrication approach guarantees the precise alignment of InAs QDs in the center of a GaAs Tapers, injecting photons in the SiN WGs underneath. In quasi-resonant p-shell excitation, we demonstrate the generation of indistinguishable photons from a single InAs QD in a hybrid quantum photonic device with a post-selected Hong-Ou-Mandel visibility of 0.89 [2].

[1] Schnauber et al., Nano Letters 18 (4), 2336 (2018)
[2] Schnauber et al., Nano Letters 19 (10), 7164 (2019)

HL 36.4 Tue 15:00 POT 51

Voltage dependent photoluminescence of GaAs/AlGaAs quantum dots — •Nandlal Sharma, Robert Keil, Caspar Hopfmann, and Oliver G. Schmidt — Institute for Integrative

Nanosciences, Leibniz Institute for Solid State and Material Research (IFW), Helmholtzstraße 20, 01069 Dresden, Germany

The semiconductor quantum dots (QDs) are promising candidate for high quality photon sources and the biexciton cascade decay in such dots is most advanced technique for the generation of entangled photon pairs. In this work the GaAs/AlGaAs QDs are grown by droplet epitaxy in a n-i Schottky diode structure. The back contact is prepared by thermal diffusion and top contacts is prepared by deposition of semi-transparent 2 nm/4 nm Cr/Au metals. The optical emission (photoluminescence) from different charging state of a GaAs QDs is controlled by application of external bias. The voltage dependent photoluminescence spectrum is recorded at 4K. The effect of external bias on the fine structure splitting and coherence time is studied.

Invited Talk HL 36.5 Tue 15:15 POT 51

Classical computing with quantum states of light — •Stefanie Barz — University of Stuttgart, Germany

Secure delegated computing is a key task for both classical and quantum networks. There exist both classical and quantum protocols for performing secure (quantum) computations in networks.

In this talk, I will show how to use quantum states of light for computing in such networks.

Here, each party in the network has limited computational resources; quantum states increase the computational power of the individual parties. As particular examples, I will show how single qubits and XOR gates allow for universal classical computation. Further, I will demonstrate how quantum resources and linear classical processing enable non-linear computation.

Finally, I will show proof-of-concept implementations using photonic qubits. Thus, this work highlights how minimal quantum and classical resources can be combined and exploited for classical computing.

HL 37: 2D semiconductors and van der Waals heterostructures IV (joint session HL/DS/O)

Time: Tuesday 14:00–16:00 Location: POT 81

HL 37.1 Tue 14:00 POT 81

Resolving the interlayer charge transfer in van der Waals heterostructures by ultrafast THz emission nanoscopy — •Markus Plankl[1], Martin Zizlsperger[1], Fabian Mooshammer[1], Felix Schiegl[1], Fabian Sandner[1], Markus A. Huber[1], Tom Siday[1], Jessica L. Boland[2], Tyler L. Cocker[3], and Rupert Huber[1] — [1]Department of Physics, University of Regensburg, 93053 Regensburg, Germany — [2]Photon Science Institute, University of Manchester, Manchester M13 9PL, UK — [3]Department of Physics and Astronomy, Michigan State University, 48824 Michigan, USA

In van der Waals heterostructures composed of two transition metal dichalcogenide monolayers, photogenerated electron-hole pairs are spatially separated on ultrafast timescales, giving rise to the formation of interlayer excitons. Yet, the underlying interlayer charge transfer has only been investigated in a spatially averaged manner. Consequently, probing nanoscale transfer efficiencies and tunneling rates has so far remained elusive. Since the tunneling of photoexcited charge carriers between adjacent layers represents an ultrafast current along the out-of-plane direction, a concomitant electromagnetic pulse in the terahertz spectral range is emitted. By combining electro-optic time-domain spectroscopy with near-field microscopy, we resolve this characteristic fingerprint of the interlayer carrier dynamics on the nanoscale with sub-cycle temporal resolution. Thereby, we infer tunneling characteristics, which we relate with the nanoscale conductivity of the heterostructure.

HL 37.2 Tue 14:15 POT 81

Influence of dark states on excitonic spin relaxation in transition metal dichalcogenides — •Malte Selig, Dominik Christiansen, and Florian Katsch — Technische Universität Berlin, Berlin, Germany

Energetically low lying dark exciton states with momenta well above the radiative cone manifest a significant relaxation channel for optically pumped excitons in transition metal dichalcogenides (TMDCs). While they have been demonstrated to influence the optical linewidth [1], lineshape [2], relaxation and luminescence properties [3], they can also be expected to play a crucial role for the spin relaxation of excitons.

Here we present a Heisenberg equation of motion theory for the intervalley exchange coupling, mediating the spin relaxation, and exciton phonon coupling. We demonstrate that the interplay of both mechanisms leads to unintuitive signatures in pump probe experiments where the A transition is pumped and either A or B transition are probed [4]. Additionally we reveal that the presence of energetically low lying dark excitons significantly quenches the efficiency of intervalley exchange coupling [5]. Our theoretical results shine new light on existing experimental data.

[1] M. Selig et al.,Nature Commun. 7,13279 (2016)
[2] D. Christiansen et al., Phys. Rev. Lett. 119, 187402 (2017)
[3] M. Selig et al., 2D Mat. 5, 035017 (2018)
[4] M. Selig et al., Phys. Rev. Research 1, 022007(R) (2019)
[5] M. Selig et al., arXiv:1908.11178 (2019)

HL 37.3 Tue 14:30 POT 81

Kelvin probe force microscopy-based direct measurements of contact resistance in 2D semiconductor thin film transistors — •Aleksandar Matkovic[1], Andreas Petritz[2], Gerburg Schider[2], Markus Krammer[4], Markus Kratzer[1], Michael Gärtner[3], Andreas Terfort[3], Christian Teichert[1], Egbert Zojer[4], Karin Zojer[4], and Barbara Stadlober[2] — [1]Institute of Physics, Montanuniversität Leoben, Leoben, Austria. — [2]Joanneum Research MATERIALS, Institute for Surface Technologies and Photonics, Weiz, Austria. — [3]Institute of Solid State Physics, Graz University of Technology, Graz, Austria. — [4]Institut für Anorganische und Analytische Chemie, Goethe-University Frankfurt, Frankfurt am Main, Germany.

This study aims at direct determination of the contact resistance in MoS_2-based thin film transistors (TFTs). Exfoliated single-crystal flakes of MoS_2 have been used in a bottom-contact TFT configuration. Pyrimidine-containing self-assembled monolayers (SAMs) were employed to tune the work function of gold electrodes. Kelvin probe force microscopy measurements were carried out during operation of the devices in order to directly image potential drops across the channel and to study the influence of different SAM treatments on the contact resistance. By independently imaging potential drops at both, carrier injection and extraction points, we demonstrate the asymmetry of contact resistances in MoS_2-based TFTs, as well as their non-linear and bias-dependent behavior.

HL 37.4 Tue 14:45 POT 81

MOVPE of large-scale 2D-2D heterostructures for optoelectronic applications — Annika Grundmann[1], Clifford McAleese[2], Ben Richard Conran[2], Andrew Pakes[2], Dominik Andrzejewski[3], Tilmar Kümmel[3], Gerd Bacher[3], Kenneth Bo Khin Teo[2], •Michael Heuken[1,4], Holger Kalisch[1], and Andrei Vescan[1] — [1]Compound Semiconductor Technology, RWTH Aachen University, Aachen, Germany — [2]AIXTRON Ltd., Cambridge, United Kingdom — [3]Werkstoffe der Elektrotechnik and CENIDE, University Duisburg-Essen, Duisburg, Germany — [4]AIXTRON SE, Herzogenrath, Germany

Vertical heterostructures of two (or more) different 2D layer provide many fascinating opportunities by combining the unique intrinsic chemical, physical and (opto)electronic properties of 2D materials. Without the need of consideration of lattice matching, a nearly infinite number of potential combinations of 2D layers are possible. Transition metal dichalcogenide (TMDC) monolayers are the most widely studied 2D semiconductors beyond graphene and thus provide a strong basis for understanding the properties of 2D heterostructures. Unlike mechanical exfoliation, direct successive growth of 2D-2D heterostructures requires a controlled synthesis of the respective monolayers with pristine interlayer interfaces and no intermixing of disparate layers. Here, we report on direct successive MOCVD of vertical MoS_2-WS_2 and WS_2-MoS_2 heterostructures as well as MOCVD of WS_2 and MoS_2 onto graphene previously deposited in another MOCVD reactor.

HL 37.5 Tue 15:00 POT 81

Efficient Hot Electron Transfer at Graphene-WS2 van der Waals Bilayers — SHuai Fu and •Hai Wang — Max Planck Insti-

tute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Hybridization of (semi-)metallic and semiconducting monolayers, such as graphene and layered transition metal dichalcogenides (TMDs), enables efficient and sensitive photodetectors, by combing the synergetic properties of strong absorption at exciton resonances in TMDs, efficient charge transfer cross the interfaces and ultrahigh charge mobility in graphene. In spite of the great advance in devices, the fundamental understanding of the mechanism underlying the ultrafast charge flow across the heterostructures lags far behind, and effective means of controlling its efficiency have not been established.

Employing Terahertz spectroscopy, we shed light on the fundamentals of ultrafast interfacial nonequilibrium dynamics in graphene-WS2 van der Waals bilayers. We report an efficient and ultrafast hot electron injection from graphene to WS2, which competes with hot carrier heating process in graphene. We will discuss the mechanism underlying the hot electron charge transfer process, and factors governing its efficiency and lifetime of interfacial charge states, which are critical for efficient optoelectronics (i.e. photodetectors) based on van der Waals heterostructures.

HL 37.6 Tue 15:15 POT 81

Excitation Induced Dephasing in Monolayer Transition Metal Dichalcogenides — •Florian Katsch, Malte Selig, and Andreas Knorr — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, 10623 Berlin, Germany

Exceptionally strong Coulomb interactions in atomically thin transition metal dichalcogenides lead to tightly bound electron-hole pairs (excitons) dominating their linear and nonlinear optical response. The latter involves bleaching [1], energy renormalizations [2], and higher-order Coulomb correlation effects like biexcitons [3] and excitation induced dephasing (EID) [4]. Whereas bleaching, energy renormalizations, and biexcitons are widely investigated, EID in exciton dominated semiconductors so far lacks microscopic calculations. Within a Heisenberg equations of motion formalism we identify the coupling between excitons and exciton-exciton scattering continua as the most prominent process causing EID and sideband formation. Evaluating the EID for single-layers of transition metal dichalcogenides, we find a good agreement with recent experiments [5,6].

[1] M. Selig *et al.*, Physical Review Research **1**, 022007 (2019).
[2] J. Shacklette and S. Cundiff, Physical Review B **66**, 045309 (2002).
[3] E. Sie *et al.*, Physical Review B **92**, 125417 (2015).
[4] H. Wang *et al.*, Physical Review Letters **71**, 1261 (1993).
[5] G. Moody *et al.*, Nature Communications **6**, 8315 (2015).
[6] E. Martin *et al.*, arXiv preprint arXiv:1810.09834 (2018).

HL 37.7 Tue 15:30 POT 81

Dirac physics in honeycomb semiconductors — •Christiaan Post[1], Nathali Franchina Vergel[2], Tomas Meerwijk[1], Jesper Moes[1], Xavier Wallart[2], Guillaume Fleury[3], Ludovic Desplanque[2], Ingmar Swart[1], Christophe Delerue[2], Bruno Grandidier[2], and Daniel Vanmaekelbergh[1] — [1]Debye Institute for Nanomaterials Science, Utrecht, The Netherlands — [2]Institute of Electronics, Microelectronics and Nanotechnology (IEMN), Lille, France — [3]Laboratory for Chemistry of Organic Polymers (LCPO), Bordeaux, France

III-V semiconductor quantum wells have obtained a central place in advanced logics and opto-electronics. In more recent research, the effects of a nano scale geometry forming a periodic scattering potential in the lateral directions of the quantum well have been discussed and calculated. In case of a nano-scale honeycomb geometry, Dirac cones are formed similar as for graphene, creating massless fermions while the semiconductor quantum well band gap remains nearly unaltered.

In this research, we report on the electronic characterization of a modulated InGaAs quantum well with a honeycomb symmetry. The honeycomb symmetry is fabricated by perforating the quantum well with a triangular symmetry using nano-scale lithography. By performing scanning tunneling microscopy experiments, the electronic properties of the sample are intensively investigated, showing the combined electronic properties of a two-dimensional material and Dirac-like features. Muffin-tin calculations support the obtained experimental results, revealing the exciting properties of these novel materials.

HL 37.8 Tue 15:45 POT 81

Structural and electronic properties of twisted MoS_2 bilayers — •Somepalli Venkateswarlu, Andreas Honecker, and Guy Trambly de Laissardière — Laboratoire de Physique Théorique et Modélisation, CNRS (UMR 8089), Université de Cergy-Pontoise, France

Vertically stacked transition metal dichalcogenides of multilayer structures have gained increasing attention because of their fascinating features in electronics and optical properties [1]. We performed calculations of structural and electronic properties of nontwisted and twisted MoS_2 bilayers using first-principle calculations [ABINIT][2] and the tight-binding (TB) method. Our results reveal significant differences in the band structures of twisted and nontwisted ones: the appearance of a crossover between direct and indirect band gap, gap variation, and atomic relaxations. For rather large angles, the band structures are very similar for different rotation angles [3]. For the smallest angles, TB calculations predict some flat bands in the valence band and conduction band. As in twisted bilayer graphene, the corresponding states are localized in the AA stacking region of the Moiré pattern.

[1] E. S. Kadantsev, P. Hawrylak, Solid State Comm. **152**, 909 (2012).

[2] X. Gonze *et al.*, Comp. Mat. Sci. **25**, 478 (2002). https://www.abinit.org.

[3] Z. Wang *et al.*, J. Phys. Chem. C **119**, 4752 (2015).

HL 38: Focus Session: Magnon Polarons – Magnon-Phonon Coupling and Spin Transport (joint session MA/HL)

The coupling of spin waves and atomic lattice vibrations in solid magnetic states, so-called magnon polarons (MPs), can have large impact on spin transport properties as recently explored for spin-Seebeck effect, spin pumping and nonlocal spin transport. This resonant enhancement can be reached when the magnon dispersion is shifted by a magnetic field and crosses the phonon dispersion with sufficient overlap. While initially observed at low temperatures and large magnetic fields, further material and device developments have led to MPs at room temperature and moderate magnetic fields. Thus, MPs become important for the manipulation and amplification of spin currents in spintronic and spin caloritronic devices, e.g. by carrying the spins much further than using uncoupled magnons. This focus session highlights the main important research outcomes for MPs, state-of-the-art techniques to detect MPs, such as Brillouin light scattering and neutron scattering, and to study MP transport, e.g. by spin Seebeck effect and nonlocal spin transport, as well as the investigation of MPsin different material classes such as garnets, ferrites and antiferromagnets. In addition, the excessive theoretical work on MPs performed recently is addressed in this focus session.

Organizer: Timo Kuschel (Bielefeld University)

Time: Wednesday 9:30–13:00 Location: HSZ 04

Invited Talk HL 38.1 Wed 9:30 HSZ 04 **Magnon-polaron transport in magnetic insulators** —

•Benedetta Flebus — University of Texas at Austin, Austin, USA

In this talk, I will introduce the anomalous features in the magnetic field and temperature dependence of the spin Seebeck effect observed by Kikkawa et al. [PRL 117, 207203 (2016)] and explain how they can be interpreted as a signature of magnon-polaron transport.

Specifically, I will discuss how magnetoelastic coupling between magnetic moments and lattice vibrations in ferromagnets can gives rise to magnon-polarons, i.e., hybridized magnon and phonon modes. I will derive a Boltzmann transport theory for the mixed magnon-phonon modes and show that magnon-polaron formation can lead to transport anomalies when the disorder scattering in the magnetic and elastic subsystems is sufficiently different.

Invited Talk HL 38.2 Wed 10:00 HSZ 04

Spin-phonon coupling in non-local spin transport through magnetic insulators — •Rembert Duine — Institute for Theoretical Physics, Utrecht University, Princetonplein 5, 3584 CC Utrecht, The Netherlands — Department of Applied Physics, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands

Long-range spin transport through ferromagnetic and antiferromagnetic insulators has recently been demonstrated. In this talk I will discuss how spin-phonon interactions influence this transport. In the first part of the talk I will discuss how bulk spin-phonon interactions lead to magnon-polaron formation and how this composite boson influences the non-local transport. In the second part, I will discuss how spin-phonon interactions across an interface give rise to long-distance spin transport that is carried purely by phonons.

Invited Talk HL 38.3 Wed 10:30 HSZ 04

Anisotropic transport of spontaneously accumulated magneto-elastic bosons in yttrium iron garnet films — •Alexander A. Serga — Fachbereich Physik and Landesforschungszentrum OPTIMAS, Technische Universität Kaiserslautern, 67663 Kaisersalutern, Germany

It is well known that bosonic quasiparticles as excitons, polaritons or magnons are able to spontaneously form Bose-Einstein condensates (BECs). However, interactions between quasiparticles of a different nature, for example, between magnons and phonons, can significantly alter their properties and, thus, modify the condensation scenarios.

Here, I present a novel condensation phenomenon mediated by the magnon-phonon interaction: a bottleneck accumulation of hybrid magneto-elastic bosons—magnon polarons. Similar to the magnon BEC, the phenomenon is observed in a microwave-driven single-crystal ferrimagnetic film. However, unlike BEC, which is a consequence of equilibrium Bose statistics, the bottleneck accumulation is determined by varying interparticle interactions. Furthermore, the accumulated quasiparticles possess a nonzero group velocity. Our recent 2D transport measurements show the simultaneous formation of a few distinct magnon-polaron groups, which propagate in film plane as spatially localized beams with different group velocities. The role of the magnetoelastic anisotropy in the beam formation and interaction of the accumulated quasiparticles with the magnon BEC are discussed.

Financial support of this work by the European Research Council Advanced Grant "SuperMagnonics" is gratefully acknowledged.

HL 38.4 Wed 11:00 HSZ 04

Formation of magnon polarons in ferromagnetic nanogratings — •Felix Godejohann[1], Alexey Scherbakov[1,2], Serhii Kukhtaruk[1,3], Alexander Poddubny[2], Dmytro Yaremkevych[1], Mu Wang[5], Achim Nadzeyka[4], Dmitri Yakovlev[1,2], Andrew Rushforth[5], Andrey Akimov[5], and Manfred Bayer[1,2] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44227 Dortmund, Germany. — [2]Ioffe Inst., RAS, St. Petersburg, Russia — [3]Dept. of Theo. Phys., V.E. Lashkaryov Inst. of Semiconductor Phys., Kyiv, Ukraine — [4]Raith GmbH, 44263 Dortmund, Germany — [5]School of Phys. and Astronomy, Univ. of Nottingham, UK

In our time-resolved experiments with ferromagnetic nanogratings (NGs), the formation of coherent magnon polarons is confirmed by direct evidence of the avoided crossing effect, as well as by several bright indirect manifestations. The NGs have been produced by focused ion beam milling into a 105 nm-thick $Fe_{0.81}Ga_{0.19}$ film. They have a lateral period of 200 nm and consist of parallel grooves of 100-nm width and 7-21 nm depth milled along the [100]-crystallographic direction. We perform transient magneto-optical measurements in a conventional pump-probe scheme with micron spatial resolution, where the femtosecond pump pulse excites the NGs, while the probe pulse serves to detect coherent lattice and magnetic responses. Using an external magnetic field, the magnon modes can be brought into resonance with the localized phonon modes of the NG resulting in the formation of magnon polarons, where the coupling strength is determined by the spatial overlap of the interacting modes.

Invited Talk HL 38.5 Wed 11:15 HSZ 04

Boltzmann approach to the longitudinal spin Seebeck effect — Piet Brouwer and •Rico Schmidt — Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany

We develop a Boltzmann transport theory of coupled magnon-phonon transport in ferromagnetic insulators. The explicit treatment of the magnon-phonon coupling within the Boltzmann approach allows us to calculate the low-temperature magnetic-field dependence of the spin-Seebeck voltage. We consider both a high-temperature regime, in which magnon and phonon branches are coupled incoherently, and a low-temperature regime, which has strongly coupled magnon-polaron excitations. For the magnetic field dependence of the spin Seebeck voltage in both limits we observe similar features as found by Flebus et al. [Phys. Rev. B 95, 144420 (2017)] for a strongly coupled magnon phonon system that forms magnon-polarons, consistent with experimental findings in yttrium iron garnet by Kikkawa et al. [Phys. Rev. Lett. 117, 207203 (2016)].

Invited Talk HL 38.6 Wed 11:45 HSZ 04

Magnon-polaron excitations in the noncollinear antiferromagnet Mn_3Ge — •Aleksandr Sukhanov — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

In this talk, the detailed inelastic neutron scattering measurements of the noncollinear antiferromagnet Mn_3Ge will be discussed. Time-of-flight and triple-axis spectroscopy experiments showed that the magnetic excitations in Mn_3Ge have a 5-meV gap and display an anisotropic dispersive mode reaching $\simeq$ 90 meV at the boundaries of the magnetic Brillouin zone. The spectrum at the zone center shows two additional excitations that demonstrate characteristics of both magnons and phonons. The *ab initio* lattice-dynamics calculations show that these can be associated with the magnon-polaron modes resulting from the hybridization of the spin fluctuations and the low-energy optical phonons. The observed magnetoelastic coupling agrees with the previously found negative thermal expansion in this compound and resembles the features reported in the spectroscopic studies of other antiferromagnets with the similar noncollinear spin structures.

Invited Talk HL 38.7 Wed 12:15 HSZ 04

Magnon-Polarons in different flavors: (anti)ferromagnetic to topological — •Akashdeep Kamra — Center for Quantum Spintronics, Norwegian University of Science and Technology, Trondheim, Norway

Due to magnetoelastic coupling, magnons and phonons in a magnetic material can combine to form hybrid quasiparticles, inheriting properties from both, called magnon-polarons. In this talk, we will examine and clarify the essential requirements for their hybridization in terms of the typical conservation laws and the nature of the magnetoelastic coupling. This will allow us to deduce the properties, such as spin, of the magnon-polarons thus formed by examining the general symmetries of the material and excitation propagation direction. In carrying out this general discussion, we will refer to the cases of magnon-polarons in ferromagnets as examples. What is their spin? What kind of phonons can the magnons hybridize with? Then, we will apply the general principles developed to the cases of antiferromagnets and topological magnonic insulators thereby demonstrating magnon-polarons with novel, tunable, and chiral properties. We will conclude the discussion with an outlook on some open questions and possible future avenues in this context.

References: [1] A. Kamra, H. Keshtgar, P. Yan, and G. E. W. Bauer. Phys. Rev. B 91, 104409 (2015). [2] H. T. Simensen, R. E. Troncoso, A. Kamra, and A. Brataas. Phys. Rev. B 99, 064421 (2019). [3] E. Thingstad, A. Kamra, A. Brataas, and A. Sudbø. Phys. Rev. Lett. 122, 107201 (2019).

HL 38.8 Wed 12:45 HSZ 04

Topological Magnon-Phonon Hybrid Excitations in Two-Dimensional Ferromagnets with Tunable Chern Numbers — •Gyungchoon Go[1], Se Kwon Kim[2], and Kyung-Jin Lee[1,3] — [1]Department of Materials Science and Engineering, Korea University,

Seoul 02841, Korea — [2]Department of Physics and Astronomy, University of Missouri, Columbia, Missouri 65211, USA — [3]KU-KIST Graduate School of Converging Science and Technology, Korea University, Seoul 02841, Korea

We theoretically investigate magnon-phonon hybrid excitations in two-dimensional ferromagnets. The bulk bands of hybrid excitations, which are referred to as magnon polarons, are analytically shown to be topologically nontrivial, possessing finite Chern numbers. We also show that the Chern numbers of magnon-polaron bands and the number of band-crossing lines can be manipulated by an effective magnetic field. For experiments, we propose to use the thermal Hall conductivity as a probe of the finite Berry curvatures of magnon-polarons. Our results show that a simple ferromagnet on a square lattice supports topologically nontrivial magnon polarons, generalizing topological excitations in conventional magnetic systems.

HL 39: Materials and devices for quantum technology II

Time: Wednesday 9:30–12:45 Location: POT 112

Invited Talk HL 39.1 Wed 9:30 POT 112

Quantum communication with entangled photons from quantum dots — •Rinaldo Trotta — Department of Physics, Sapienza University of Rome, Piazzale Aldo Moro 5, 00185 Rome, Italy

The prospect of using the quantum nature of light for secure quantum communication keeps spurring the search of quantum emitters capable of delivering entangled photons on-demand, with high quality, and efficiency. Despite recent advances, however, the exploitation of deterministic quantum light sources in advanced quantum communication protocols remains a major open challenge. In this talk, I will show that photons generated on-demand by quantum dots can be used to implement a teleportation protocol whose fidelity violates the classical limit for any arbitrary input states [1]. Moreover, I will present the first experimental demonstration of all-photonic entanglement swapping using pairs of entangled photons from a quantum dot [2]. A discussion on future perspectives and challenges will conclude the talk. [1] M. Reindl, et al., Sci. Adv. 4, eaau1255 (2018). [2] F. Basso Basset, et al., Phys. Rev. Lett. 123, 160501 (2019).

HL 39.2 Wed 10:00 POT 112

Tools for the Performance Optimization of Single-Photon Quantum Key Distribution — Timm Kupko[1], Martin v. Helversen[1], Lucas Rickert[1], Jan-Hindrik Schulze[1], André Strittmatter[1,2], Manuel Gschrey[1], Sven Rodt[1], Stephan Reitzenstein[1], and •Tobias Heindel[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany — [2]Institut für Experimentelle Physik,Otto-von-Guericke Universität Magdeburg, 39106 Magdeburg, Germany

Solid-state quantum light sources have the potential to boost quantum communication [1,2]. Here, we report on tools to optimize the performance of quantum key distribution (QKD) implemented with single-photon sources (SPSs). We analyze the performance of a receiver module designed for polarization-encoded QKD using deterministically-fabricated quantum dot SPSs. Exploiting two-dimensional temporal filtering and real-time security monitoring, we analyze the sifted key fraction, the quantum bit error ratio, and $g^{(2)}(0)$ expected in full implementations of the BB84 protocol as a function of the acceptance time-window. This routine enables us to choose optimal filter settings depending on the losses of the quantum channel [3]. Our findings are relevant for the development of QKD-secured communication networks based on quantum-light sources.

[1] T. Heindel et al., New J. Phys. 14, 083001 (2012)
[2] E. Waks et al., Phys. Rev. A **66**, 042315 (2002)
[3] T. Kupko et al., arXiv:1908.02672 (2019)

HL 39.3 Wed 10:15 POT 112

Efficient single photon extraction out of a photonic beer-glass — •Jonathan Jurkat[1], Magda Moczała-Dusanowska[1], Ana Predojevic[2], Niels Gregersen[3], Christian Schneider[1], and Sven Höfling[1] — [1]Technische Physik, Julius-Maximilians Universität Würzburg, 97074 Würzburg — [2]department of Physics, Stockholm University, 106 91 Stockholm — [3]Department of Photonics Engeneering, Technical University of Denmark, 2800 Kgs. Lyngby

We demonstrate the fabrication and functionality of a photonic beer-glass cavity. This device combines the Purcell enhancement of a photonic micro-pillar structure with broadband photonic mode shaping of a vertical, tapered waveguide (sometimes referred to as a photonic trumpet). Our device is based on a MBE grown GaAs/AlGaAs heterostructure containing a low density layer of InAs Quantum Dots. Carefull optimization of the subsequent reactive ion etching step allows us to implement beer-glass shaped photonic microcavities, which support broadband optical resonances and promise efficient photon extraction efficiencies and significant Purcell effects over a spectral range up to 11 nm.

HL 39.4 Wed 10:30 POT 112

Deterministic fabrication of quantum dot single-photon sources with emission in telecom c-band — •Niklas Kanold[1], Andrei Kors[2], Sven Rodt[1], Johann Peter Reithmaier[2], Mohamed Benyoucef[2], and Stephan Reitzenstein[1] — [1]Institute of Solid State Physics, Technische Universität Berlin, Berlin, Germany — [2]Institute of Nanostructure Technologies and Analytics, CINSaT, University of Kassel, Kassel, Germany

The availability of reliable single-photon sources (SPS) with emission wavelength compatible with long-range communication in existing fiber-networks is one crucial requirement to implement large-scale quantum key distribution. Beyond that, applications in quantum metrology and information can profit form the availability of such non-classical light sources. Self-assembled semiconductor quantum dots (QDs) are very attractive candidates to realize on-demand SPS as they combine high emission rates with excellent single-photons purity and high indistinguishability, however almost exclusively at emission wavelengths in the 900-950 nm range. Here, we report on the development of QD SPSs in the InAs/InP-material system with emission at 1.55 micron. The QDs are grown via molecular beam epitaxy and include a back-side on a distributed Bragg reflector. We apply in-situ electron-beam lithography to deterministically integrate such QDs e.g. into mesa structures in order to maximize the photon extraction efficiency. The realized telecom SPSs are studied by optical and quantum optical tools to evaluate for instance the single-photon purity of emission.

HL 39.5 Wed 10:45 POT 112

High-frequency electronics for quantum technologies — •Kai J. Spychala, Alex Widhalm, Björn Jonas, Sebastian Krehs, Dirk Reuter, and Artur Zrenner — Department of Physics, University of Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany

The implementation of quantum effects in computation, simulation, sensing and communication in commercial technology requires a miniaturization and standardization effort which interfaces it with current technology. A very important aspect for scalability is the implementation of state of the art electronics in order to provide a link to the known digital technologies. As quantum phenomena are mostly short-lived and observed under cryogenic environments, robust high-frequency electronics which can operate in the cryogenic regime is needed. Further, the integration between quantum systems and high-frequency electronics plays an important role.
We show results on the ultrafast electric phase manipulation of an exciton qubit [1], the rapid adiabatic passage of an exciton qubit and present a scheme for Ramsey-based optoelectronic sampling. Additionally, we present electronics for a spin-photon interface which consists of a QD molecule controlled by a BiCMOS chip. Our chip generates electric pulses in order to entangle the spins of the electrons trapped in the QD molecule.

Ref: [1] A.Widhalm et al., APL112, 111105(2018)

30 min. break.

HL 39.6 Wed 11:30 POT 112

Spin shuttling in a silicon double quantum dot — •Florian Ginzel[1], Adam R. Mills[2], Jason R. Petta[2], and Guido

Burkard[1] — [1]Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — [2]Department of Physics, Princeton University, Princeton, New Jersey 08544, USA

Motivated by the demand[1] for long and intermediate range interaction in quantum information devices and recent developments[2,3] we theoretically analyze the dynamics of an electron during a detuning sweep in a silicon double quantum dot (DQD) occupied by one electron, and investigate possibilities and limitations of spin transport. Spin-orbit interaction and an inhomogeneous magnetic field which can introduce errors are included in our model. Interactions that couple the position, spin and valley degrees of freedom open a number of avoided crossings in the spectrum allowing for diabatic transitions and interfering paths. The outcome of a spin shuttling protocol is explored by means of numerical simulations and an approximate analytical model based on the solution to the Landau-Zener problem. We find that constructive interference can ensure a high transport fidelity even for a fast protocol. Exploiting destructive interference between different paths the DQD can also act as a spin or valley filter.

This work was supported by the ARO grant W911NF-15-1-0149.

[1] J. M. Taylor *et al.*, Nat. Physics **1**, 177 (2005)
[2] T. Fujita *et al.*, npj Quan. Inf. **3**, 22 (2017)
[3] A. R. Mills *et al.*, Nat. Communs. **10**, 1063 (2019)

HL 39.7 Wed 11:45 POT 112

Purcell enhancement in hemispherical Fabry-Perot fiber-microcavities with InAs-QDs — •Sascha Böhrkircher[1], Stefen Both[1], Thomas Herzog[2], Michael Jetter[2], Simone Luca Portalupi[2], Peter Michler[2], and Thomas Weiss[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, 70550, Stuttgart, Germany — [2]Institut für Halbleiteroptik und Funktionelle Grenzflächen (IHFG), Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, D-70569 Stuttgart, Germany

The Purcell effect is responsible for the modification of spontaneous emission rate of quantum emitters when embedded and resonant with cavities. Recent investigations of quantum-dot (QD) transitions in Fabry-Perot-based fiber microcavities demonstrate clearly the presence of Purcell enhancement [1]. That depends significantly on the resonant states of the cavity and their capability to couple to the QD. We discuss possible limitations of calculating these resonant states within the paraxial approximation [2] by comparing the results with finite-element simulations, and we provide design rules for an optimal Purcell enhancement.

[1] T. Herzog et al. , Quantum Sci. Technol. **3** 034009 (2018)
[2] Dustin Kleckner et al. , Phys. Rev. A, **81** 043814 (2010)

HL 39.8 Wed 12:00 POT 112

Local vibrational modes of Si vacancy spin qubits in SiC — •Z. Shang[1], Y. Berencén[1], A. Hashemi[2], A. Krasheninnikov[1,2], G. Astakhov[1], H-P. Komsa[2], and P. Erhart[3] — [1]Institute of Ion Beam Physics and Materials, HZDR, Dresden, Germany — [2]Department of Applied Physics, Aalto University, Aalto, Finland — [3]Department of Physics, Chalmers University of Technology, Gothenburg, Sweden

Since the first demonstration of promising quantum properties of intrinsic point defects in SiC, they have been used to implement room-temperature quantum emitter as well as to realize quantum sensing. Radiative recombination of these point defects is accompanied by phonon emission due to the interaction with crystal vibrations. This process results in the so-called phonon side band (PSB). A high ratio of the emitted light from the zero-phonon line (ZPL) to the all emitted light, the Debye-Waller factor, is required for the implementation of quantum repeaters. Although the understanding of the PSB is important for quantum applications, it has not been yet investigated systematically in SiC.In this work, we uncover the local vibrational modes of the Si vacancy spin qubits in pristine 4H-SiC. The ZPL and six equally separated phonon replicas are observed in the optically-detected magnetic resonance spectra. We present first-principles calculations of the photoluminescence line-shape, which are in excellent agreement with the experiments. We experimentally obtain the resonance phonon energy and the Debye-Waller factor associated with the Si vacancy qubits. Our approach can be applied to a large variety of optically-active spin defects in wide-bandgap materials.

HL 39.9 Wed 12:15 POT 112

Rectifying the zero-field splitting of the NV centers in silicon carbide — •Timur Biktagirov, Wolf Gero Schmidt, and Uwe Gerstmann — University of Paderborn, Paderborn, Germany

The negatively charged nitrogen-vacancy (NV) center in silicon carbide is an attractive class of spin-triplet qubits, analogous to its counterpart in diamond [1]. One of the key spectroscopic fingerprints of the NV center is the splitting of its spin sublevels in the absence of external magnetic fields [2]. Herein, we show that the theoretical prediction of the zero-field splitting with the density functional theory is challenged by the so-called spin contamination of the two-particle spin density [3]. Subsequently, an efficient scheme to correct the zero-field splitting is devised showing excellent agreement with the experiment.

[1] H. J. Von Bardeleben, *et al.*, *PRB* **94**, 121202 (2016).
[2] T. Biktagirov, W. G. Schmidt, and U. Gerstmann *PRB* **97**, 115135 (2018).
[3] S. Sinnecker, and F. Neese, *J. Phys. Chem. A* **110**, 12267-12275 (2006).

HL 39.10 Wed 12:30 POT 112

Incoherent effects in hot-electron quantum optics — •Lewis Clark[1], Clarissa Barratt[1], Masaya Kataoka[2], and Clive Emary[1] — [1]Joint Quantum Centre Durham-Newcastle, School of Mathematics, Statistics and Physics, Newcastle University, Newcastle upon Tyne NE1 7RU, United Kingdom — [2]National Physical Laboratory, Hampton Road, Teddington, Middlesex TW11 0LW, United Kingdom

Using dynamical quantum dot single electron pumps, high-energy (hot) single electrons may be injected into semiconductor systems both reliably and at a high rate. When combined with energy and time-resolved detection, electrons from these sources provide us with a new platform to probe fundamental semiconductor physics in unprecedented detail.

In this contribution, we discuss coupling single-electron sources into interferometer geometries, such as the Mach-Zehnder interferometer, where the visibility of the quantum interference acts as a sensitive probe of the properties both of the electrons and their environment. We investigate the effect of the uncertainty in injection energy on the phase contributions of the path lengths and quantum point contacts.

We also present theoretical calculations of the decay rate of a hot electron subject to phonon scattering, and determine how these rates are affected by parameters such as the injection energy and the magnetic field. Using our calculations for both phase averaging and phonon rates, we derive strategies for minimising the effects of these processes, thus maximising the quantum-coherent properties of the electrons.

HL 40: Thermal, acoustic and transport properties

Time: Wednesday 9:30–12:30 Location: POT 151

HL 40.1 Wed 9:30 POT 151

Thermal stability of tellurium-hyperdoped silicon — •Mohd Saif Shaikh[1,2], Mao Wang[1], Zichao Li[1,3], Yufang Xie[1,3], Teresa Isabel Madeira[2], Dietrich R.T. Zahn[2], Slawomir Prucnal[1], and Shengqiang Zhou[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, 01328 Dresden, Germany — [2]Semiconductor Physics, Chemnitz University of Technology, 09126 Chemnitz, Germany — [3]Dresden University of Technology, 01062 Dresden, Germany

Si doped with Te, a deep level impurity, at concentrations higher than the solid solubility limit (hyperdoping) was achieved by ion-implantation and nanosecond pulsed laser melting. The resulting material exhibit a strong sub-bandgap optical absorption, showing potential for room-temperature broadband infrared photodetectors. Te-hyperdoped Si is supposed to be meta-stable i.e. Te atoms tend to move out from the substitutional sites forming inactive clusters and precipitates. Here, we examine the thermal stability of Te-hyperdoped Si after furnace annealing. We conclude that the samples are stable up to 400°C for 60 minutes but at higher annealing temperatures Te-impurities tend to form clusters and the sub-bandgap optical ab-

sorption decreases. Rapid thermal annealing was also applied to Te-implanted Si and the results will be compared. Understanding the deactivation process upon thermal annealing is crucial during device fabrication steps, to maintain the satisfactory performance of devices utilizing such chalcogen hyperdoped Si structures.

HL 40.2 Wed 9:45 POT 151

Optimized internal-coordinates Gartstein potential for graphene, boron nitride and their nanotubes — •Francesco Libbi[1], Nicola Bonini[2], and Nicola Marzari[1,3] — [1]Theory and Simulation of Materials (THEOS), École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [2]Physics Department, King's College, London, United Kingdom — [3]National Centre for Computational Design and Discovery of Novel Materials (MARVEL)

The lattice dynamics and, in particular, the quadratic behaviour of the flexural acoustic modes in low-dimensional materials play a fundamental role in their thermo-mechanical and thermal transport properties. A first-principles evaluation of these properties can be computationally very demanding and can be affected by numerical errors which break translational or rotational invariance. In order to overcome these problems in graphene-like materials, we develop an internal-coordinate potential with 13 parameters tuned on first-principles phonon calculations. We show that the potential not only reproduces very well the phonon dispersion of graphene, but that the same potential also describes correctly the vibrational properties of carbon nanotubes of arbitrary diameter and chirality. In addition, it is very easy to modify it adding a cubic term to reproduce the dominant anharmonic force constants. This allows a good estimate of lattice thermal conductivities. The potential form works well also for other 2D honeycomb lattice materials, including the case of hexagonal, polar, boron nitride.

HL 40.3 Wed 10:00 POT 151

Probing curling of current induced electric field in real space in graphene using KPFM — •Sayanti Samaddar[1], Kevin Janssen[1,2], Tjorven Johnsen[1], Zhengzhing Wang[3], Daniel Neumaier[3], Marcus Liebmann[1], and Markus Morgenstern[1] — [1]II. Institute of Physics B, RWTH Aachen University and JARA-FIT, Otto-Blumenthal-Str., 52074 Aachen, Germany — [2]Peter Grünberg Institute (PGI-6,9), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [3]Advanced Microelectronic Center Aachen (AMICA), AMO GmbH, Otto-Blumenthal-Str. 25, 52074 Aachen

We conduct local transport measurements using Kelvin Probe Force Microscopy (KPFM) to investigate gated single layer graphene on SiN (150 nm)/Si substrate at room temperature. This allows us to image two quantities: (1) doping fluctuations and (2) local electric fields due to electric current. As charge neutrality is approached, the initially homogeneous and uniformly directed electric field lines start developing prominent curvature that ultimately lead to inversion at certain locations that are dominated by short range scattering. The inverted electric field implies a local back flow of current i.e. formation of current vortices. These current vortices systematically disappear at high source to drain current. Since vortex formation could be a manifestation of viscous flow of electrons [1], we investigate the plausibility of a hydrodynamic description by deducing the relevant transport length scales, from the gate dependent electric field maps at large gate voltages, taking different possible scattering mechanisms into account.

[1] D.A. Bandurin et al., Science 351, 1055-1057 (2016)

HL 40.4 Wed 10:15 POT 151

Transport properties of natural and synthetic $FeAs_xS_{2-x}$ ($0 \leq x \leq 0.01$) pyrites — •Esteban Zuñiga-Puelles[1,2], Raul Cardoso-Gil[2], Matej Bobnar[2], Igor Veremchuk[2], Cameliu Himcinschi[1], Jens Kortus[1], and Roman Gumeniuk[1] — [1]TU Bergakademie Freiberg, Freiberg, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

Synthetic polycrystalline and natural (Schönbrunn mine, Saxony, Germany) pyrites show comparable electrical resistivities (corresponding to the energy gaps $\sim$ 0.7-0.9 eV) and Seebeck coefficients (-350 to -400 μV K^{-1} at 600 K). On the other hand, their thermal conductivities are similar (*i.e.* nearly temperature independent $\sim$40-20 W m^{-1} K^{-1}) above 200 K. Below this temperature natural pyrite reveal a strong and well pronounced maximum, which became strongly reduced in synthetic samples. Such an effect is caused by much smaller grain size ($\leq$ 100 μm) in synthetic FeS_2, which results in additional scattering mechanisms (*i.e.* on point defect and/or grain boundaries). Therefore, mineral from Schönbrunn is further considered as a model system.

Interestingly, electrical transport properties of pyrites from other mines in Saxony varies from metallic (n-type conductivity) to semiconducting (p-type conductors). To shed light on such a behavior, $FeAs_xS_{2-x}$ ($0 \leq x \leq 0.01$) compounds were synthesized. The increase of As-content x in this system results in a decrease of the electrical resistivity as well as in the shift of the type of conducting mechanism towards hole-like one.

HL 40.5 Wed 10:30 POT 151

Magneto-transport properties via exact solution of the linearised Boltzmann equation — •Francesco Macheda[1] and Nicola Bonini[2] — [1]King's College London, Strand, London, UK — [2]King's College London, Strand, London, UK

Understanding and predicting the electrical and thermal transport in crystalline materials is crucial for the development of a new generation of electronic devices. In solids, transport coefficients can be conveniently calculated via the solution of the linearized Boltzmann transport equation (BTE), where the electronic and vibrational properties of the system, including electron-phonon interactions, are computed using density functional theory. Here we will present our recent developments to compute a wide range of transport coefficients in doped semiconductors and metals, such as Hall and drift mobilities, Seebeck and magneto-Seebeck coefficients and Lorenz number, also including the effects of phonon drag. We will show several examples of these calculations for semiconductors and metals that are of interest for technological applications. We will also discuss the application of this method to mono-layer graphene, whit a particular focus on magneto-transport effects.

HL 40.6 Wed 10:45 POT 151

Photo-induced metal-insulator transition in Cu(d_6-DCNQI)$_2$ single crystals — •Lisa Schraut-May[1], Sebastian Hammer[1], Florian Hüwe[1], and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Low dimensional organic metals based on radical anion salts offer a wide range of exciting electronic as well as photo-physical phenomena. For instance, dicyanoquinonediimine (DCNQI) coordinated by metal atoms forms a complex showing a pronounced metal-insulator transition from the quasi-1D metallic ground state to the Peierls insulating state upon cooling. This transition is accompanied by a conductivity change of up to seven orders of magnitude [1]. By photo-exciting the insulating phase, a reverse Peierls transition occurs back to the metallic state followed by a lattice rearrangement on picosecond time scale [2]. We characterize this photo-induced switching in Cu(d_6-DCNQI)$_2$ single crystals by transient conductivity measurements as function of temperature and light intensity. The underlying mechanisms governing the dynamics of the reverse Peierls transition are characterized by a preliminary phenomenological model based on various decay processes for the excess energy upon photo-excitation. Finally, we will evaluate the potential of this material class for application as ultra-fast photoswitches.

[1] F. Karutz, et al., Phys. Rev. Lett. **81** (1998) 140
[2] B. Smit, et al., Adv. Mater. **31** (2019) 1900652

30 min. break

HL 40.7 Wed 11:30 POT 151

Large non-reciprocal transmission of surface acoustic waves in GaAs coated with epitaxial Fe_3Si film — •Alberto Hernández-Mínguez[1], Ferran Macià[2], Joan Manel Hernàndez[2], Jens Herfort[1], and Paulo Santos[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]University of Barcelona, Barcelona, Spain

Non-reciprocal propagation of sound, that is, the different transmission of acoustic waves traveling along opposite directions, is a challenging requirement for the realization of devices like acoustic diodes and circulators. Here, we demonstrate the efficient non-reciprocal transmission of surface acoustic waves (SAWs) with 3.45 GHz frequency propagating along a GaAs substrate coated with a 50-nm-thick epitaxial Fe_3Si film. Fe_3Si is a binary Heusler-like ferromagnetic metal with potential applications in semiconductor-based spintronic devices. For well-defined orientations of the magnetization in the Fe_3Si film, the magneto-elastic (ME) coupling transfers energy from the acoustic into the magnetic system, thus inducing SAW attenuation. The strength

of the ME coupling depends on the relative angle between magnetization and SAW wave vector, and leads to attenuation differences of up to 20% for SAWs propagating along opposite directions. We attribute the non-reciprocal behavior to the dependence of the magnetization dynamics on the helicity of the elliptically polarized ME field associated to the SAW. Our simulations confirm these results and show that Fe_3Si/GaAs is a promising platform for the realization of efficient on-chip, semiconductor-based non-reciprocal SAW devices.

HL 40.8 Wed 11:45 POT 151

Topological nanomechanical states by band inversion — •Martin Esmann[1], Fabrice R. Lamberti[1], Guillermo Arregui[2], Omar Ortiz[1], Carmen Gomez-Carbonell[1], Pascale Senellart[1], Clivia Sotomayor-Torres[2], Pedro David Garcia[2], Aristide Lemaitre[1], and Daniel Lanzillotti-Kimura[1] — [1]CNRS, Centre for Nanoscience and Nanotechnology (C2N), Palaiseau, France — [2]Catalan Institute of Nanoscience and Nanotechnology (ICN2), Barcelona, Spain

Many concepts studied in nanomechanics to control the confinement and propagation of acoustic phonons were inspired by their counterparts in optics and electronics. In these fields, the consideration of topological invariants has had a great impact for the generation of robust confined states. Here, we introduce this concept of topological invariants to nanophononics [1,2] and experimentally implement a GaAlAs heterostructure supporting a robust topological interface state at 350 GHz. The state is constructed through band inversion[3], by concatenating two semiconductor superlattices with inverted spatial mode symmetries. We experimentally evidenced the mode through Brillouin spectroscopy [1] and study its dynamics by picosecond optical pump-probe spectroscopy [3]. The reported robust topological interface state could become part of nanophononic devices requiring robust resonances such as mass sensors or phonon lasers.

[1] M. Esmann et al., PRB 97, 155422 (2018). [2] M. Esmann et al. PRB 98, 161109(R) (2018). [3] M. Xiao et al., Phys. Rev. X 4, 021017 (2014). [4] G. Arregui et al. APL Photonics 4, 030805 (2019).

HL 40.9 Wed 12:00 POT 151

Generation and propagation of superhigh-frequency bulk acoustic waves in GaAs — Diego H. O. Machado[1,2], •Antonio Crespo-Poveda[1], Alexander S. Kuznetsov[1], Klaus Biermann[1], Luis V. A. Scalvi[2], and Paulo V. Santos[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany — [2]UNESP, Department of Physics, 17033-360 Bauru (SP), Brazil

Coherent superhigh-frequency (SHF) vibrations provide an excellent tool for the modulation and control of excitations in semiconductors. Here, we investigate the piezoelectric generation and propagation of longitudinal bulk acoustic waves (LBAWs) with frequencies up to 20 GHz in GaAs crystals using monolithic bulk acoustic-wave resonators based on piezoelectric thin ZnO films. The transducers are used to investigate the propagation of the LBAWs in the frequency and temperature ranges from 1 to 20 GHz and 10 and 300 K, respectively. We find that the acoustic absorption of GaAs in the temperature range from 80 K to 300 K is dominated by scattering with thermal phonons. In contrast, at lower temperatures, the acoustic absorption saturates at a frequency-dependent value. Experiments carried out with different propagation lengths indicate that the saturation is associated with losses during reflections at the sample boundaries. We also demonstrate devices with a high quality factor fabricated on top of acoustic Bragg reflectors. These findings prove the feasibility of high-quality acoustic resonators embedding GaAs-based nanostructures, opening exciting new technological opportunities, such as acoustic carrier control and nanomechanics in the SHF range.

HL 40.10 Wed 12:15 POT 151

Brillouin scattering in optophononic micropillar resonators at 300 GHz — •Martin Esmann[1], Fabrice R. Lamberti[1], Abdelmounaim Harouri[1], Isabelle Sagnes[1], Carmen Gomez-Carbonell[1], Ivan Favero[2], Olivier Krebs[1], Loïc Lanco[1], Aristide Lemaitre[1], Pascale Senellart[1], and Daniel Lanzillotti-Kimura[1] — [1]CNRS, Centre for Nanoscience and Nanotechnology (C2N), Palaiseau, France — [2]Matériaux et Phénomènes Quantiques, CNRS, Université Paris Diderot, Paris, France

Inelastic scattering of light by acoustic phonons has potential for tailored optical frequency combs, narrow-line lasers [1], and all-optical data storage [2]. To be efficient, these applications require strong optical fields featuring a large overlap with the acoustic modes. So far, patterned waveguides and photonic crystal fibers allow tailoring the acoustic spectrum up to few tens of gigahertz.

Here, we introduce a monolithic Brillouin generator [3] based on a high-frequency nanoacoustic GaAlAs resonator operating at 300 GHz, which is embedded inside an optical micropillar cavity. This decouples the design of the Brillouin spectrum and the optical device. We develop a free-space filtering technique to detect the generated Brillouin signals. The micropillars could be readily integrated into fibered and on-chip architectures, and are compatible with epitaxial quantum dots, making them relevant for quantum communication.

[1] N. T. Otterstrom et al. Science 360, 1113 (2018).
[2] M. Merklein et al. Nature Commun. 8, 574 (2017).
[3] M. Esmann et al. Optica 6, 854 (2019).

HL 41: Perovskite and photovoltaics III (joint session HL/CPP)

Time: Wednesday 9:30–12:30 Location: POT 251

HL 41.1 Wed 9:30 POT 251

Efficiency dependence on incident angle for CIGS solar cells — •Lilén Vöhringer[1], Janet Neerken[1], Hippolyte Hirwa[1], Jörg Ohland[1], Alfons Weber[2], Robert Lechner[2], Thomas Dalibor[2], Sascha Schäfer[1], and Stephan Heise[1] — [1]Ultrafast Nanoscale Dynamics, Institute of Physics, University of Oldenburg, D-26111 Oldenburg, Germany — [2]Avancis GmbH, Otto-Hahn-Ring 6, D-81739 München, Germany

Facing climate change, renewable energies are becoming more and more relevant. Hence, understanding their mechanisms in detail is important to improve their use. In photovoltaics, solar cells are used to convert solar energy into electrical energy. In general, the efficiency of a solar cell is measured and compared under standard test conditions, which may vary vastly from real conditions. Hence, it is important to investigate the dependence of the efficiency on different parameters, in order to find the best solar cell for each case of non-standard conditions. One of these parameters is the incident angle of light, which varies according to the suns position, but also depends on the orientation of the solar cell. Its influence on the efficiency is being tested in this study for $Cu(In,Ga)(S,Se)_2$ (CIGS) solar cells using IV-measurements. CIGS solar cells are thin-film solar cells which can reach efficiencies up to 23%. In particular, the role of the front glass for the angular-dependent efficiency is studied by investigating different front glass variations. The measurements show that the efficiency dependence on the incident angle cannot be explained by the reduced photon flux only.

HL 41.2 Wed 9:45 POT 251

Reaching Efficiency Limts for Blue $CsPbBr_3$ based Light Emitting Diodes — •Tassilo Naujoks[1], Thomas Morgenstern[1], Carola Lampe[2], Alexander Urban[2], Matthew Jurow[3], Yi Liu[3], and Wolfgang Brütting[1] — [1]University of Augsburg, 86135 Augsburg, Germany — [2]Ludwig-Maximilians-Universität München, 80539 Munich, Germany — [3]Lawrence Berkeley National Laboratory, Berkeley, CA 94720, United States of America

The unique optical properties of lead halide perovskites have drawn significant attention towards their application in light emitting devices. While quantum yield, emission wavelength and stability are already in the focus of many research groups, the orientation of the emissive transition dipoles is rarely investigated.

In this work, we investigate $CsPbBr_3$ nanoplatelets of variable thickness and determine the orientation of their transition dipole moments from thin film radiation patterns.

We use a thickness variation for nanoplatelets reaching from 2 to 6 monolayers to systematically study the tunability of the TDM orientation and the concomitant color shift, while the emission peak stays as narrow as it is for the green emitting nanocubes. Together with high photoluminescent quantum yields the efficiency limit of lead-halide perovskite based light emitting diodes can be re-estimated.

The present data reveal very promising new efficiency limits, for

solution-processed light emitting diodes: A solution-processed, highly efficient blue emitter with strong horizontal orientation can be made of $CsPbBr_3$ nanoplatelets.

HL 41.3 Wed 10:00 POT 251

Frenkel-Holstein Hamiltonian Applied to Quaterthiophene-based 2D Hybrid Organic-Inorganic Perovskites — •Svenja M. Janke[1], Mohammad B. Qarai[2], Volker Blum[1], and Frank C. Spano[2] — [1]Duke University, Durham, NC, USA — [2]Temple University, Philadelphia, PA, USA

In two-dimensional hybrid organic-inorganic perovskites (HOIPs), both the organic and inorganic components can contribute to the electronic properties at the electronic frontier levels and hence open up a wide area for design of new materials with high tunability. For development of new devices like solar cells or light emitting diodes, the understanding of electronic excitations and their photophysical signatures play a fundamental roll. Here, we show at the example of quaterthiophene-based lead-halide HOIPs that the organic contribution to 2D HOIP absorption and emission spectra can be theoretically investigated employing a Frenkel-Holstein Hamiltonian that treats electronic coupling and electron-phonon coupling on equal footing. We relate changes in the spectra to structural changes in the organic layer that in turn are caused by variation of the halide anion. Furthermore, we take first steps towards including the contribution of the Wannier exciton on the inorganic component into the framework of the Frenkel-Holstein Hamiltonian. Supported by the German Science Foundation (DFG), grant number 393196393.

HL 41.4 Wed 10:15 POT 251

Environmental Stability of High Efficiency PbS Quantum Dot Solar Cells — •David Becker-Koch[1,2], Miguel Albaladejo-Siguan[1,2], Vincent Lami[3], Fabian Paulus[2], Hengyang Xiang[4], Zhuoying Chen[4], and Yana Vaynzof[1,2] — [1]IAPP, TU Dresden, Germany — [2]cfaed, TU Dresden, Germany — [3]KIP, Uni Heidelberg, Germany — [4]ESPCI, CNRS, Université Pierre et Marie Curie, Paris, France

Colloidal inorganic quantum dot (CQD) solar cells (SCs) are an emerging class of photovoltaics, which can be processed from solution at low temperature and their optoelectronic properties can easily be tuned by changing their size, shape and surface passivation. While power conversion efficiencies of ~12% have been demonstrated by employing lead sulphide (PbS) CQDs, their stability remains an unresolved issue preventing them from being integrated into industrial applications. In this work we focus on the influence of different atmospheres on the performance of high efficiency PbS CQDs SCs. We find that while N2 and humidity lead to a quick decline in performance, oxidation dominates the initial improvement and the subsequent deterioration of the device function. By applying a range of spectroscopic methods, we identify the pivotal layer for these processes and furthermore, we propose a model for the performance evolution. We conclude that the stability and performance can be improved by exchanging the extraction layer (EL) ubiquitously used in these devices. Finally, we present several promising organic, semiconducting replacement ELs and show preliminary results of their application as ELs in PbS CQDs solar cells.

HL 41.5 Wed 10:30 POT 251

How does strain impact the solar cell performance at grain boundaries? — •Michael Stuckelberger[1], Irene Calvo-Almazán[2], Martin Holt[2], Megan Hill[3], Siddharth Maddali[2], Mariana Bertoni[4], Xiaojing Huang[5], Hanfei Yan[5], Evgeny Nazaretski[5], Yong Chu[5], Andrew Ulvestad[2], and Stephan Hruszkewycz[2] — [1]DESY, Hamburg, Germany — [2]ANL, Lemont IL, USA — [3]Northwestern University, Evanston IL, USA — [4]ASU, Tempe AZ, USA — [5]BNL, Upton NY, USA

Grain boundaries (GB) often limit the conversion efficiency of polycrystalline solar cells. Strain is particularly detrimental there, as it enhances the defect concentration and band fluctuations, leading to increased recombination rates. Unfortunately, standard methods cannot easily measure the strain distribution in working thin-film devices.

Based on nanodiffraction experiments, we demonstrate the assessment of the strain distribution at sub-100-nm resolution. In a multimodal detector design, we combined nanodiffraction with X-ray fluorescence (XRF) and X-ray beam induced current (XBIC) measurements. Mapping individual grains, this enabled us to correlate point-by-point the strain with composition and performance within grains and at GB.

In CIGS solar cells, we found that the strain increases towards GB, which is accompanied by an increase of the charge collection efficiency. In contrast, we found a decreasing lattice constant towards GB in CdTe solar cells. Similar correlative experiments are ongoing on perovskite solar cells, and we will present the latest results.

30 min. break

HL 41.6 Wed 11:15 POT 251

Tuning Perovskite Halide Content to Engineer Environmental Stability — •Katelyn P. Goetz[1,2], Fabian Thome[1,2], Paul Fassl[1,2], Lukas M. Falk[1,2], Vincent Lami[1,2], Alexander D. Taylor[1,2], Qingzhi An[1,2], Fabian Paulus[1,2], and Yana Vaynzof[1,2] — [1]IAPP, Technical University of Dresden, Germany — [2]CFAED, Technical University of Dresden, Germany

The presence of surface defects in perovskite films has been linked to their stability; however, many questions remain regarding details of the degradation process. Here, we incrementally tune the iodine or bromide content in MAPbI3 or MAPbBr3 thin-films and examine the impact on optoelectronic properties. X-ray photoelectron spectroscopy is used to identify the density and type of surface defect. We examine the interaction of the defect with the environment by exposing the films to controlled levels of oxygen and humidity under light, and monitor changes to the films via photoluminescence (PL) spectroscopy. Here, we observe that, while halide-rich films exhibit lower PL quantum efficiency (PLQE) than halide-poor films, exposure to low levels of oxygen enhances the luminescence of all films. In solar cells, iodine-poor MAPbI3 samples show a tremendous drop in the short-circuit current after exposure to oxygen, while those with excess show no change. The MAPbBr3 solar cells show little dependence of the initial photovoltaic performance on the halide content, but upon exposure to air and light, bromide-deficient solar cells undergo a large Jsc boost, resulting in a near tripling of their initial PCE. These results highlight the strong role that chemical composition plays in stability.

HL 41.7 Wed 11:30 POT 251

Enabling Versatile High-Efficiency Perovskite Photovoltaics by Charge-Selective Contact Design — •Amran Al-Ashouri[1], Artiom Magomedov[2], Marcel Ross[1], Marko Jošt[1], Martynas Talaikis[3], Ganna Christiakova[1], José M. Prieto[1], Eike Köhnen[1], Ernestas Kasparavičius[2], Bernd Rech[1], Tadas Malinauskas[2], Thomas Unold[1], Lars Korte[1], Gediminas Niaura[3], Vytautas Getautis[2], and Steve Albrecht[1] — [1]HZB, Berlin, Germany — [2]KTU, Kaunas, Lithuania — [3]FTMC, Vilnius, Lithuania

By establishing a simple, low-cost and robust perovskite solar cell device structure that employs self-assembled monolayers (SAMs) [1], we realized power conversion efficiencies of over 21 % for single junction cells, over 23 % for CIGSe/perovskite and well over 27 % for silicon/perovskite tandem solar cells. Using time-resolved and absolute photoluminescence spectroscopy together with an analysis of the energetic alignment between hole-selective contact and absorber, we identify design guidelines for an hole-selective interface without non-radiative recombination losses. A SAM model system further allows to study voltage and fill factor losses for an increased understanding of how to experimentally explore pathways towards theoretical efficiency limits.

[1] Al-Ashouri et al. *Energy Environ. Sci.* 2019, **12**, 3356

HL 41.8 Wed 11:45 POT 251

Anharmonicity, short-range correlated disorder, and small Urbach energies in halide perovskites — •Christian Gehrmann and David A. Egger — Department of Physics, Technical University Munich, 85748 Garching, Germany.

Halide perovskites (HaPs) are known to show complex nuclear dynamics and structural effects. But seemingly in contrast to this effects, a low amount of disorder is implied by measurements of small Urbach energies and sharp optical absorption edges. Using density functional theory (DFT) and DFT-based molecular dynamics, we calculated spatial correlations in the disorder potential induced for electronic states due to nuclear dynamics in representative HaPs [1]. We find sizeable anharmonicity in the nuclear vibrations and a dynamic shortening of correlations in the disorder potential: the motion of especially A-site and X-site ions are found to have an important impact on the length of spatial correlations in the disorder potential, such that they become as short as atomic bonds in the material. We explicitly establish that these short-range correlated disorder potentials lead to narrow band-

energy distributions, which imply small Urbach energies. We conclude that effective collection of sunlight in HaP based photovoltaic devices, as indicated by small Urbach energies and sharp optical absorption edges, is facilitated by this mechanism.

[1] C. Gehrmann & D. A. Egger, Nat. Commun. 10, 3141 (2019).

HL 41.9 Wed 12:00 POT 251

Combined Multi-Photon-Excitation and Multi-Exciton-Generation Processes in $CsPbBr_3$ Supercrystals — •Anja Barfüsser[1], Alexander F. Richter[1], Aurora Manzi[1], Shixun Wang[2], He Huang[1], Andrey L. Rogach[2], and Jochen Feldmann[1] — [1]Chair for Photonics and Optoelectronics, Nano-Institute Munich and Department of Physics, Ludwig-Maximilians-Universität (LMU), Königinstr. 10, 80539 Munich, Germany — [2]Department of Materials Science and Engineering and Centre for Functional Photonics (CFP), City University of Hong Kong, Kowloon, Hong Kong

A fundamental problem limiting the power conversion efficiency of solar cells are photons with energies below the band gap, as they cannot be absorbed by linear processes, and above the band gap, as the excess energy typically is lost as heat. Multi-photon-excitation (MPE) and multi-exciton-generation (MEG) target this issue. Up to now, these processes have only been observed independently. Here, their combined effect is demonstrated for bulk-like $CsPbBr_3$ perovskite nanocubes forming a superlattice. For below-band-gap excitation energies (0.5-0.8 E_g) nonlinear absorption is observed. Interestingly, when the energy of multiple below-band-gap photons resonantly matches the energy of multiple excitons, a strong photoluminescence enhancement of up to 10^5 takes place. Excitation power dependent measurements reveal a high-order absorption process deviating from the typical two-photon absorption.

HL 41.10 Wed 12:15 POT 251

The Versatility of Polyelemental Perovskite Compositions — •Michael Saliba — TU Darmstadt

Perovskites have emerged as low-cost, high efficiency photovoltaics with certified efficiencies of 22.1% approaching already established technologies. The perovskites used for solar cells have an ABX3 structure where the cation A is methylammonium (MA), formamidinium (FA), or cesium (Cs); the metal B is Pb or Sn; and the halide X is Cl, Br or I. Unfortunately, single-cation perovskites often suffer from phase, temperature or humidity instabilities. This is particularly noteworthy for CsPbX3 and FAPbX3 which are stable at room temperature as a photoinactive *yellow phase* instead of the more desired photoactive *black phase* that is only stable at higher temperatures. Moreover, apart from phase stability, operating perovskite solar cells (PSCs) at elevated temperatures (of 85 °C) is required for passing industrial norms.

HL 42: Oxide semiconductors

Time: Wednesday 9:30–12:15 Location: POT 51

HL 42.1 Wed 9:30 POT 51

Modelling native defects in transparent conducting oxides using the hybrid QM/MM embedded cluster technique — •Qing Hou, John Buckeridge, Alexey A. Sokol, Jingcheng Guan, and C. Richard A. Catlow — Kathleen Lonsdale Materials Chemistry, Department of Chemistry, University College London, 20 Gordon Street, London WC1H 0AJ, UK

For n-type transparent conducting oxide (TCO) materials such as SnO2, In2O3 and ZnO, native defects play a key role in electronic conductivity. Depending on their electronic structure, energetics and geometries, defects can act as donors, resulting in intrinsic n-type conductivity, or can compensate extrinsic donors such as Sn in In2O3. Predictive modelling of the properties of defects in such systems requires a detailed description of the dielectric response of the host material, which can be difficult to obtain using standard supercell techniques. Here, we employ the hybrid quantum mechanical/molecular mechanical (QM/MM) embedded cluster method, a multi-region approach that allows us to model defects at the true dilute limit, with polarisation effects described in an accurate and consistent manner. Moreover, we develop techniques to analyse the energetic balance between electrons bound to donors in diffuse and compact states, a difficult problem regardless of the model employed. We benchmark our results where possible and find good agreement with experiments for a variety of defect-related properties.

HL 42.2 Wed 9:45 POT 51

CVD based growth of ZnO layers on Si(111) w/ and w/o AlN nucleation layers. — •Raphael Müller[1], Okan Gelme[1], Florian Huber[1], Jan-Patrick Scholz[2], Martin Mangold[1], Alexander Minkow[2], Ulrich Herr[2], and Klaus Thonke[1] — [1]Institute of Quantum Matter / Semiconductor Physics Group, Ulm University — [2]Institute for Functional Nanosystems, Ulm University

The epitaxial growth of high quality zinc oxide (ZnO) layers on silicon (Si(111)) is a challenging task, because the formation of an amorphous SiO_x layer at the interface usually inhibits the growth of a well oriented ZnO layer. One way to circumvent this is the prior growth of a thin AlN nucleation layer, grown by MOVPE. Such nucleation layers were optimized and finally overgrown with ZnO layers under different growth conditions by a chemical vapor deposition (CVD)-based growth method, in order to find the best combination of growth parameters for both processes. The resulting ZnO layer quality was characterized by atomic force microscopy, electron backscattering diffraction, high resolution X-ray diffraction, low temperature photoluminescence and high resolution TEM measurements. A drastic increase in layer quality was observed comparing such layers to those w/o AlN nucleation layer, proofing the critical role of SiO_x at the interface. Growth temperature and thickness of the AlN nucleation are critical parameters, too, and have to be adjusted, as well as the temperature and II/VI-ratio of the ZnO growth. Finally we achieved perfectly aligned ZnO layers with a surface roughness RMS value of $1.2\,nm$, and a FWHM in ω-scan of $715\,arcsec$ for the ZnO (0002) reflection.

HL 42.3 Wed 10:00 POT 51

Magnetic-field-induced second harmonic generation of excitons in Cu_2O — •Andreas Farenbruch, Johannes Mund, Dietmar Fröhlich, Dmitri Yakovlev, and Manfred Bayer — Experimentelle Physik 2, Technische Universität Dortmund, Germany

We report on magnetic-field-induced second harmonic generation (SHG) of higher excitons ($n \geq 3$) of the lowest exciton series in Cu_2O. SHG is allowed for the $1S$ orthoexciton and higher excitons in low symmetry directions (e.g. [111] and [112]). By application of a magnetic field in Voigt geometry SHG gets also allowed for excitation along the [110]-axis. Magnetic-field experiments in Voigt configuration are of special interest, since one expects besides the Zeeman effect also the magneto-Stark effect, which leads to an effective electric field perpendicular to the light propagation and magnetic-field direction. With a group theoretical analysis we derive polarization selection rules for SHG. Of special elegance are 2D polarization diagrams (SHG intensity versus incoming and outgoing polarization angle). By a special choice of the experimental settings one can separate the spectral features due to the Zeeman effect and the magneto-Stark effect or observe an interference of both effects. The SHG signals are large enough to measure the full polarization dependence for the whole spectrum. It is shown, that the magneto-Stark effect dominates the Zeeman effect for higher principal quantum numbers.

HL 42.4 Wed 10:15 POT 51

A Koopman*s compliant exchange correlation potential for semiconductors — •Michael Lorke, Peter Deak, and Thomas Frauenheim — BCCMS, Universität Bremen

Density functional theory is the workhorse of theoretical materials investigations. Due to the shortcoming of (semi-)local exchange correlation potentials, hybrid functionals have been established for practical calculations to describe surfaces, molecular adsorption, and defects. These functionals operate by mixing between semi-local and Hartree-Fock exchange semi-emprically. However, their parameters have to be optimized for every material separately. To treat materials with a more physics driven approach and without the need of parameter optimization is possible with many-body approaches like GW, but at an immense increase in computational costs and without the access to total energies and hence geometry optimization.

HL 42.5 Wed 10:30 POT 51

Investigations on the electronic structure of strongly correlated electron system Cr-doped PrFeO3 — •Anil Kumar. and Pankaj R Sagdeo — Indian Institute of technology Indore, Indore-453552, India

High-resolution powder x-ray diffraction (SXRD), Soft x-ray absorption (SXAS) Raman and optical absorption spectroscopy (OAS) studies have been carried out to estimate the possible correlation between tolerance factor, structural bandwidth (w) , eg electron bandwidth (W) estimated from SXAS and charge transfer parameter (Δ) on one of the strongly correlated system Cr-doped PrFeO3. The present investigation suggests that tolerance factor, w and W scale in a similar fashion with Cr-doping, which infers the governance of these parameters by a common factor. The observed variation in eg electron bandwidth and has been understood in terms of variation in the Fe-O bond length and Fe-O-Fe bond angles with Cr-doping, which enhances the overlapping between Fe-O orbitals. Further, Resonant and power dependent Raman spectroscopy experiments were carried out to understand the origin of local oxygen breathing mode in the mixed Fe-Cr orthorhombic perovskite through the orbital mediated electron-phonon coupling (EPC) mechanism. Thus, by using the combination of SXAS, SXRD, Raman and OAS, a crucial information related to tolerance factor, structural bandwidth, eg electron bandwidth and Δ has been demonstrated. Additionally, present investigations strongly reveal the orbital mediated EPC is not limited to Jahn-Teller active materials and this series can be used as a model for study on orbital mediated EPC.

30 min. break

HL 42.6 Wed 11:15 POT 51

Highly Doped Transparent Conductive Oxides — •Alexander Koch, Jura Rensberg, Martin Hafermann, and Carsten Ronning — Institute of Solid State Physics, Friedrich-Schiller University Jena

Transparent conductive oxides have recently gained a lot of attention for applications in plasmonics and nanophotonics due to their low optical loss, metal-like behavior, tailorable optical properties, and well-established fabrication procedures. In particular, n-type doped zinc oxide (ZnO), such as gallium doped ZnO (GZO) is very attractive, because its dielectric permittivity can be engineered over a broad range from near to far IR. Here we show, that a very high doping concentrations in GZO can be reached by ion implantation and post implantation annealing treatment, where we have to face the competition between dopant activation and dopant diffusion. Furthermore, ion implantation offers the great opportunity to selectively dope ZnO by using appropriate lithography techniques. By this means, subwavelength structure elements, typically used for metasurfaces, fabrication can be formed.

HL 42.7 Wed 11:30 POT 51

Exciton Lattices in Curprous Oxide — •Martin Bergen — Experimentelle Physik 2, Technische Universität Dortmund, D-44221 Dortmund, Germany

Excitons are a heavily studied topic within the field of semiconductor physics and generally well understood. For example they can be created in highly excited states as so called Rydberg-excitons. This specific form of exciton is characterized by a large spatial extension and strong interaction between the excitons as well as external fields. However, currently only a few select materials with comparatively large binding energies like cuprous oxide (Cu_2O) can be effectively studied. In Cu_2O excited states with principal quantum number up to n=25 can be observed, which corresponds to an exciton extension of over $2\,\mu m$. Due to the large dipole-dipole interaction a so called Rydberg-blockade can be observed, which prevents the creation of additional excitons in the vicinity of already existing excitons.
In atom physics optical lattices with cold atoms are an often used tool to study the atom's physics. In analogy to this our most recent findings on the influence of lattices on Rydberg-excitons in Cu_2O will be shown. One example is an enhanced Rydberg-blockade as compared to a homogeneous exciton distributon.

HL 42.8 Wed 11:45 POT 51

H_2S detection for medical breath analysis with surface functionalized ZnO nanowires — •Angelika Kaiser[1], Erick Torres[1], Tanja Mauritz[1], Yujia Liu[1], Florian Huber[1], Ulrich Herr[2], and Klaus Thonke[1] — [1]Institute of Quantum Matter, Ulm University — [2]Institute of Functional Nanosystems, Ulm University

Numerous publications in the past years highlighted the potential importance of hydrogen sulfide (H_2S) detection for therapeutic applications and early diagnostics. It was suggested that an abnormal production of H_2S in the human respiratory system functions as an early biomarker for inflammatory diseases like asthma etc. Reliable breath analysis with respect to H_2S detection demands a reproducible and selective sensor device. Therefore, we present a planar resistive gas sensor based on the gas sensing approach of a ChemFET for medical breath analysis in an electronic nose approach. Here, the CVD grown zinc oxide (ZnO) nanowire (NW) surface operates as the gas sensitive open gate, while the conductive core serves as the source-drain channel. We investigated the benefit of surface modification of ZnO NWs, which are used for the detection of gaseous H_2S in the very low parts per billion (ppb) concentration range. In particular, we studied the catalytic effect of thin nanoparticle layers of gold (Au) or platinum (Pt) deposited on the ZnO NW surface in order to improve H_2S sensor sensitivity, selectivity and limit of detection. We find that surface modification with Au nanoparticles improves the overall sensor performance and allows for an exceptional detection limit below 10 ppb for H_2S diluted in synthetic air at room temperature.

HL 42.9 Wed 12:00 POT 51

defect compensation in the p-type transparent oxide Ba2BiTaO6 — •Diana Dahliah, Gian-Marco Rignanese, and Geoffroy Hautier — institute of Condensed Matter and Nanoscience (IMCN), Universit e catholique de Louvain (UCLouvain), Louvain-la-Neuve, Belgium

Transparent Conducting Oxides TCOs, combine a wide bandgap with good conductivity properties, such an unusual combination can be obtained by doping (n-type or p-type) a wide band gap oxide. p-type conductors are lagging behind in their performance because of the low hole mobility due to the presence of localized O 2p orbitals in the valence band. Breaking this localization and finding a p-type material with good conductivity as the one of n-type TCOs will make a revolution in the industry and will flip the type of materials that are used in some industrial applications. In a recent paper, Ba2BiTaO6 was reported as remarkable high mobility p-type TCOs though its conductivity is limited by charge compensation[1]. Here, we used first principles computations to investigate the reasons behind such a low conductivity from a defects physics standpoint. The calculated defect formation energies confirm that K is an adequate p-type shallow extrinsic dopant but that high p-type doping is prevented by the presence of compensating defects. Our work stresses the inherent difficulty in doping Ba2BiTaO6, we also highlight the potential directions for future improvements in its conductivity.
[1] A. Bhatia et al., Chem. Mater. 28, 30-34 (2016)

HL 43: 2D semiconductors and van der Waals heterostructures V (joint session HL/DS/O)

Time: Wednesday 9:30–13:00 Location: POT 81

HL 43.1 Wed 9:30 POT 81

Impurity effects in graphene: resonances, localized states and Mott-transitions — Yuriy G. Pogorelov[1], •Denis Kochan[2], and Vadim M. Loktev[3] — [1]IFIMUP-IN, Departamento de Física, Universidade do Porto, Porto, Portugal — [2]Institute for Theoretical Physics, University of Regensburg, Regensburg, Germany — [3]N.N. Bogolyubov Institute of Theoretical Physics, NAS of Ukraine, Kyiv, Ukraine

Impurities modify electronic spectrum of graphene in several ways. For example, they can shift charge neutrality point, tilt the Fermi level, open spectral (quasi)gaps, form resonances, and localized states.

In the presentation we discuss formation of resonances, and localized states in graphene for Anderson-like impurities (Hydrogen, Copper, Fluorine) in top, bridge and hollow positions. Particularly, we focus on spectral transition between resonant and localized states, and Mott mobility edges, tracing dependencies on graphene Fermi energy, con-

centration of impurities, their sub-lattices distribution, and impurity hybridization strength.

Employing the group expansion of the Green's functions we calculated reconstructed band structure of graphene hosting Anderson impurities. Applying Ioffe-Regel-Mott criterion, we obtained system-specific critical concentrations at which system undergoes resonance-to-bound-state transition.

HL 43.2 Wed 9:45 POT 81

Twisted Bilayer Graphene Produced by Atomic Force Microscopy Techniques — •Lina Bockhorn, Lucas Gnörich, Johannes C. Rode, Christopher Belke, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany

The electronic properties of bilayer graphene strongly depend on relative orientation of the two atomic lattices. The rotational mismatch between both layers opens up a whole new field of rich physics, especially around the magic angle.
Twisted bilayer graphene can be obtained by different methods. Here, we use atomic force microscopy techniques to generate twisted bilayer graphene. A diagonal cut is applied at high contact force through a monolayer graphene. Several folds spread from the newly created edge. The self-assembled twisted bilayer graphene is separated in folds with one or two rips.
We estimate the relative orientation of twisted bilayer graphene which is prepared by folding monolayer graphene [1, 2, 3].

[1] H. Schmidt, J. C. Rode, D. Smirnov, R.J. Haug,
Nature Communications 5, 5742 (2014)
[2] J. C. Rode, D. Smirnov, C. Belke, H. Schmidt, R.J. Haug,
ANNALEN DER PHYSIK 529 (11), 1700025 (2017)
[3] J. C. Rode, D. Zhai, C. Belke, S. J. Hong, H. Schmidt, N. Sandler, R. J. Haug, 2D Materials, 6(1), 015021 (2019)

HL 43.3 Wed 10:00 POT 81

Magneto-Raman Spectroscopy for Probing Electron-Phonon and Electron-Electron Interactions in Graphene — •Jens Sonntag[1,2], Sven Reichardt[1,3], Ludger Wirtz[3], Mikhail Katsnelson[4], Bernd Beschoten[1], and Christoph Stampfer[1,2] — [1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, Germany — [3]Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg — [4]Radboud University, Institute for Molecules and Materials, Nijmegen, Netherlands

We present charge carrier density-dependent magneto-Raman spectroscopy measurements on suspended graphene and hBN/graphene heterostructures to investigate electron-phonon and electron-electron interactions, both without applied magnetic field and within the quantum Hall regime. Strikingly, at $B = 0\,\mathrm{T}$ we do not observe the expected strong renormalization of the G-mode energy as a function of charge carrier density n. We identify Laser induced heating and a limited electron-hole lifetime as possible origins.
Utilizing gate-tunable magneto-phonon resonances, we extract the charge carrier density-dependence of the Landau level transition energies and the associated effective Fermi velocity v_F. In contrast to the logarithmic divergence of v_F at zero magnetic field, we find a piecewise linear scaling of v_F as a function of n, due to a magnetic field-induced suppression of the long-range Coulomb interaction. Furthermore, we can estimate the excitonic correction to the energies of the Landau level transistions to $\approx 6\,\mathrm{meV}$.

HL 43.4 Wed 10:15 POT 81

Tip-enhanced Raman spectroscopy combined with other Scanning Probe Microscopy Methods: Focus on 2D Materials — •Jana Kalbacova[1], Marc Chaigneau[2], and Andrey Krayev[3] — [1]HORIBA Jobin Yvon GmbH, Germany — [2]HORIBA Scientific, France — [3]HORIBA Scientific, USA

New two dimensional materials are on the rise. After the wonder material graphene, new materials such as MoS2, MoSe2, WSe2 have an intrinsic bandgap and as such are opening new doors for semiconductor applications. Raman spectroscopy offers information on the chemical structure of materials but cannot provide information on the electronic properties such as surface potential or photocurrent of our sample. Co-localized measurements combining scanning probe microscopy (SPM) with Raman spectroscopy can already bring a wealth of information; however, further improvements can be obtained by a tip that will act as an antenna and amplify the Raman signal and thus breaking the diffraction limit in a method called Tip-enhanced Raman spectroscopy (TERS). Typically spatial resolution of 10 - 20 nm can be achieved. In this contribution, we investigate different 2D materials by a combination of TERS, tip-enhanced photoluminescence, Kelvin probe microscopy, and other SPM methods to show very locally for example doping variations or defects that would otherwise go unnoticed with other macro- and microscopic techniques.

HL 43.5 Wed 10:30 POT 81

Edge photogalvanic effect driven by optical alignment in bi-layer graphene — •Susanne Candussio[1], Mikhail V. Durnev[2], Jun Yin[3], Artem Mishchenko[3], Helene Plank[1], Vasily V. Bel'kov[2], Sergey A. Tarasenko[2], Vladimir Fal'ko[3], and Sergey D. Ganichev[1] — [1]University of Regensburg, 93040 Regensburg, Germany — [2]Ioffe Institute, 194021 St. Petersburg, Russia — [3]University of Manchester, Manchester M13 9PL, UK

We report on the observation of the edge electric current excited in bi-layer graphene by terahertz laser radiation. We show that the current generation belongs to the class of second order in electric field phenomena and is controlled by the orientation of the THz electric field polarization plane. Application of a magnetic field normal to the graphene plane leads to a phase shift in the polarization dependence. In strong magnetic field the current exhibit 1/B-magnetooscillations with a period consistent with that of the Shubnikov-de-Haas effect and amplitude by an order of magnitude large as compared to the current at zero field measured under the same conditions. The developed microscopic theory shows that the current is formed in the edges vicinity limited by the mean-free path and originates from optical alignment of free carriers and scattering at the edges, which naturally break the P-symmetry. The observed magnetooscillations of the photocurrent are attributed to the formation of the Landau levels.

HL 43.6 Wed 10:45 POT 81

Electronic Properties of Two-Dimensional $ZrSe_3$-Films — •Lars Thole[1], Christopher Belke[1], Sonja Locmelis[2], Peter Behrens[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Institut für Anorganische Chemie, Leibniz Universität Hannover, 30167 Hannover, Germany

The family of 2d materials offers a big variety of different material classes [1]. This includes the transition metal trichalcogenides (TMTC) of the form MX_3, where M is a transition metal and X is a chalcogen [2, 3]. Here we exfoliated $ZrSe_3$ into thin films and contacted them with electron beam lithography. These thin flakes were investigated by means of optical microscopy, atomic force microscopy and electrical measurements. During this, it was shown that the material degrades in ambient condition. Furthermore, an activation energy of about 0.6 eV was measured. Inducing charge carriers showed the samples to be n-doped semiconductors. Finally, a mean free path for the bulk material was determined.

[1] A. K. Geim et al., Nature, 499, 419-425 (2013).
[2] J. O. Island et al., 2D Materials, 4, 0220033 (2017).
[3] J. Dai et al., WIREs Comput. Mol. Sci., 6, 211-222 (2016).

30 min. break

HL 43.7 Wed 11:30 POT 81

ultraviolet photodetectors based on mechanically exfoliated few-layer FePS3 and ZnO quantum dots with high responsivity — •juanmei duan[1,2], liang hu[3], yujia zeng[3], manfred helm[1,2], shengqiang zhou[1], and slawomir prucnal[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, D-01328 Dresden, Germany — [2]Technische Universität Dresden, D-01062 Dresden, Germany — [3]College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen 518060, P. R. China

Metal-phosphorus-trichalcogenides (MPTs), FePS3, are newly developed 2D wide-bandgap semiconductors and have been proposed as excellent candidates for ultraviolet (UV) optoelectronics. In this work, few-layer FePS3/ZnO quantum dots heterojunction were studied with Transmission electron microscopy (TEM), scanning electron microscope (SEM), X-ray photoelectron spectroscopy (XPS), and Raman measurement. The photoresponse characteristic of UV detectors based on FePS3/ZnO were investigated under 365nm, 405nm illumination and bias voltages. The high photoresponse property paves the way for the further development of 2D MPTs/ZnO quantum dots in high-

performance UV photodetectors.

HL 43.8 Wed 11:45 POT 81

Selectively grown Topological Insulator Nanodevices — •Daniel Rosenbach[1], Abdur Rehman Jalil[1], Jonas Kölzer[1], Nico Oellers[1], Michael Schleenvoigt[1], Tobias Werner Schmitt[2], Peter Schüffelgen[1], Gregor Mussler[1], Hans Lüth[1], Detlev Grützmacher[1], and Thomas Schäpers[1] — [1]Peter Grünberg Institut (PGI-9) and JARA-Fundamentals of Future Information Technology, Jülich-Aachen Research Alliance, Forschungszentrum Jülich, 52425 Jülich, German — [2]JARA-FIT Institute Green IT, RWTH Aachen University, 52062 Aachen, Germany

1-dimensional topological insulator nanoribbons in close proximity to elemental superconductors can be utilized to create localized Majorana modes for topological quantum computation architectures. We employ a selective area growth method using molecular beam epitaxy in order to define topological insulator nanodevices without harmful post processing steps. Using the transmission line method the interface of Bi_2Te_3 nanorribons towards ex situ applied Ti/Au contacts is probed at low temperatures. Furthermore, magnetotransport measurements on nano-Hallbars of down to 50 nm wide Bi_2Te_3 nanoribbons show indications of highly mobile charge carriers originating from 2-dimensional, topological surfaces. Finally, making use of a stencil mask on-chip, elemental superconductors like Nb and Al are deposited to define in situ, lateral topological Josephson junctions. Superconducting properties of proximitized topological nanoribbons are presented and discussed.

HL 43.9 Wed 12:00 POT 81

Investigation of one-dimensional materials — •Hadeel Moustafa, Peter Larsen, Morten Gjerding, and Karsten Jacobsen — Technical University of Denmark (DTU), department of physics.

1D materials are an interesting subset of materials with promising applications in batteries, photonic crystals and as electronic interconnects. 1D materials also present the possibility of combining them with other 1D materials or higher dimensional materials to create new hetero-structures with novel physical properties. Another potential application could be in heterogeneous catalysis, where the restricted geometry of 1D materials might lead to new types of atomic sites with different chemical characteristics. We identify potential 1D materials through a screening procedure applied to the ICSD and the COD. We employ the dimensionality scoring parameter defined in ref [1], which is based exclusively on the atomic geometry. The algorithm extract one-dimensional components from periodic three-dimensional crystals. So far around 300 compounds have been studied. Their basic properties like atomic structure, stability (heat of formation and convex hull), band structure, density of states and work function have been calculated. They are furthermore characterized using symmetry and grouped together using a clustering algorithm based on the root-mean-square-distance. In the future we expect to construct new potential 1D materials by element substitution in the constructed database. [1] http://doi.org/10.1103/PhysRevMaterials.3.03400.

HL 43.10 Wed 12:15 POT 81

Proximity exchange effects in excitons of TMDC/ferromagnet van der Waals heterostructures — •Paulo E. Faria Junior, Klaus Zollner, and Jaroslav Fabian — Universität Regensburg, Germany

Proximity effects in two-dimensional van der Waals heterostructures are an efficient way to modify intrinsic electronic properties[1]. In particular, proximity exchange offers the possibility of inducing magnetic properties in nominally nonmagnetic materials. Furthermore, this induced synthetic Zeeman spltting exhibits strong signatures in the optical spectra. Combining ab initio calculations with tight-binding modeling and the effective Bethe-Salpeter equation for excitons, we investigate the proximity exchange in TMDC/ferromagnet systems: (i) (Mo,W)Se2 on the ultrathin van der Waals ferromagnet CrI3[2] and (ii) (Mo,W)S2/hBN on ferromagnets Co and Ni[3]. Since stacking different 2D materials requires adjusting the lattice parameters to obtain commensurate supercells, we also discuss the impact of biaxial strain in monolayer TMDCs[4]. We show the evolution of different optical transitions and the role of excitonic effects in the direct transitions. [1] Zutic et al., Mater. Today 22, 85 (2019). [2] Zollner, Faria Junior, Fabian, PRB 100, 085128 (2019). [3] Zollner, Faria Junior, Fabian, arXiv:1910.13223 (2019). [4] Zollner, Faria Junior, Fabian, PRB 100, 195126 (2019). Supported by: Alexander von Humboldt Foundation, Capes, DPG SFB 1277.

HL 43.11 Wed 12:30 POT 81

Decreasing Activation Energies with Thickness of Thin $HfTe_5$ layers — •Christopher Belke[1], Sonja Locmelis[2], Lars Thole[1], Peter Behrens[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Institut für Anorganische Chemie, Leibniz Universität Hannover, 30167 Hannover, Germany

Hafnium pentatelluride ($HfTe_5$) is a layered two dimensional material from the class of Transition Metal Penta Chalcogenide with the chemical formula MX_5, where M is a transition metal and X a chalcogenide [1]. $HfTe_5$ shows a resistivity anomaly and is expected to be a topological insulator [2] with a bulk band gap of about 22 meV [3]. In addition, theory predicts that a single layer should show a band gap of about 400 meV and should be a quantum spin hall insulator [1].

We present that the electronic properties of $HfTe_5$ drastically change with decreasing thickness. We prepared samples with different thicknesses under 100 nm and made temperature dependent measurements to determine the activation energy in an Arrhenius plot. We found that the band gap increases with decreasing thickness. Conductivity measurements also show an anomaly due to a mobility change at around 120 K.

[1] H. Weng et al., Phys. Rev. X 4, 011002 (2014)
[2] S. Liu et al., APL Materials 6, 121111 (2018)
[3] H. Wang et al., Phys. Rev. B 93, 165127 (2016)

HL 43.12 Wed 12:45 POT 81

Tailoring of electronic and magnetic properties of hematene: a computational study — •Yidan Wei, Mahdi Ghorbani, and Arkady Krasheninnikov — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Exfoliation of non van der Waals materials has established new class of two dimensional materials, such as hematene btained from hematite. In order to exploit and design potential applications, understanding the electronic and magnetic properties is crucial. Using density functional theory calculations, the atomic structures, electronic and magnetic properties of hematene are systematically investigated. Bare hematene in the ferromagnetic states is less stable than that in the anti ferromagnetic states, and it has a direct band gap. The stability, electronic and magnetic properties of hematene can change significantly with different terminations. Hematene covered with OH is a semiconductor with surface states removed, while hematene covered with H changes from semiconductor to half metal. Further, changes in the electronic characteristics are possible under with mechanical deformation. Applying strain causes significant changes in the electronic properties of hematene. In case of non-terminated hematene, both compressive and tensile strain can result in a reduction of the band gap in the anti-ferromagnetic state under biaxial and uniaxial deformation, and the band gap increases in case of OH terminated hematene. The band gap also increases under tensile strain in the ferromagnetic states. The deformation can lead to the enhancement of polarization.

HL 44: Focus: Exploitation of Anisotropy in Organic Semiconductors II (joint session CPP/HL)

Time: Wednesday 9:30–11:15 Location: ZEU 222

Invited Talk HL 44.1 Wed 9:30 ZEU 222

Structural and photophysical properties of blends of weakly interacting organic semiconductors — •Katharina Broch[1], Clemens Zeiser[1], Giulio Cerullo[2], Roel Tempelaar[3], and Christopher Bardeen[4] — [1]Institute for Applied Physics, University of Tübingen, Germany — [2]Department of Physics, Polytechnic University of Milan, Italy — [3]Department of Chemistry, Northwestern University, USA — [4]Department of Chemistry, University of California at Riverside, USA

Blends of organic semiconductors are functional parts in many organic electronic devices and their structural, electronic and photophysical properties have been studied in great detail. So far, research focussed mainly on electron donating and accepting organic semiconductors due to their relevance for devices. However, also blends of weakly interacting compounds can be interesting from the viewpoint of a fundamental understanding of mixing behavior [1,2], or as tool to study the details of complex photophysical processes [3,4]. Anisotropies in structure formation and their impact on photophysical properties will be discussed using the example of acene blends.

[1] J.-O. Vogel et al., J. Mater. Chem. 20 (2010); [2] A. Aufderheide et al., Phys. Rev. Lett. 109 (2012); [3] D. Lubert-Perquel et al., Nat. Commun. 9, 4222 (2018); [4] K. Broch et al., Nat. Commun. 9, 954 (2018)

HL 44.2 Wed 10:00 ZEU 222

Influence of alkyl chain variation on co-crystal formation and molecular charge transfer — •Nadine Russegger, Oleg Vladimirov, Alexander Hinderhofer, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, Germany

A very important and fundamental process for organic semiconductors is the charge transfer effect between electron donor and electron acceptor molecules in the ground state and in the excited state.

In this work, the charge transfer effect of weakly interacting organic semiconductor mixtures is comprehensively investigated depending on the influence of alkyl chain variation with different acceptor molecules. We choose dinaphtho[2,3-b:2',3'-f]thieno[3,2-b]thiophene (DNTT) and diindenoperylene (DIP) as donor and several perylene-diimide derivatives with different alkyl chain length in the imide position as acceptor molecules (PDIF-CN_2, PDI-C3, PDI-C5, and PDI-C8-CN_2).

For a full structural overview of the resulting molecularly mixed co-crystals, the bulk-heterojunction films were evaluated by surface X-ray scattering. The optical and electronic properties of the intermolecular interactions were characterized by optical absorption, photoluminescence as well as *in-situ* differential reflectance spectroscopy. For the various equimolar mixed systems of DNTT as well as DIP and different perylene-diimide derivatives charge transfer effects were estimated [1].

The results allow us to correlate the structural morphology and the charge transfer effects depending on the chain length and their configuration of the different mixed systems.

[1] V. Belova et al., *J. Am. Chem. Soc.*, **2017**, 139, 8474-8486.

HL 44.3 Wed 10:15 ZEU 222

Favored face-on crystal orientation in poly(3-(6-bromohexyl)-thiophene) on graphene as a result of modified interfacial interactions — •Oleksandr Dolynchuk[1], Philip Schmode[2], Matthias Fischer[1], Mukundan Thelakkat[2], and Thomas Thurn-Albrecht[1] — [1]Experimental Polymer Physics, Martin Luther University Halle-Wittenberg, Germany — [2]Applied Functional Polymers, University of Bayreuth, Germany

Directed crystallization on a substrate could be advantageous for inducing molecular orientation in semicrystalline conjugated polymers whose charge transport properties are anisotropic. Although a preferred face-one molecular orientation was shown in monolayers of poly(3-hexylthiophene) (P3HT) on graphite, a full face-one orientation in thicker P3HT films has not been realized so far. We assume that it is a result of two competing interfacial orientations initiated at the interfaces to vacuum and graphite. Here it is shown that modification of the chemical structure of P3HT side chains can alter the surface interactions and result in fully face-on oriented crystals. Specifically, we present a comparative study of the substrate induced orientation in thin films of poly(3-(6-bromohexyl)-thiophene) (P3BrHT) and P3HT on graphene. The crystal orientation in films of both polymers was explored by surface-sensitive grazing incidence XRD. The results indicated that P3BrHT on graphene had solely face-on oriented crystals in films up to 26 nm, whereas P3HT showed the mixed face-on and edge-on crystal orientation with edge-on crystals formed at the top surface that supports our assumption about competing interfacial orientations.

HL 44.4 Wed 10:30 ZEU 222

Determining Anisotropic Effects in Strongly Coupled Metal Organic Hybrid Structures — •Maximilian Rödel[1], Thomas Stark[2], Markus Hecht[3], Jochen Manara[2], Matthias Stolte[3], Frank Würthner[3], and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg — [3]Institut für Organische Chemie &Center for Nanosystems Chemistry (CNC), Julius Maximilian University of Würzburg, 97074 Würzburg

Coupling phenomena in metal organic hybrid structures enable unique possibilities to tune the properties of opto-electronic devices. Furthermore, the strong coupling between surface plasmons and excitons in organic semiconductors leads to novel hybrid states, which are termed plexcitons. By means of surface plasmon resonance spectroscopy we investigate these plexcitonic states in liquid-crystalline perylene bisimide (PBI) thin films exhibiting J-type coupling deposited on gold surfaces processed via doctor blading from solution. These new states show a characteristic coupling strength of ≈110 meV. Alignment of hydrogen-bonded PBI molecules and, thus, their transition dipoles results in long-range ordered films with a pronounced spatially anisotropy of structural and optical characteristics. A ratio of 2.78 can be evaluated between strongest and weakest coupling strength of the anisotropic system. Understanding the correlation between molecular order and optical properties will enable new device concepts utilizing the presented opto-electronic directionality in future applications.

HL 44.5 Wed 10:45 ZEU 222

Anistropic Charge Transfer Formation at Crystalline Pentacene/Perfluoropentacene Interfaces — •Sebastian Hammer[1], Clemens Zeiser[2], Katharina Broch[2], and Jens Pflaum[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Institute for Applied Physics, University of Tübingen, 72076 Tübingen — [3]ZAE Bayern, 97074 Würzburg

Strongly bound charge transfer (CT) states critically influence the performance of devices based on donor/acceptor (D/A) heterojunctions such as light emitting diodes or photovolatic cells. Whereas the excited states in the archetypical CT system Pentacene:Perfluoropentacene (P:PFP) have been vastly studied in thin films [1][2], the role of molecular orientation on CT formation and energetics has not been evaluated to the same extent, so far. Utilizing heteroepitaxial growth of PFP on P (001) single crystals surfaces we were able to prepare long-range ordered D/A heterojunctions in an edge-on molecular configuration as confirmed by XRD. Optical analyses by temperature dependent cw-fluorescence spectroscopy and *in-situ* differential reflectance spectroscopy on the PFP/P interfaces revealed no indication for CT formation in case of edge-on molecular orientation, in contrast to the face-to-face geometry. By means of bilayer as well as heterojunction diode structures we demonstrate that by controlling the molecular orientation at the PFP/P interface, thus, utilizing the anisotropic CT characteristics, the overall performance can be significantly improved.

[1] K. Broch et al., *Phys. Rev. B* **83**, 245307 (2011)
[2] T. Breuer, G. Witte, *J. Chem. Phys.* **21**, 138 (2013)

HL 44.6 Wed 11:00 ZEU 222

On the Origin of Electronic Gap States in Molecular Semiconductor Thin Films — •Alexander Hinderhofer[1], Jan Hagenlocher[1], Satoshi Kera[2], and Frank Schreiber[1] — [1]Universität Tübingen, Institut für Angewandte Physik, 72076 Tübingen, Germany — [2]Institute for Molecular Science, Myodaiji, 444-8585, Japan

Electronic gap states within the HOMO-LUMO gap of molecular semiconductors play a key role in the energy level alignment of organic-organic and organic-inorganic interfaces and therefore are a defining parameter for device functionality and efficiency. The density of gap states originates from structural defects acting as dopants and it can be varied by different film preparation methods, e.g. by temperature variation during film deposition.

We present a systematic study of anisotropic structural parameters in thin films, including grain size, strain, dislocation density, mosaicity and coherently ordered domain size (in-plane and out-of-plane) studied by X-ray scattering and atomic force microscopy. The structural properties of several molecular semiconductors (Pentacene (PEN), Perfluoropentacene (PFP), 6-Phenacene (6Phen), etc.) are correlated with their electronic gap state density studied by ultra-low background ultraviolet photoelectron spectroscopy (UPS). We discuss which types of structural parameters have the strongest impact on the gap state density. Finally, we present examples of the energy level alignment in organic-organic heterojunctions controlled by their gap state density.

HL 45: Hybrid Perovskite and Photovoltaics I (joint session CPP/HL)

Time: Wednesday 9:30–12:45 Location: ZEU 260

HL 45.1 Wed 9:30 ZEU 260

Growth of High-quality $(FAPbI_3)_{0.9}(MAPbBr_3)_{0.1}$ Perovskite Single Crystals and their Optoelectronic Properties — •Julian Höcker[1], Mathias Fischer[1], Mehmet Özcan[2], Benedikt Bichler[2], Sebastian Hammer[1], Melina Armer[1], Volker Drach[1], Bert Nickel[2], and Vladimir Dyakonov[1] — [1]Experimental Physics VI, JMU, 97074 Würzburg — [2]Soft Condensed Matter Group, LMU, 80539 München

Organo lead trihalide perovskites are potentially highly interesting class of semiconductors. Particularly the perovskite $(FAPbI_3)_{0.9}(MAPbBr_3)_{0.1}$ is one of the most important representatives of this material class. In order to further develop this complex perovskite system and thus foster its use, it is essential to investigate the chemical and physical properties of high-quality single crystals with the same stoichiometry. However, the liquid growth of perovskite crystals without seed crystals is usually challenging and becomes even more challenging with mixed cations/halides crystals, making it difficult to assess their properties. For this purpose, we have developed a new efficient re-fill crystallization method (RFCM) based on the Inverse Temperature Crystallization (ITC), which avoids seed crystals. We applied qualitative and quantitative analyses to identify the elemental composition and the exact stoichiometry of the grown crystals and studied their crystallographic properties, demonstrating a high single crystal quality. Optical and electrical measurements completed the structural and elemental analysis, and enabled us to derive relevant properties of this perovskite material.

HL 45.2 Wed 9:45 ZEU 260

Revealing the Impact of Cesium/Rubidium Incorporation on the Photophysics of Multiple-Cation Lead Halide Perovskites — Yajun Gao, Kai Wang, Mingcong Wang, Jafar Khan, Ahmed Balawi, Stefaan De Wolf, and •Frédéric Laquai — King Abdullah University of Science and Technology (KAUST), KAUST Solar Center, Thuwal, Saudi Arabia

The incorporation of cesium (Cs) and rubidium (Rb) ions in multiple-cation mixed lead halide perovskites increases their photovoltaic performance. Here, the reasons for the performance increase are investigated by steady-state and transient spectroscopy techniques. The band edge absorption shows that the Cs/Rb-ion incorporation increases the band gap, while exciton binding energies remain low, in the range of a few milli-electronvolts. Low Urbach energies determined by photothermal deflection spectroscopy suggest optimized microstructures upon Cs/Rb incorporation. The charge carrier recombination dynamics indicate that Cs/Rb-incorporation reduces not only the first-order (trap-assisted) recombination, but also the second-order recombination. Upon photoexcitation, carrier density-induced broadening of the photo-bleaching following the Burstein-Moss model is observed and effective carrier masses are determined to be in the range of a few tenths of the electron rest mass, explaining the excellent charge carrier mobilities of these perovskite films. Sub-picosecond hot carrier cooling is observed, indicating a strong charge-phonon coupling. Our results reveal the impact of cesium/rubidium incorporation on the photophysics of multiple-anion lead halide perovskites.

HL 45.3 Wed 10:00 ZEU 260

Unraveling origin of performance instability in mixed perovskite solar cells — •Małgorzata Kot[1], Chittaranjan Das[2], Tim Hellmann[2], Carolin Wittich[2], Iwan Zimmermann[3], Mohammad Khaja Nazeeruddin[3], Wolfram Jaegermann[2], and Jan Ingo Flege[1] — [1]BTU Cottbus-Senftenberg, Germany — [2]TU Darmstadt, Germany — [3]EPFL Lausanne, Switzerland

A degradation mechanism of mixed perovskite solar cells is mostly attributed to the segregation of halide phases in the perovskite film. However, our studies have revealed, that the mixed perovskites degrade due to the migration of iodine and methylammonium ions across the solar cell. Nonetheless, an ultrathin RT-ALD-Al_2O_3 layer deposited on top of perovskite can very effectively limit this migration thanks to the reactive property of this interface.[1-3] Namely, there is a closed cycle of the charge transfer between ALD and perovskite films. Such ALD film doesn't cause any drastic changes in the perovskite morphology, chemical composition, optoelectronic properties or crystallinity. What more, it helps to preserve the initial properties of the film during exposure to the light and ambient air under real operating conditions and thus improves the stability of the solar cells. This ultra-thin Al_2O_3 layer prepared in an unusual RT process for ALD method significantly increases the lifetime of perovskite solar cells at a very low cost bringing thus the introduction of the perovskite solar cells into mass production. [1] M. Kot et al., ChemSusChem 11 (2018) 3640. [2] M. Kot et al., Energy Technol. 7 (2019) 1900975. [3] D. Schmeißer et al., J. Phys. Chem. C 123 (2019) 23352.

HL 45.4 Wed 10:15 ZEU 260

Phase transitions of hybrid and inorganic perovskites simulated by machine-learning force fields — Ryosuke Jinnouchi[1,2], Jonathan Lahnsteiner[1], Ferenc Karsai[3], Georg Kresse[1], and •Menno Bokdam[1] — [1]University of Vienna, Vienna, Austria — [2]Toyota Central R&D Labs, Aichi, Japan — [3]VASP Software GmbH, Vienna, Austria

Finite-temperature simulations of complex dynamic solids are a formidable challenge for first-principles methods. Long simulation times and large length scales under isothermal-isobaric (NPT) conditions are required, demanding years of compute time. We applied the recently developed on-the-fly Machine-Learning Force Field (MLFF) scheme[1] to generate force fields for several hybrid and inorganic perovskites (APbX3, A={MA,Cs},X={I,Br,Cl}). The MLFFs open up the required time and length scales, while retaining the distinctive chemical precision of first principles methods. We study the entropy driven phase transitions of hybrid perovskites, which have never been accurately described in simulations. Simulations using machine learned potentials give direct insight into the underlying microscopic mechanisms. The ordering of the Methylammonium (MA) molecules as function of temperature is obtained. Furthermore, we relate the phase transition temperatures of different perovskites to the radii of the involved species, and we determine the order of the transitions in Landau theory.

[1] R. Jinnouchi et al., Phys. Rev. Lett. 122, 225701 (2019)

HL 45.5 Wed 10:30 ZEU 260

The tetragonal to orthorhombic crystal phase transition in MAPI studied by time-resolved photoluminescence microscopy — •Alexander Biewald[1], Nadja Giesbrecht[1], Richard Ciesielski[1], Thomas Bein[1], Pablo Docampo[2], and Achim Hartschuh[1] — [1]LMU München, Butenandtstr. 11, 81377 Munich, GER — [2]Newcastle University, Newcastle upon Tyne, UK

Perovskite-based thin-film solar cells today reach power conversion efficiencies of more than 22% [1]. Methylammonium lead iodide (MAPI) is prototypical for this material class of hybrid halide perovskite semiconductors and at the focal point of interest for a growing community in research and engineering. We investigated the diffusion properties for the orthorhombic and tetragonal phase using time-resolved photoluminescence (PL) microscopy before [2]. Now we focus on the PL dynamics at the phase transition. First, the phase transition is observed in temperature dependent PL spectra, which show the correlated decrease and rise of two spectrally distinct bands. This indicates the coexistence of both phases in a limited temperature range. Second, at the phase transition, which is found to vary between grains, diffusive transport suddenly stops and only reappears upon further cooling or heating, respectively. Our spatio-temporal studies provide detailed microscopic insights into the phase transition and its influence on the carrier dynamics in large crystal MAPI thin films.

[1] M.A.Green et al.,Prog.Photovolt:Res.Appl.,26,427-436,2018
[2] A. Biewald et al.,ACS Appl.Mat.&Interfaces,11,20838-20844,2019

HL 45.6 Wed 10:45 ZEU 260

Structural, optical and dielectric properties of $Cs_2AgBiBr_6$, a lead-free perovskite for photovoltaic applications — •Melina Armer[1], Maximilian Sirtl[2], Patrick Dörflinger[1], Julian Höcker[1], Thomas Bein[2], and Vladimir Dyakonov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Ludwigs Maximilian University München, 81377 München

As conventional perovskite solar cells contain lead and therefore suffer toxicity and stability issues, finding alternative and stable lead-free materials for the application in perovskite photovoltaics has become

an essential problem to be solved. In this work, lead-free $Cs_2AgBiBr_6$ single crystals have been synthesized using different solution based approaches, permitting a detailed characterization of the optical and structural properties of this material. The morphology and quality of the as grown crystals has been evaluated using scanning electron microscopy (SEM), energy dispersive X-ray microscopy (EDX) and X-ray diffraction (XRD). The crystals have been characterized using steady-state and time-resolved photoluminescence (PL) spectroscopy. We observed PL in the visible region characterized by large PL lifetimes. Furthermore, the dielectric constant of $Cs_2AgBiBr_6$ crystals has been measured at 9 GHz by time resolved microwave conductivity (TRMC). Using the obtained value of the dielectric constant the mobility of $Cs_2AgBiBr_6$ thin films could be estimated using TRMC.

HL 45.7 Wed 11:00 ZEU 260

Characterization of Perovskite Precursor Solutions in order to achieve High-Performance Solar Cells — •Marion Flatken[1], Nga Phung[1], Robert Wendt[1], Armin Hoell[1], and Antonio Abate[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie (HZB) — [2]Department of Chemical, Materials and Production Engineering, University of Naples Federico II

Despite the current success of Perovskite Solar Cells, there are still open questions how to explain intrinsic parameters in terms of stability and general photovoltaic performance of varying perovskite compositions. Deeper knowledge in coordination chemistry of the perovskite itself is one key parameter to improve and control crystallization in the solution based fabrication. Using small angle scattering we can prove, that the coordination starts in the perovskite precursor solution and differs according to the perovskite composition. The observed colloidal structures are characterized via small angle neutron scattering (SANS) and is further compared to synchrotron based small angle x-ray scattering (SAXS). Based on nuclear magnetic resonsance spectroscopy the chemical composition of the complexes can be revealed, which leads us to a possible starting mechanism for nucleation and growth in perovskite precursor solutions. In our work we compare the precursor solutions of MAPbI3 and MAPbI3 x SrI2 to a cesium containing triple cation perovskite solution, which is known to be a highly efficient and stable perovskite. Observed differences and similarities might give one reason for the divergence in photovoltaic properties of the respective full device solar cells.

15 min. break

HL 45.8 Wed 11:30 ZEU 260

Solution-Processed Perovskite Solar Cells — Florian Mathies[1], Gopinath Paramasivam[1], Janardan Dagar[1], and •Eva Unger[1,2] — [1]Helmholtz Zentrum Berlin — [2]Lund University, Sweden

Metal halide perovskites (MHP) are being intensively researched for solar energy conversion applications and are the best solution-processable solar cell technology to date. For scaling the technology, high throughput and material-efficient printing and coating techniques can be utilised to make larger area devices. We will here present our systematic approach translating successful processing strategies developed for spin-coating to slot-die coating and inkjet printing through in-depth rationalisation of MHP formation gained from in-situ optical monitoring. Depending on the composition of MHP precursors and solvents as well as process conditions and process quenching by e.g. an antisolvent, thin film formation proceeds via crystalline intermediate phases or directly into the perovskite phase. Optimisation of MHP precursors composition and processing conditions enabled us to recently achieve 22% power conversion efficiency in small area devices by spin-coating and 15% on large are mini-modules that are being further optimised in the near future. We are currently working on translating process conditions to obtain high quality perovskite thin films to scalable solution based deposition methods such as slot-die coating and inkjet printing. To date, we have demonstrated slot-die coating and inkjet printed small area devices with power conversion efficiencies $> 15\%$.

HL 45.9 Wed 11:45 ZEU 260

How do solvent molecules determine the electronic structure of halide perovskite precursors? — •Ana M. Valencia[1], Richard Schier[1], Oleksandra Shargaieva[2], Eva Unger[2], and Caterina Cocchi[1] — [1]Physics Dept., Humboldt-Universität zu Berlin und IRIS Adlershof — [2]Helmholtz-Zentrum Berlin, HySPRINT Innovation Lab, Berlin

Hybrid metal-halide perovskites have been demonstrated as excellent candidates for opto-electronic applications such as high-performing solar cells and light-emitting devices. The quality of the resulting materials, and hence their performance, strongly depends on the solution processing conditions. For this reason, it is of paramount importance to gain insight into their initial steps of formation of the solid-state materials. To do so, we investigate the inorganic building blocks of lead-iodide perovskites in DMSO solution. In order to mimic the initial steps of the perovskite nucleation, we consider PbI2(DMSO)4, Pb2I4(DMSO)6, and Pb3I6(DMSO)8, as model compounds treated fully atomistically and quantum-mechanically in the framework of density-functional theory and many-body perturbation theory. Through the analysis of the computed molecular orbitals, optical spectra, and electron and hole densities we discuss and rationalize the role of electronic hybridization between solute and solvent, and the mechanisms that are responsible for the absorption and emission peaks observed in the experiments.

HL 45.10 Wed 12:00 ZEU 260

Photodoping through local charge carrier accumulation in alloyed hybrid perovskites for highly efficient luminescence — •Sascha Feldmann, Stuart Macpherson, Satyaprasad Senanayak, Mojtaba Abdi-Jalebi, Jasmine Rivett, Guangjun Nan, Gregory Tainter, Tiarnan Doherty, Kyle Frohna, Emilie Ringe, Richard Friend, Henning Sirringhaus, Michael Saliba, David Beljonne, Samuel Stranks, and Felix Deschler — Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom

Metal-halide perovskites have emerged as exceptional semiconductors for optoelectronic applications. Substitution of the monovalent cations has advanced luminescence yields and device efficiencies. Here, we control the cation alloying to enhance optoelectronic performance through alteration of the charge carrier dynamics in mixed-halide perovskites. In contrast to single-halide perovskites, we find high luminescence yields for photo-excited carrier densities far below solar illumination conditions. Using time-resolved spectroscopy we show that the charge-carrier recombination regime changes from second to first order within the first tens of nanoseconds after excitation. Supported by microscale-mapping of the optical bandgap, electrically-gated transport measurements and first-principles calculations, we demonstrate that spatially-varying energetic disorder in the electronic states causes local charge accumulation, creating p- and n-type photo-doped regions, which unearths a strategy for efficient light emission at low charge-injection in solar cells and LEDs.

HL 45.11 Wed 12:15 ZEU 260

Perovskite solar cells from direct co-evaporation: Impact of hole transport materials on device performance — •Marcel Ross[1], Amran Al-Ashouri[1], Erica Magliano[1], Marko Jošt[1], and Steve Albrecht[1,2] — [1]Helmholtz-Zentrum Berlin, D-12489 — [2]Technical University Berlin, D-10587

Deposition of perovskite solar cell absorbers by co-evaporation offers a variety of advantages over solution based preparation such as homogeneous coating of large substrates and conformal coverage of different textures. Nevertheless, the majority of reported publications focusses on solution-based preparation of perovskite solar cells. This is likely due to the challenging evaporation characteristic of organic precursors and the limited understanding of the perovskite co-evaporation process itself. To achieve a better process control, we implement an evaporation setup with a thermal management system. This enables the deposition of high quality Methylammonium Lead Iodide perovskite films as confirmed by XRD, PL and optical measurements. To analyse the influence of substrate properties on film formation, perovskites are deposited on different hole transport materials (HTMs) such as PTAA and self-assembling monolayer (SAM) molecules. Furthermore, the impact of the substrate temperature during deposition of the perovskite is investigated. While the substrate temperature is mainly influencing the incorporation of methylammonium iodide into the film, the p-i-n solar cell performance is strongly affected by the used HTM. Finally, a stabilized efficiency over 20% is realized with the SAM hole transport layer and a proper substrate temperature.

HL 45.12 Wed 12:30 ZEU 260

The impact of mobile ions on the open cicuit voltage decay of perovskite solar cells explained by time resolved drift-diffusion simulations. — •Mathias Fischer, David Kiermasch, Kristofer Tvingstedt, and Vladimir Dyakonov — Experimental Physics VI, Julius Maximilian University of Würzburg, 97074

Würzburg

The open circuit voltage decay (OCVD) is a characteristic transient response of an operating solar cell after the illumination is turned off. By analyzing such transients correctly, it is possible to obtain valuable information about charge carrier dynamics in a fully functional device. When additional charged species like mobile ions are present, extraordinary features can be observed during the OCVD. We use a self-programmed transient drift-diffusion simulator involving mobile ions with sub-nanoseconds time resolution, to show how quantitative information about the ionic species, such as concentration and diffusion coefficient can be obtained. The simulated transients showing characteristic ionic features are in excellent agreement with experimental data from methylammonium lead iodide ($CH_3NH_3PbI_3$) devices. Further, the ionic contributions to the OCVD are clearly visualized by specially resolved carrier profiles. This approach opens up new ways to interpret transient electrical measurements on perovskite based devices.

HL 46: Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions III (joint session O/HL/CPP/DS)

Time: Wednesday 10:30–13:30 Location: GER 38

Invited Talk HL 46.1 Wed 10:30 GER 38

Hybrid Perovskites: polarons, excitons and phase diagrams — •Georg Kresse, Menno Bokdam, and Ryosuke Jinnouchi — University of Vienna, Faculty of Physics and Center for Computational Materials Sciences

Halide perovskites are very promising solar cell materials. The first part of this presentation studies the formation of polarons and excitons in MAPbI3. We show that both, polarons and excitons, possess about similar binding energies. To obtain accurate results, the calculations have to be carefully converged with respect to the k-point sampling, something that has been often "overlooked" in the past [1].

The second part of the talk presents studies on the finite temperature behavior of MAPbI3. To achieve the required long simulation time and large length scales, an on-the-fly machine learning scheme that generates force fields automatically during first principles molecular dynamics simulations is used. This force field opens up the required time and length scales, while retaining the distinctive chemical precision of first principles methods [2]. Using machine learned potentials, isothermal-isobaric simulations give direct insight into the underlying microscopic mechanisms of the phase transitions. We observe that MAPbI3 is an very dynamic material even at room temperature, putting some question marks on the hereto considered static models.

[1] M. Bokdam, T. Sander, A. Stroppa, S. Picozzi, D. D. Sarma, C. Franchini, G. Kresse, Scientific Rep. 6, 28618 (2016); [2] R. Jinnouchi, J. Lahnsteiner, F. Karsai, G. Kresse, M. Bokdam, PRL 122, 225701 (2019).

HL 46.2 Wed 11:00 GER 38

Assessing ab-initio methodology to compute electronic properties of organic-inorganic metal halide perovskites — •Cecilia Vona, Dmitrii Nabok, and Claudia Draxl — Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

Organic-inorganic metal halide perovskites (HaPs) are materials widely studied for their light-harvesting properties. Owing to the interplay between strong electron-electron interaction and spin-orbit coupling, their theoretical investigation is still a challenge. Here we evaluate the methodology to compute their electronic structure. To this extent, we explore several approaches, within density-functional theory and many body perturbation theory, to compute the electronic structure of PbI_2, which is the precursor of many HaPs. Spin-orbit coupling effects are taken into account, and the hybrid functionals PBE0 and HSE are at the center of the investigation. We first explore several methods to determine the mixing parameter α, which in PBE0 and HSE defines the amount of Hartree-Fock exchange mixed with the semi-local functional PBE. We then use the results obtained from HSE and PBE0 for different values of α as starting point of G_0W_0 calculations. All the calculations are performed with the full-potential all-electron computer package `exciting`, in which LAPW+lo bases are implemented. We observed that hybrid functionals with a proper α value are most suitable to compute the electronic structure of PbI_2. Moreover, we show that the methodology is transferable to $CsPbI_3$, and we expect the same behavior for the lead-iodine perovskites.

HL 46.3 Wed 11:15 GER 38

Rashba-Dresselhaus Effect in Two Dimensional Layered Halide Perovskites — •Benedikt Maurer[1,2], Claudia Draxl[1,2], and Christian Vorwerk[1,2] — [1]Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, 12489 Berlin — [2]European Theoretical Spectroscopy Facility

It has been shown that huge spin-orbit coupling in bulk hybride organic inorganic perovskites in combination with broken inversion symmetry leads to Rashba-Dresselhaus splitting, which influences the optoelectronic properties. This indicates that such effects also affect the optoelectronic properties of their two dimensional layered relatives, which are promising candidates as new light emitting materials. In this work, we aim at understanding which inversion symmetry breaking can lead to the Rashba-Dresselhaus effect in those materials. For this purpose, we develop model structures, where we replace the organic compounds by Cs atoms and disregard possible distortions in the inorganic layers, resulting in the structural composition $Cs_{n+1}Pb_nI_{3n+1}$. Using the all-electron full-potential density-functional-theory code `exciting`, we systematically study how atomic distortions impact the band structure for n=1, 2 and ∞. We identify displacement patterns that yield Rashba-Dresselhaus splitting, and determine the size of the splitting as a function of the displacement. Furthermore, we analyze the spin textures in electronic states around the band gap to differentiate between Rashba and Dresselhaus effect. Our study reveals in-plane lead displacements as the origin of the Rashba-Dresselhaus splitting.

HL 46.4 Wed 11:30 GER 38

Intrinsic polarons on polar surfaces — •Michele Reticcioli[1,2], Zhichang Wang[2], Igor Sokolovic[2], Michael Schmid[2], Ulrike Diebold[2], Martin Setvin[2], and Cesare Franchini[2,3] — [1]University of Vienna, Center for Computational Materials Science, Vienna, Austria — [2]Institute of Applied Physics, Technische Universitaet Wien, Vienna, Austria — [3]University of Bologna, Department of Physics and Astronomy, Bologna, Italy

Uncompensated charge at the surface boundary of polar materials is conventionally expected to form a two dimensional electron gas (2DEG), as a result of the alternating charged-plane stacking in the ionic crystals, interrupted by the surface cut. By means of density-functional theory calculations and surface-sensitive experiments, we propose a different paradigm able to accommodate the uncompensated charge in a more effective way, establishing a more favorable ground state for the system, that is the polaron formation (local lattice distortions coupled with charge localization). In fact, the intrinsic uncompensated charge tends to spontaneously localize and form polarons, rather than a 2DEG. Only beyond the critical polaron density, excess charge arising from external doping or defects starts to build dispersed electronic states. Here, we show how polarons and 2DEG compete on the polar KTaO3(001) surface.

HL 46.5 Wed 11:45 GER 38

Polarons in extended p-conjugated systems: the role of electron correlation. — •Daniele Fazzi[1], Klaus Meerholz[1], and Fabrizia Negri[2] — [1]Institut für Physikalische Chemie, Universität zu Köln, Luxemburger str. 116, 50939 Köln, Germany — [2]Dipartimento di Chimica, Università di Bologna, via F. Selmi, 2, 40126 Bologna, Italy

Polarons play a crucial role in governing charge transfer in organic materials. An accurate description of their electronic structure and electron-phonon couplings is mandatory to understand their response and transport properties.

We report a comprehensive investigation of polarons in extended p-conjugated systems (ladder-type polymers, graphene nano-ribbons, and cyanine-based compounds [1-2]). We show how spin polarized DFT lead to solutions of the polarons wavefunction which are not the

most stable ones. This aspect, can be traced back to the multireference character of polarons. Broken symmetry DFT can address the electronic and structural properties of polarons, providing a correct assessment of charge transport parameters, otherwise incorrectly computed [3]. Multi-reference wavefunction methods are also considered to take into account correlation effects in charged and excited states.

Our study calls for a careful assessment in the description of charged/excited states in conjugated materials.

[1] Wang, S., et al., Adv. Mater. 2018, 30, 1801898. [2] Medina, S. et al., Phys. Chem. Chem. Phys., 2019, 21, 7281-7288. [3] Fazzi, D. et al, J. Mat. Chem. C., 2019, 7, 12876-12885.

HL 46.6 Wed 12:00 GER 38

Optical and x-ray absorption spectra of MgO from first-principles including many-body effects — •Vijaya Begum, Markus E Gruner, and Rossitza Pentcheva — Faculty of Physics and Centre for Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg, Germany

We discuss the optical and x-ray absorption (XAS) spectra of MgO – a wide band gap oxide with versatile applications – in the framework of density functional theory (DFT) including many-body and excitonic corrections. The quasi-particle band gap improves over DFT with PBEsol as the starting exchange-correlation functional (4.58 → 7.52 eV) and is overcorrected with the hybrid functional HSE06 (6.58 → 8.53 eV) when compared to experiment (7.7 eV). Including excitonic effects by solving the Bethe-Salpeter equation (BSE) leads to excellent agreement with the experimental spectrum both for the real and imaginary part of the dielectric function, when starting with the HSE06 functional. Furthermore, the x-ray absorption spectra of the O and Mg K-edge calculated with the Exciting code exhibit good agreement with experiment regarding the positions of the prominent peaks, underlining the importance of including the core-hole and electron interactions within the G_0W_0+BSE. Projection of the electron-hole coupling coefficients from the BSE eigenvectors on the band structure allows to explore the origin of the peaks and identify the orbital character of the relevant contributions.

Funding by DFG CRC1242, project C02 is gratefully acknowledged.

HL 46.7 Wed 12:15 GER 38

Strain effects on the lattice-dynamical properties of titanium dioxide — •Peter Weber, Sebastian Tillack, Pasquale Pavone, and Claudia Draxl — Humboldt-Univeristät zu Berlin, Physics Department and IRIS Adlershof, Germany

A fingerprint of temperature-related anharmonic effects in a crystal is the change of the phonon frequencies with the volume. For anisotropic crystals, this variation must be generalized by the introduction of the mode Grüneisen tensor, which expresses the change of the phonon frequencies with respect to any applied strain. In this work, we present the results of an *ab-initio* investigation of the strain effects on the lattice-dynamical properties of the rutile and anatase phases of TiO_2. In particular, we focus our attention to the determination of the generalized Grüneisen parameters at the Brillouin zone center. In order to obtain all independent components of the Grüneisen tensor for these phases, all polar and nonpolar phonon frequencies at the Γ point are calculated for several strained configurations. These calculations are performed using density-functional theory as implemented in the full-potential all-electron software package `exciting` [1]. The connection between the Grüneisen tensors of the acoustic branches and the elastic constants of these materials is analyzed and discussed. Our results are also compared with available Raman scattering data for strained TiO_2.

[1] A. Gulans *et al.*, J. Phys.: Condens. Matter **26** (2014) 363202

HL 46.8 Wed 12:30 GER 38

Ab-initio phonon self-energies and fluctuation diagnostics of phonon anomalies: lattice instabilities from Dirac pseudospin physics in transition-metal dichalcogenides — •Jan Berges[1], Erik van Loon[1], Arne Schobert[1], Malte Rösner[2], and Tim Wehling[1] — [1]Institute for Theoretical Physics and Bremen Center for Computational Materials Science, University of Bremen, Germany — [2]Institute for Molecules and Materials, Radboud University Nijmegen, The Netherlands

We present an ab-initio approach for the calculation of phonon self-energies and their fluctuation diagnostics, which allows us to identify the electronic processes behind phonon anomalies. Application to the prototypical transition-metal dichalcogenide 1H-TaS_2 reveals that coupling between the longitudinal–acoustic phonons and the electrons from an isolated low-energy metallic band is entirely responsible for phonon anomalies like mode softening and associated charge-density waves observed in this material. Our analysis allows to distinguish between different mode-softening mechanisms including matrix-element effects, Fermi-surface nesting, and Van Hove scenarios. We find that matrix-element effects originating from a peculiar type of Dirac pseudospin textures control the charge-density-wave physics in 1H-TaS_2 and similar transition-metal dichalcogenides.

HL 46.9 Wed 12:45 GER 38

Toward a general non-local polarizability density functional for van der Waals dispersion interactions — •Szabolcs Góger, Dmitry Fedorov, Péter Szabó, and Alexandre Tkatchenko — University of Luxembourg, 1511 Luxembourg, Luxembourg

Density functional theory (DFT), while being a workhorse for electronic structure calculations, struggles with describing long-range electron correlations including van der Waals (vdW) dispersion interactions. Various promising approaches have been developed to include vdW interactions in DFT, but a broadly applicable method is yet to be found [1,2]. The first key issue is developing a general density functional for non-local polarizability in molecules and solids. In this work, we use different known properties of atomic and molecular polarizabilites including the direct relation between the dipole polarizability and vdW radius unveiled recently [3]. Diverse methods starting with the Slater-Kirkwood approach [4] are applied to simple quantum mechanical systems like the Drude oscillator and the hydrogen atom under the effect of various electric fields. Our model studies along with prior work on semi-local polarizability functionals [5] pave the way toward developing a unified non-local polarizability functional for molecules and materials.

[1] Hermann *et al.*, Chem. Rev. **117**, 4714 (2017)
[2] Stöhr *et al.*, Chem. Soc. Rev. **48**, 4118 (2019)
[3] Fedorov *et al.*, Phys. Rev. Lett. **121**, 183401 (2018)
[4] Slater and Kirkwood, Phys. Rev. **37**, 682 (1931)
[5] Vydrov and Van Voorhis, Phys. Rev. Lett. **103**, 063004 (2009)

HL 46.10 Wed 13:00 GER 38

Insights into van der Waals interactions from the quantum Drude oscillator model — •Dmitry Fedorov, Martin Stöhr, and Alexandre Tkatchenko — University of Luxembourg, 1511 Luxembourg, Luxembourg

The quantum Drude oscillator (QDO) model [1] represents the response of all valence electrons in an atom by a single Drude particle with its charge, mass, and characteristic frequency. Due to the simple form, this model serves as an insightful approach for the description of atomic response properties and van der Waals (vdW) interactions [2]. Recently, the QDO model helped to unveil a non-trivial relation between the dipole polarizability and the atomic volume, $\alpha_{\mathrm{dip}} \propto V^{4/3}$, [3] as well as the surprising direct relation between the multipole polarizabilities and the equilibrium distances in vdW-bonded atomic dimers [4]. Here, we provide a detailed insight into the physical background of the aforementioned findings. The connection between different striking scaling laws obtained by diverse ways shows the inner consistency and power of this simple but efficient model. We discuss the importance of the revealed quantum-mechanical relations between response and geometric properties of atoms for computational models like the Tkatchenko-Scheffler [5] and the many-body dispersion [2] methods.

[1] Jones *et al.*, Phys. Rev. B **87**, 144103 (2013)
[2] Hermann *et al.*, Chem. Rev. **117**, 4714 (2017)
[3] Kleshchonok and Tkatchenko, Nat. Commun. **9**, 3017 (2018)
[4] Fedorov *et al.*, Phys. Rev. Lett. **121**, 183401 (2018)
[5] Tkatchenko and Scheffler, Phys. Rev. Lett. **102**, 073005 (2009)

HL 46.11 Wed 13:15 GER 38

Conical intersections in molecular systems: 3D vs 2D models — •Erik Pillon, Dmitry Fedorov, Péter Szabó, and Alexandre Tkatchenko — University of Luxembourg, 1511 Luxembourg

The molecular Aharonov-Bohm effect [1], covering various phenomena caused by the Berry (geometric or topological) phase in molecular systems, is an important playground for understanding fundamental quantum physics as well as for building quantum electronic devices. The related non-adiabatic effects, stemming from the coupling between the electron and nuclear degrees of freedom, are especially pronounced in systems possessing conical intersections (CI) in potential energy surfaces, ubiquitous in condensed matter and molecular physics. Many toy models have been introduced to study the influence of CIs on the nuclear dynamics from a general point of view. However, most of them,

including the linear vibronic coupling model [2, 3] widely used in literature, employ two-dimensional (2D) real Hamiltonians. In our work, we check whether such models capture all the important features of real molecular systems. To this end, we perform a comparison of the conventional approaches with the general treatment of a CI within the three-dimensional (3D) complex Hamiltonian possessing SU(2) symmetry [4]. The features present within the 3D model but missing in the 2D case are identified and discussed.

[1] Zygelman, J. Phys. B: At. Mol. Opt. Phys. **50**, 025102 (2017)
[2] Longuet-Higgins *et al.*, Proc. R. Soc. A **244**, 1 (1958)
[3] Jahn and Teller, Proc. R. Soc. A **161**, 220 (1937)
[4] Berry, Proc. R. Soc. A **392**, 45 (1984)

HL 47: 2D Materials IV: Interfacial Interactions (joint session O/HL/CPP)

Time: Wednesday 10:30–13:45 Location: WIL B321

HL 47.1 Wed 10:30 WIL B321

Interplay between electronic instability and moiré structure of monolayer V_2S_3 on Au(111) — •Sahar Pakdel[1], Umut Kamber[2], Raluca-Maria Stan[1], Anand Kamlapure[2], Brian Kiraly[2], Fabian Arnold[1], Andreas Eich[2], Arlette S. Ngankeu[1], Marco Bianchi[1], Jill A. Miva[1], Charlotte Sanders[1], Philip Hofmann[1], Alexander A. Khajetoorians[2], and Nicola Lanata[1] — [1]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, Aarhus, Denmark — [2]Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands

The formation of Moiré superstructures between 2D-materials and their substrates has attracted considerable attention, as it can influence their physical properties. Here we study monolayer V_2S_3 grown on an Au(111) substrate. Scanning tunneling microscopy experiments exhibit multiple domains with different Moiré structures. Comparing the calculated Fermi surfaces with angle resolved photo-emission spectroscopy data, we find that the substrate induces a substantial shift in the chemical potential. We show that the computed Lindhart function of V_2S_3 (at the measured chemical-potential) has a pronounced peak corresponding to a second-order reciprocal point of the prevalent Moiré structure. This suggests that the system tends to favor Moiré structures with modulations able to accommodate underlying electronic instabilities of V_2S_3. We speculate that this could be the manifestation of a more general mechanism and a promising route for tailoring the electronic structure of 2D-materials.

HL 47.2 Wed 10:45 WIL B321

Probing the electronic structure of twisted transition metal dichalcogenide bilayers by photoemission — •bharti parashar[1], sven borghardt[2], kevin janssen[1], mateo jugovac[1], vitaliy feyer[1], dorota wilgocka slezak[3], józef korecki[3], lukasz plucinski[1], and claus m. schneider[1] — [1]PGI-6, FZ Jülich, Germany — [2]PGI-9, FZ Jülich, Germany — [3]Polish Academy of Sciences, Kraków, Poland

Moire bands in twisted transition metal dichalcogenide (TMDC) bilayers are predicted to host novel topological and correlated electronic phases [1]. We performed angle-resolved photoemission studies with few micrometer resolution (μ-ARPES) on several hetero- and homobilayers made from MoS_2 and WSe_2 by mechanical exfoliation and dry transfer technique. The twist angle between the layers was determined in a separate experiment by μ-LEED.

We determine the hybridization between the layers through monitoring the formation of new spectral features in normal emission spectra, that are not present in respected monolayers. The existence of hybridization indicates high quality of the interface that is critical to enable formation of interesting moire bands. Furthermore, our results allow to shed light on whether the valence band maximum is located at Γ or at K at various bilayers. This is improtant for predicted moire physics, since only at K the bands are spin-momentum locked.

[1] See e.g.: F. Wu, T. Lovorn, E. Tutuc, I. Martin, and A. H. MacDonald, Phys. Rev. Lett. 122, 086402 (2019), and refs. therein.

HL 47.3 Wed 11:00 WIL B321

Electronic vs Structural Effects in the Moiré Pattern of MoS_2 on Au(111) — Caio C. Silva[1,2], Daniela Dombrowski[1,2], Nicolae Atodiresei[3], Wouter Jolie[2], Ferdinand Farwick zum Hagen[2], Jiaqi Cai[2], Paul T. P. Ryan[4], Pardeep Thakur[5], Vasile Caciuc[3], Stefan Blügel[3], David A. Duncan[5], Thomas Michely[2], Tien-Lin Lee[5], and •Carsten Busse[1,2,6] — [1]WWU Münster, Germany — [2]Universität zu Köln, Germany — [3]FZ Jülich and JARA, Germany — [4]Imperial College London, U. K. — [5]Diamond Light Source Ltd, U. K. — [6]Universität Siegen, Germany

The lattice mismatch between a monolayer of MoS_2 and its Au(111) substrate induces a moiré superstructure. The local variation of the registry between sulfur and gold atoms at the interface leads to a periodic pattern of strongly and weakly interacting regions. In consequence, also the electronic bands show a spatial variation.

We use scanning tunneling microscopy and spectroscopy (STM/STS), x-ray photoelectron spectroscopy (XPS) and x-ray standing wave (XSW) for a determination of the atomic structure and the resulting electronic properties. The experimental results are corroborated by density functional theory (DFT). We deduce the structure of the supercell with high precision, identify the fraction of interfacial atoms that are strongly interacting, and analyze the variation of the electronic structure in dependence of the location within the moiré cell and the nature of the band.

HL 47.4 Wed 11:15 WIL B321

Complex moiré structures in rotated monolayer V_2S_3 on Au(111) — •Umut Kamber[1], Sahar Pakdel[2], Raluca-Maria Stan[2], Anand Kamlapure[1], Brian Kiraly[1], Fabian Arnold[2], Andreas Eich[1], Arlette S. Ngankeu[2], Marco Bianchi[2], Jill A. Miwa[2], Charlotte Sanders[2], Nicola Lanata[2], Philip Hofmann[2], and Alexander A. Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands — [2]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, Aarhus, Denmark

Moiré superlattices have led to the emergence of tunable many-body states of matter like superconductivity and Mott insulator states absent in the individual layers [1,2]. For transition metal dichalcogenides (TMDCs), there has been a strong interest in how electronic structure is modified near the single layer limit and potentially affected by the dielectric environment. Here, we show spatially periodic modifications to the electronic structure of single layer V_2S_3 grown on Au(111) varying with the underlying moiré pattern [3]. Similar modifications were observed in multiple moiré patterns, each arising from a different relative orientation between the monolayer and the Au(111) substrate. We characterize these spatial variations in electronic structure with respect to the atomic and moiré lattices via scanning tunneling microscopy and spectroscopy, with the help of ab initio calculations.

[1] Y. Cao et al., Nature, 556, 43 (2018).
[2] Y. Cao et al., Nature, 556, 80 (2018).
[3] F. Arnold et al., 2D Mater. 5, 045009 (2018).

HL 47.5 Wed 11:30 WIL B321

Screening effects at the internal interfaces of bulk-like MoS_2 — •Philipp Marauhn, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

The two-dimensional nature of TMDCs is intrinsically linked to reduced screening. This renders the materials sensitive to their dielectric environment. Quasiparticle calculations of MoS_2 deposited on different substrates have shown the importance to account for environmental screening [1]. In this talk we discuss how screening effects modify the electronic structure across the internal interfaces of bulk-like MoS_2.

In a first step we use a tight-binding model to reproduce the band structure on a level of density functional theory. To include polarization effects, we extend the model by introducing a self-energy operator constructed from layer-resolved quasiparticle corrections calculated within the framework of *GW*. Using this *GW*-tight-binding approach, we show that environmental screening has strong impact on the formation of the subbands which originate from interlayer interactions. Most striking, at the K-point, the surface layer decouples from lower lying layers forming a direct gap which is distinctly different from that of the total system.

[1] M. Drüppel et al., Nat. Commun. **8**(1), 2117 (2017)

HL 47.6 Wed 11:45 WIL B321

Charge density wave and superconductivity of single-layer NbSe2 on different screening environments — •Wen Wan, Paul Dreher, Marco Gobbi, and Miguel M. Ugeda — Donostia International Physics Center and Centro de Física de Materiales, San Sebastián-Donostia, Spain

Superconductivity and charge density wave order, typical collective electronic phases of transition metal chalcogenides (TMD), are highly sensitive to external perturbations. In the 2D limit, the properties, and even the mere existence, of these phases in monolayers of TMDs become mostly dependent on the supporting substrate due to charge doping/screening and hybridization effects [1,2]. Here, we carry out low-temperature STM/STS (350 mK) measurements to study the electronic structure of single-layer NbSe2 grown on different substrates by molecular beam epitaxy. In particular, we explore and compare the fate and fundamental properties of the superconducting and CDW states of single-layer NbSe2 on both highly metallic, semi-metallic and insulating TMD substrates [3].

[1] M. M. Ugeda, et al. Nature Physics 12, 92 (2016).
[2] Stan, et al. Phys. Rev. Mat. 3, 044003 (2019).
[3] W. Wan, et al., in preparation.

HL 47.7 Wed 12:00 WIL B321

Incorporation of K and Cs into hBN/Ir(111) and hBN/Ru(0001) — •Jiaqi Cai[1,2,3], Caio Silva[2,3], Wouter Jolie[2], Thais Chagas[1], Kai Mehlich[1], David Duncan[4], Christoph Schlueter[4], Tien-Lin Lee[4], and Carsten Busse[1,2,3] — [1]Department Physik, Universität Siegen, Walter-Flex-Str. 3, 57068 Siegen — [2]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln — [3]Institut für Materialphysik, WWU Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [4]Diamond Light Source, Didcot OX11 0DE, Oxfordshire, United Kingdom

The bi-atomic unit cell of monolayer hexagonal boron nitride (hBN) makes its interaction with the substrate more complex in comparison with its famous cousin, graphene. To probe this interaction, we incorporate alkali metals into hBN/substrate systems. We choose alkali metals for two reasons: i) they tend to lose the electron in the out-most orbitals, thus introducing a strong electronic effect into the hBN/substrate system; ii) the alkali metal ions have full-shell structure, making them unlikely to chemically bond to hBN.

In this talk, we report our experimental results on K as well as Cs incorporation into epitaxial hBN on Ir(111) and Ru(0001). We rely on STM, LEED, XPS, and XSW for the determination of the atomic coordinates with high precision. We report a rich pool of structures (adsorption and/or intercalation of alkali metals), and find that the location of the alkali metal ions are determined by the hBN-substrate interaction strength, and the size of the alkali metal ions.

HL 47.8 Wed 12:15 WIL B321

Control of interface alloying between silicene and a silver substrate — •Johannes Küchle[1], Aleksandr Baklanov[1], Felix Haag[1], David Duncan[2], Paul Ryan[2,3], Ari Seitsonen[4], Willi Auwärter[1], and Francesco Allegretti[1] — [1]Physics Department E20, Technical University of Munich, Germany — [2]Diamond Light Source, Didcot, UK — [3]Imperial College London, UK — [4]Département de Chimie, École Normale Supérieure, Paris, France

Silicene, the silicon analogue of graphene, is a promising material with unique structural and electronic properties, which has been the focus of intense research in the past decade. The epitaxial growth *via* deposition of silicon on solid substrates is an established strategy for silicene preparation, however, strong interfacial interactions may modify the functional properties of the resulting layer. On metal substrates, interfacial alloying may occur, but surprisingly, its role is often underestimated. Here, we present our recent experiments with soft X-ray photoelectron spectroscopy (SXPS) at various Si coverages, indicating that during the growth of the most commonly studied (4 × 4) superstructure of silicene on Ag(111) a Si-Ag surface alloy is formed. Our scanning tunneling microscopy studies resolve a yet unreported phase, which we relate to the Si-Ag alloy. Notably, we show that the alloy related component in SXPS can be largely suppressed by growing silicene on a $GeAg_2$ surface alloy on Ag(111). In this case, a number of distinct structures are observed by low-energy electron diffraction, which differ significantly from all previously reported superstructures of silicene.

HL 47.9 Wed 12:30 WIL B321

Curvature-Induced Charge Baskets in Two-Dimensional Semiconducting Monolayers — •bong gyu shin[1], jz-yuan juo[1], soon jung jung[1], and klaus kern[1,2] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, DE-70569 Stuttgart, Germany — [2]Institut de Physique, École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

The localized quantum states in two-dimensional (2D) materials are attractive for valley- and spin- related optoelectronics or other quantum applications. However, achieving these quantum states is still challenging due to technical difficulties. Here, we investigated strain-induced charge localization and quantum confinement in monolayer MoS_2 on a SiO_2/Si substrate using a gate-tunable home-built scanning tunneling microscope at ∼4.9K. Monolayer MoS_2 follows surface roughness of the substrate, which exhibits a bending strain with band gap reduction. This band gap reduction at a local regime acts like a potential well leading to charge localization. When the bending strain in MoS_2 is larger than 2% at a local region of ∼4 nm, quantum-confined energy levels are observed near the conduction or valence band edge due to the significant band gap reduction of ∼1 eV. Moreover, our theoretical results show that spatial flattening of the conduction (valence) band edge occurs by heavy electron- (hole-) doping of over $\sim 10^{13}$ cm^{-2}. The strain-induced quantum confinement in 2D materials can play an important role in the future development of quantum devices.

HL 47.10 Wed 12:45 WIL B321

Long-range charge order induced by strain in layered $IrTe_2$ revealed by ARPES — •Chris W. Nicholson[1], Maxime Rumo[1], Geoffroy Kremer[1], Thomas Jaouen[1], Baptiste Hildebrand[1], Marie-Laure Mottas[1], Björn Salzmann[1], Aki Pulkinnen[2], Bernardo Barbiellini[2], Timur Kim[3], Saumya Mukherjee[3], Cephise Cacho[3], Matthias Muntwiler[4], Fabian von Rohr[5], Philipp Aebi[1], and Claude Monney[1] — [1]University of Fribourg, Switzerland — [2]LUT University, Finland — [3]Diamond Light Source, UK — [4]Swiss Light Source, Switzerland — [5]University of Zurich, Switzerland

Uniaxial strain combined with ARPES offers a relatively new route to studying the interplay between the lattice and electronic structure. The wide range of properties displayed by layered transition metal dichalcogenides makes them intriguing candidates for exploring this.

Here we present ARPES data revealing the influence of tensile strain on the electronic structure of $IrTe_2$, which exhibits a complicated mixture of one dimensional charge ordered phases at low temperatures but very broad electronic bands [1]. The application of strain induces a single, long-range ordered phase, with clear quasi-1D features at the Fermi level and sharp bands over a wide binding energy range. By comparison with electronic structure calculations, we will discuss the mechanism of this strain-induced stabilization with reference to the redistribution of charge between Ir and Te bonds [2].

[1] Ko et al, Nat. Comm 6, 7342 (2015)
[2] Nicholson et al, in preparation

HL 47.11 Wed 13:00 WIL B321

Seeking 2D Ferromagnets among TMD materials — •Paul Dreher[1,2], Wen Wan[1,2], Adolfo O. Fumega[5], Md N. Huda[4], Shawulienu Kezilebieke[4], Santiago Blanco[2,3], Victor Prado[5], Hannu-Pekka Komsa[4], Marco Gobbi[2,3], Peter Liljeroth[4], and Miguel M. Ugeda[1,2] — [1]Donostia International Physics Center, San Sebastián, Spain — [2]Centro de Física de Materiales, San Sebastián, Spain — [3]CIC nanoGUNE, San Sebastián, Spain — [4]Department of Applied Physics, Aalto University School of Science, 00076 Aalto, Finland — [5]Departamento de Física Aplicada, Universidade de Santiago de Compostela, Campus Sur s/n, E-15782 Santiago de Compostela,Spain

We study the magnetic character of various monolayer TMD candidates (VSe2, CrSe2) grown by MBE on different substrates (NbSe2, graphene, graphite) by combining various characterization techniques. Our findings reveal that the substrate plays a crucial role on the magnetic order in the grown TMD monolayer. The CDW order in single-layer VSe2 causes a strong reduction in the DOS at EF incompatible with ferromagnetism. When grown on graphene substrates, the CDW persists VSe2 and it becomes paramagnetic [1]. Instead, the electronic structure of single-layer VSe2 on a superconducting substrate (NbSe2) shows features compatible with magnetism [2]. Finally, XMCD measurements on Cr-based TMD monolayers indicate the presence of an uncompensated spin in Cr, which retains a paramagnetic behavior even at low temperatures. [1] J.Phys.Chem.C, 123, 27802 (2019), [2] ArXiv:1909.10208 (2019).

HL 47.12 Wed 13:15 WIL B321

Signatures of strong coupling between WS_2 excitons and surface plasmon polariton waves — Moritz Gittinger[1], Sven Stephan[1], Trung Nguyen[1], Antonietta deSio[1], •Martin Silies[1], Christoph Lienau[1], Alison Cadore[2], Ilya Goykhman[2], and Andrea Ferrari[2] — [1]Institute of Physics and Center of Interface Science, Carl von Ossietzky Universität Oldenburg — [2]Cambridge Graphene Centre, University of Cambridge, UK

All-solid-state strong coupling systems with large vacuum Rabi splitting energies are of great potential in future technologies such as quantum information processing. Here, atomically thin layers of transition metal dichalcogenides in close vicinity to metallic nanoparticles have recently been explored as excellent candidates for the observation of this coherent energy transfer from the exciton to its localized surface plasmon counterpart [1]. We here present first results of the interaction between surface plasmon polariton (SPP) waves induced in focused-ion beam written gratings in planar silver films with excitons from atomically-thin WS_2 flakes. By using confocal angle-resolved reflectance spectroscopy, the dispersion relation of the coupled system is mapped at room temperature. We observe a clear anti-crossing of the exciton and the SPP resonance with a normal mode splitting of up to 50meV. We take this splitting as a first signature for a strong coupling between the WS_2 exciton and the SPP wave in the silver grating [2].

[1] Schneider C. et al, Nature Comm. 9, 2695 (2018) [2] Vasa P, and C. Lienau, ACS Photonics 5, 2-23 (2018)

HL 47.13 Wed 13:30 WIL B321

Substrate-dependent charge transfer mechanisms between monolayer MoS2 and molecular dopants — •Patrick Amsalem[1], Soohyung Park[1,2], Thorsten Schultz[1,3], Xiaomin Xu[1], Berthold Wegner[1,3], Areej Aljarb[4], Ali Han[4], Lain-Jong Li[4,5], Vincent C . Tung[4,6], and Norbert Koch[1,3] — [1]Humboldt-Universität zu Berlin, Institut für Physik & IRIS Adlershof, Berlin, Germany — [2]Korea Institute of Science and Technology (KIST), Seoul, South Korea — [3]Helmholtz-Zentrum für Materialien und Energie GmbH, Berlin, Germany — [4]King Abdullah University of Science and Technology, Thuwal, Saudi Arabia — [5]The University of New South Wales, Sydney, Australia — [6]Lawrence Berkeley National Lab, Berkeley, CA, USA

2D transition metal dichalcogenides monolayer films have recently gained enormous attention. Yet, to extend the range of applications of these emerging materials, tuning their Fermi level is of crucial importance. Here, we report on the adsorption of a strong p-type organic dopant, F6TCNNQ, as an efficient route for doping of MoS2 [1]. More specifically, we employ angle-resolved UV and X-ray photoelectron spectroscopy to reveal the charge transfer (CT) mechanisms taking place at a TMDC/organic interface as a function of the electrical properties of the employed supporting substrate, here sapphire, graphite and gold. The present findings can be exploited for the design of advanced hybrid heterostructures with tailored electronic properties.

[1] S. Park et al., Communications Physics 2, 109 (2019).

HL 48: Organic semiconductors II (joint session HL/CPP)

Time: Wednesday 15:00–17:30 Location: POT 112

Invited Talk HL 48.1 Wed 15:00 POT 112

Ultrafast nonadiabatic dynamics and intermolecular conical intersections in organic photovoltaic materials — •Antonietta De Sio — Institut für Physik, Universität Oldenburg

Conjugated polymer and molecular aggregates, used as photoactive materials in organic optoelectronic devices, are large supramolecular assemblies which often present complex energy landscapes and many vibrational degrees of freedom. Coupling of electronic and nuclear motion in molecules may lead to special topologies of potential energy surfaces, such as conical intersections (CoIns). At CoIns, strong vibronic couplings drive ultrafast and efficient nonadiabatic transitions between electronic states and may thus profoundly influence the ultrafast pathways of energy flow and motion of charges. CoIns are of key importance in many photochemical and biological intramolecular processes. So far, however, not much is known about their possible occurrence and relevance for intermolecular excitations in functional condensed-phase assemblies. Here we discuss how ultrafast two-dimensional electronic spectroscopy (2DES) can provide detailed insight into vibronic couplings and nonadiabatic dynamics in technologically relevant organic materials. Specifically, high-time resolution 2DES allows us to experimentally reveal the ultrafast, sub-50-fs passage of a coherent vibrational wavepacket through an intermolecular CoIn in molecular aggregate thin films used in organic photovoltaics. Our results suggest that vibronic couplings and CoIns may help to efficiently steer the energy flow in functional nanostructures, thus opening up new opportunities for controlling transport in organic-based devices.

HL 48.2 Wed 15:30 POT 112

Photoemission Spectroscopy of Organic Charge Transfer Interfaces — •Robert Kuhrt, Martin Hantusch, and Martin Knupfer — IFW Dresden, Helmholtzstraße 20, 01069 Dresden

Understanding physical processes at interfaces involving organic semiconductors plays a key role in optimizing the performance of electronic devices such as solar cells, where absorber and transport layers form interfaces involving metals as well as organic semiconductors. Furthermore, charge transfer between organic molecules might result in interesting properties such as metallic conductivity or correlated electronic states like superconductivity.

In this contribution, we present photoemission spectroscopy studies of various interfaces involving the strong electron acceptor hexafluorotetracyanonaphthoquinodimethane (F6TCNNQ). We compare the electronic properties of organic based donor, acceptor systems. Significant changes are observed in both the core levels and the valence orbitals at the interface, indicating a charge transfer between the materials. Origin and character of the charge transfer as well as the influence of substrate and film structure are discussed.

Acknowledgement: Financial support by the DFG (KN393/25; KN393/26) is gratefully acknowledged.

HL 48.3 Wed 15:45 POT 112

Vacuum processed single crystalline organic semiconductor thin films for high-performance electronic and optoelectronic device applications — •Shu-Jen Wang[1,2], Michael Sawatzski[1], Ilia Lashkov[1], Yulia Krupskaya[2], Hans Kleemann[1], Bernd Büchner[2], and Karl Leo[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), TU Dresden, Germany — [2]Leibniz Institute for Solid State and Materials Research (IFW), Germany

Organic semiconductors enable many technologically important applications such as organic light emitting diodes, solar cells and flexible circuits due to their unique physical properties and chemical structure tunability. Conventional amorphous organic semiconductors show low carrier mobility as their charge transport is limited by their structural order. Therefore, charge transport in organic semiconductors can generally be improved by higher degree of structural order and crystallinity. In this presentation, we will show efficient conversion of vacuum processed amorphous thin films to single crystalline thin films through annealing with appropriate surface treatment. We will also show functional devices such as field-effect transistors and light emitting diodes built on the single crystalline thin films and discuss their potential for high performance circuit and optoelectronics applications.

30 min. break.

HL 48.4 Wed 16:30 POT 112

Coherent Real-Space Charge Transport Across a Donor-Acceptor Interface Mediated by Vibronic Couplings — Ziyao Xu[1], Yi Zhou[1], Lynn Gross[2], Antonietta De Sio[3], ChiYung Yam[4], Thomas Frauenheim[2], GuanHua Chen[1], and •Christoph Lienau[3] — [1]Department of Chemistry, University of Hong Kong — [2]BCCMS, University of Bremen — [3]Institut für Physik, Universität Oldenburg — [4]Beijing Computational Science Research Center

Growing experimental and theoretical evidence suggests that vibronic couplings (VCs), couplings between electronic and nuclear degrees of freedom, play a fundamental role for the ultrafast excited-state dynamics in organic donor-acceptor materials. While VC has been shown to support charge separation at donor-acceptor interfaces, so far, little is known about its role for the real-space transport of charges in these

systems. Here we theoretically study charge transport in thiophene-fullerene stacks using time-dependent density functional tight-binding theory combined with Ehrenfest molecular dynamics for open systems. Our results reveal coherent oscillations of the charge density between neighboring donor sites, persisting for ¯200 fs and promoting charge transport within the polymer. At the donor-acceptor interface, vibronic wave packets are launched, propagating coherently over distances of >3 nm into the acceptor region. This supports previous experimental observations of long-range ballistic charge motion in organic photovoltaic systems and highlights the possibility of VC engineering as a concept for tailoring the functionality of organic devices

HL 48.5 Wed 16:45 POT 112

Light-assisted charge propagation in organic semiconductor networks on hexagonal boron nitride — Matkovic Aleksandar[1], Genser Jakob[1], •Kratzer Markus[1], Lüftner Daniel[2], Chen Zhongrui[3], Siri Olivier[3], Puschnig Peter[2], Becker Conrad[3], and Teichert Christian[1] — [1]Institute of Physics Montanuniversität Leoben Franz Josef Strasse 18, Leoben 8700, Austria — [2]Institute of Physics Karl-Franzens-Universität Graz NAWI Graz Universitätsplatz 5, Graz 8010, Austria — [3]Aix Marseille University CNRS CINaM UMR 7325 Campus de Luminy 13288, Marseille cedex 09, France

Electrostatic force microscopy is utilized to track charge propagation in organic semiconductor nanoneedles. As model system, crystalline dihydrotetraazaheptacene needles epitaxially grown on ultrathin hexagonal boron nitride was investigated. Due to light exposure, the specific resistivity of the crystallites changed by two orders of magnitude. Exploiting the highly anisotropic optical properties of the organic nanoneedles, selective charge propagation along the crystallites was achieved by matching the incident light's polarization direction with the direction of the molecular backbones in the crystals. Thus, it was possible to guide charge propagation along desired paths in self-assembled crystallite networks. This way, polarized light can be used as a "light gate" to control charge propagation.

HL 48.6 Wed 17:00 POT 112

Electron paramagnetic resonance in OLEDs based on dual-emitting host-guest systems — •Felix Braun[1], Tobias Grünbaum[1], Wolfram Ratzke[1], Sebastian Bange[1], Sigurd Höger[2], and John M. Lupton[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Universitätsstraße 31, 93053 Regensburg, Germany — [2]Kekulé-Institut für Organische Chemie und Biochemie, Universität Bonn, Gerhard-Domagk-Straße 1, 53121 Bonn, Germany

OLEDs exhibit strong sensitivity to magnetic fields due to spin-dependent electron-hole recombination. Employing the dual-emitting host-guest system CBP:DB, we can optically assess the spin-permutation symmetry of charge-carrier pairs by their magnetic-field dependent electroluminescence.

We monitor the interconversion between singlet-like and triplet-like populations under electron paramagnetic resonance (EPR) conditions and observe the anticipated anticorrelation in the behaviour of singlet-like and triplet-like carrier pairs. Furthermore, using a deuterated counterpart of the dual-emitting system, we can verify the influence of the hyperfine fields on the linewidth of the EPR signal. We anticipate that altering the spatial distribution of hyperfine interactions between host and guest will allow us to pinpoint the molecular site on which a charge-carrier pair is formed by analysing the EPR linewidth. With the spin-sensitivity introduced by the dual emitter, we even hope to determine whether, e.g., a singlet-like carrier pair preferentially forms on the guest emitter or on the host matrix.

HL 48.7 Wed 17:15 POT 112

Reverse Dark Current in Organic Photodetectors — •Jonas Kublitski[1], Andreas Hofacker[1], Christina Kaiser[2], Donato Spoltore[1], Hans Kleemann[1], Axel Fischer[1], Koen Vandewal[3], and Karl Leo[1] — [1]IAPP - TU Dresden, Germany — [2]Swansea University, UK — [3]IMO - Hasselt University, Belgium

Photodetectors (PDs) find broad applications in many fields of optics. While inorganic PDs are widely used, they lack in easy processability and narrow-band detection. Organic PDs can fulfill these demands, providing many further advantages in comparison to inorganic PDs. The limiting factor of OPDs is their low detectivity, mostly caused by high dark current (J_D) at reverse bias. Traps and sub-gap states are often observed in organic materials. Here, we investigate their effect on J_D. We observe that J_D follows a trend with the energies of the sub-gap CT states (E_{CT}). Furthermore, in specific donor:C_{60} blends, we find trap concentrations of around 10^{16} cm^{-3} with an energy of around 0.5 eV below the transport level of C_{60}. We intentionally vary the trap concentration in these blends and observe that*J_D scales accordingly. Dark current-voltage simulations show that the expected value of*J_D increases four orders of magnitude and rules the dark JV characteristics, when traps are included. The dependence of J_D on reverse bias can be understood as an enhanced detrapping by means of Poole-Frenkel effect. These results point out to a physical process that might be general in donor:acceptor structures, explaining the high*J_D commonly observed in OPDs. Moreover, optimized devices show J_D as low as 500 pA cm^{-2} at -1 V, and on/off ratio of 10^7.

HL 49: Quantum dots and wires II

Time: Wednesday 15:00–18:15 Location: POT 151

HL 49.1 Wed 15:00 POT 151

Charge tuning of GaAs quantum dots using Schottky diode structure — •Nand Lal Sharma[1], Robert Keil[1], Caspar Hopfmann[1], Fei Ding[2], and Oliver Schmidt[1,3] — [1]Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany — [2]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, 30167 Hannover, Germany — [3]Chemnitz University of Technology, Reichenhainer Strasse 70, 09107 Chemnitz, Germany

Semiconductor quantum dots (QDs) are promising candidates for high quality photon sources and the biexciton cascade decay in such dots is most advanced technique for the generation of entangled photon pairs. In this work the GaAs/AlGaAs QDs are grown by droplet epitaxy [1] employing a n-i Schottky diode structure. The back contact is prepared by thermal diffusion and the top contact is prepared by deposition of semi-transparent 2 and 4nm Cr and Au, respectively. The GaAs QD photoluminescence from different charging states is controlled by application of an external bias. The effects of quantum dot charging, quantum confined Stark effect, exciton fine structure and photon coherence are investigated as a function of bias voltage.

[1] Keil et. al. Nat. comm. 8, 15501(2017)

HL 49.2 Wed 15:15 POT 151

Aligning quantum dots on non-structured surfaces using roughness modulation — •Nikolai Bart[1], Christian Dangel[2], Jonathan Finley[2], Kai Müller[2], Aimeric Courville[3], Marcel Schmidt[1], Andreas D. Wieck[1], and Arne Ludwig[1] — [1]Ruhr-Universität Bochum, Lehrstuhl für Angewandte Festkörperphysik, Universitätsstraße 150, 44801 Bochum — [2]Technische Universität München, Walter Schottky Institut, Am Coulombwall 4, 85748 Garching bei München — [3]CNRS, Université Côte d'Azur, CRHEA, Rue Bernard Grégory, 06560 Valbonne, France

We present a novel approach to site selective growth of InAs/GaAs quantum dots on a smooth surface (miscut < 0.1°), without the use of ex-situ preparation of the wafer. For this, we deposit a layer of GaAs onto a (1 0 0) GaAs substrate during stopped rotation of the wafer, thereby creating a periodic modulation of the surface roughness on an atomic scale. If we deposit InAs onto this, QD nucleation is enhanced at locations of high roughness, thus creating a stripe pattern of high and low QD density. With this method, we can create stripes with periodicities between 3 and 0.3 mm and combine stripe patterns to create two-dimensional lattice patterns. Macro photoluminescence maps performed on these structures are in good agreement with simulations using a geometric approach.

HL 49.3 Wed 15:30 POT 151

Self-organized linear alignment of high-density Stranski-Krastanov quantum dots — •Tommy Müller, Udo W. Pohl, Laura Meissner, and Tore Niermann — Technische Universität Berlin, Germany

The linear alignment of high-density quantum dot (QD) ensembles is interesting for active waveguide structures. We present the fabrication of a self-organized linear array of such an ensemble in a multilayer structure without the application of post-growth lithography.

We applied the buried-stressor principle [F. Kießling et al., PRB 91, 075306 (2015)]: by selectively oxidizing buried AlGaAs-AlAs-AlGaAs layers, we produce a stripe-shaped tensile strain field in the GaAs cap layer. Here InGaAs Stranski-Krastanov QDs prefer to nucleate on top in a second epitaxy. Nucleation control of linear stressors proved more challenging than on circular stressors due to the reduction to a single lateral strain component. We still achieved a high density of QD stripes with high contrast to the side areas. Further increased QD density decreases the contrast. An improved contrast was obtained for stacked stripe structures, where a second QD layer was nucleated on top of a site-controlled buried first QD layer. The presentation outlines essential parameters for the lateral site control of the QD ensemble, confirmed by strain simulations.

HL 49.4 Wed 15:45 POT 151

Electronic structure analysis of GaAs quantum dots using correlation spectroscopy — •Robert Keil[1], Nand Lal Sharma[1], Caspar Hopfmann[1], Fei Ding[2], and Oliver Schmidt[1,3] — [1]Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany — [2]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, 30167 Hannover, Germany — [3]Chemnitz University of Technology, Reichenhainer Strasse 70, 09107 Chemnitz, Germany

Droplet etched GaAs quantum dots are promising candidates for many quantum light sources and have already demonstrated to be the best entangled photon sources to date [1]. In order to employ these devices also in other quantum optical schemes - such as carrier spin coherence based generation of photonic cluster states - a comprehensive understanding of the electronic level structure is essential. In this work we will present an electronic structure analysis based on comparative correlation spectroscopy of single photons combined with traditional photoluminescence spectroscopy methods.

[1] Zopf et. al. PRL 123, 160502 (2019)

HL 49.5 Wed 16:00 POT 151

Electrical control of spins and giant g-factors in ring-like coupled quantum dots — Heidi Potts[1], I-Ju Chen[1], •Athanasios Tsintzis[1], Malin Nilsson[1], Sebastian Lehmann[1], Kimberly Dick[1,2], Martin Leijnse[1], and Claes Thelander[1] — [1]Division of Solid State Physics and NanoLund, Lund University, SE-221 00 Lund, Sweden — [2]Centre for Analysis and Synthesis, Lund University, SE-221 00 Lund, Sweden

Emerging theoretical concepts for quantum technologies have driven a continuous search for structures where a quantum state, such as spin, can be manipulated efficiently. Central to many concepts is the ability to control a system by electric and magnetic fields, relying on strong spin-orbit interaction and a large g-factor. Here, we present a mechanism for spin and orbital manipulation using small electric and magnetic fields. By hybridizing specific quantum dot states at two points inside InAs nanowires, nearly perfect quantum rings form. Large and highly anisotropic effective g-factors are observed, explained by a strong orbital contribution. Importantly, we find that the orbital contributions can be efficiently quenched by simply detuning the individual quantum dot levels with an electric field. In this way, we demonstrate not only control of the effective g-factor from 80 to almost 0 for the same charge state, but also electrostatic change of the ground state spin.

HL 49.6 Wed 16:15 POT 151

Electronic structure of (InGa)(AsSb)/GaAs/GaP quantum dots — •Petr Klenovský[1,2], Elisa Maddalena Sala[3,4], Petr Steindl[1,5], Andrei Schliwa[3], and Dieter Bimberg[3,6] — [1]Masaryk University, Brno, Czech Republic — [2]Czech Metrology Institute, Brno, Czech Republic — [3]TU Berlin, Berlin, Germany — [4]EPSRC National Epitaxy Facility, The University of Sheffield, North Campus, Sheffield, United Kingdom — [5]Leiden University, Leiden, Netherlands — [6]Bimberg Chinese-German Center at CIOMP, Changchun, China

The electronic structure of self-assembled (InGa)(AsSb)/GaAs/GaP QDs is studied. These QD structures present an excellent example for systems exhibiting concurrently direct and indirect transitions both in real and momentum space. The structures were grown via MOVPE [1]. Our results show that they provide an easier access to applications in quantum information technology, as compared to the currently studied InGaAs/GaAs QDs. [2]. Our theoretical results are compared to and are verfied by detailed photoluminescence measurements [3]. We also compare results obtained for QDs grown on both GaP and GaAs substrates, revealing the influence of the large hydrostatic stress, particularly on valence band states, enabling the realization of the QD-Flash memory concept [1], where holes in type-II QDs act as storage units.

[1] Sala, E. M., et al., Phys. Stat. Sol. B, 1800182 (2018).
[2] Klenovsky, P., et al., Phys. Rev. B **100**, 115424 (2019).
[3] Steindl, P., et al., Phys. Rev. B **100**, 195407 (2019).

30 min. break.

HL 49.7 Wed 17:00 POT 151

Excess noise in quantum ring interferometers — Christian Riha[1], Sven S. Buchholz[1], Olivio Chiatti[1], Andreas D. Wieck[2], Dirk Reuter[3], and •Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Angewandte Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany — [3]Optoelektronische Materialien und Bauelemente, Universiät Paderborn, 33098 Paderborn

Cross-correlated noise measurements are performed in etched $Al_xGa_{1-x}As$/GaAs based quantum rings in equilibrium at a bath temperature of $T_{bath} = 4.2$ K. The measured white noise exceeds the thermal noise expected from the measured electron temperature T_e and the electrical resistance R. This excess part of the white noise decreases as T_{bath} increases and vanishes for $T_{bath} > 12$ K. Excess noise is not observed if one arm of a quantum ring is depleted of electrons or in 1D-constrictions that have a length and width comparable to the quantum rings. A model is presented that suggests that the excess noise originates from the correlation of noise sources, mediated by phase-coherent propagation of electrons.

HL 49.8 Wed 17:15 POT 151

Exciton recombination dynamics in CdSe nanocrystals in glass matrix — •Gang Qiang[1], Elena V.Shornikova[1], Dmitri R.Yakovlev[1,2], Aleksandr A. Golovatenko[2], Anna V. Rodina[2], Evgeniy A. Zhukov[1], Aleksei A. Onushchenko[3], and Manfred Bayer[1,2] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44221 Dortmund, Germany. — [2]Ioffe Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia. — [3]ITMO University, 199053, St.-Petersburg, Russia.

In this work, we studied CdSe nanocrystal (NC) with diameter from 2.8 to 6.2 nm grown in glass matrix. Temperature and magnetic field dependence of photoluminescence (PL) decay measurements demonstrate the exciton nature of the emission state. With the decreasing of NC size, due to the quantum confinement effect, the band gap of samples is blue shifted, and the bright-dark exciton splitting also becomes larger which is indicated by the deceleration of the dark exciton recombination process where a larger time constant for the long tail of the PL decay curve in the smaller sample is observed.

HL 49.9 Wed 17:30 POT 151

Carrier and energy transfer in colloidal quantum dot semiconductor hybrids — •Mikko Wilhelm, Shyam Kommadath, Salwa Khokhar, and Wolfram Heimbrodt — Philipps-Universität Marburg

Colloidal quantum dots are attractive for functionalization of semiconductors in electronic and opto-electronic devices like solar cells, field effect transistors or spintronic devices. CdS/ZnS and CdSe/ZnS core/shell quantum dots of different sizes synthesized in solution are deposited via knife coating on different semiconductor substrates. Depending on the band alignment between the quantum dots and the semiconductor substrate, energy and charge transfer is observed. The interaction between the quantum dots and semiconductor substrate is studied with optical spectroscopy. The results of continuous wave and time resolved photoluminescence measurements at different temperatures from 10K to room temperature are presented and discussed.

HL 49.10 Wed 17:45 POT 151

High-precision determination of Silicon nanocrystals — •Ronja Köthemann, Nils Weber, Jörg K. N. Lindner, and Cedrik Meier — Universität Paderborn, Deutschland

Silicon nanocrystals have atom-like discrete energy levels and exhibit strong luminescence in the visible spectral range. However, for parti-

cles embedded in a host matrix, size determination is challenging when the nanocrystals are smaller than 5 nm in diameter. Therefore, we evaluate different approaches to determine the size of the silicon nanocrystals. The nanocrystals are fabricated using a plasma-enhanced chemical vapor deposition (PECVD) process with subsequent annealing in a tube furnace. For characterization, different experimental techniques are used, including optical measurements such as photoluminescence or nonlinear optical response and analytical transmission electron microscopy. Furthermore, preliminary results for integrating the nanocrystals into photonic crystal disks are shown.

HL 49.11 Wed 18:00 POT 151

Optical properties of a double-dot rod semiconductor — •Marcel Dohrmann, Tobias Kipp, Christian Strelow, and Alf Mews — University of Hamburg, Institute of Physical Chemistry

Due to their heterogenic semiconductor band system, double dot-rod semiconductors have very interesting properties. With three different semiconductor materials, not only classical Type I or Type II systems can be achieved, but also combinations of these. For example, a system like CdSe/CdS/PbS can have two trap regions of holes and electrons. This system has been synthesized in our group and will be analyzed via confocal spectroscopy. The electron and hole wave functions and exciton energies are calculated by a numerical Schrödingers equation solver within the effective mass approximation. Our emission spectra shows two emission maxima, which are in good alignment with our calculations. Therefore this semiconductor system consist of two type I regions, is a double emitter, and could have different decay curves for each wavelength area.

HL 50: Perovskite and photovoltaics IV (joint session HL/CPP)

Time: Wednesday 15:00–17:30 Location: POT 251

HL 50.1 Wed 15:00 POT 251

Computational study of the effect of surfaces on the molecular orientation and optical properties of hybrid lead halogenide perovskites — •Gabriele Saleh, Giulia Biffi, and Sergey Artyukhin — Istituto Italiano di Tecnologia, Via Morego 30, Genova 16163 Italy

MAPbX3 perovskites (MA= CH3NH3+, X= Cl,Br,I) are attracting intense interest due to their outstanding performance in optoelectronic devices. The efficiency of MAPbX3 as photovoltaics is governed by the electronic excitation and de-excitation processes. It is widely recognized that MA molecules have an indirect yet strong influence on the band gap and on the optoelectronic properties in general. This effect is particularly intricate since it is depends on the mutual orientations of neighboring molecules (configurations), which is continuously changing at T>100 K [1]. Here we study the energetics of MA configurations near surfaces and the correlation between the dynamical behavior of MA molecules and the optical properties of MAPbX3. Force field molecular dynamics (MD) and electronic structure simulations are performed. We find a linear dependence of the band gap on the octahedral tilt angle of the PbX3 scaffold, which in turn is determined by the orientation of MA molecules. We show how the surface influences the dynamics of MA molecules, and how this affects the surface optical properties. Representative snapshots of MD simulations at different T are extracted and their electronic structure is analyzed in order to explain the measured MAPbBr3 photoluminescence spectra. [1] O. Selig et al. (2017) J. Am. Chem. Soc., 139, 4068

HL 50.2 Wed 15:15 POT 251

New insights into emerging lead-free double perovskite materials for optoelectronics — •Fabian Schmitz[1], Jonas Horn[2], Teresa Gatti[1], and Derck Schlettwein[2] — [1]Justus Liebig University Gießen, Institute of Physical Chemistry — [2]Justus Liebig University Gießen, Institute of Applied Physics

Lead-halide perovskites have become top-notch photoactive materials for application in solar cells, photodetectors and LEDs, due to their ease of synthesis, low-costs and excellent solution processability. For photovoltaics particularly, an impressive growth in power conversion efficiency (PCE) has been realized in few years, with current certified record at 25.2 %. Nevertheless, the most efficient perovskite solar cells still suffer from poor environmental stability and contain toxic elements. In this regard, there have been attempts to substitute lead by other metals such as tin or germanium, but no significant improvement in stability has been achieved. Good perspectives are emerging from the use of an all inorganic double perovskite, namely $Cs_2AgBiBr_6$. In this species, divalent lead is replaced by equal molar amounts of monovalent silver and trivalent bismuth. The material is characterized by an excellent environmental stability, but PCE of solar cells containing it are never higher than 2.5 %. Here we report on an optimized preparation of $Cs_2AgBiBr_6$ films and on a method to estimate charge carrier diffusion lengths within them. We also provide insights into novel material design strategies for improving optoelectronic performance in this material, by resorting to 2D/3D engineering and doping/alloying.

HL 50.3 Wed 15:30 POT 251

Costly efficient computational approach for calculating electronic structure of complex Organic/Inorganic Perovskites — Mohammad Moaddeli, •Mansour Kanani, and Amir Tangestani — Department of Materials Science and Engineering, School of Engineering, Shiraz University

Predictive and costly efficient computational approaches are demanding for emerging perovskite structures including heavy elements. Despite large number of research productivity on this field, there is not a consensus of multiscale material design approach. One of the main bottlenecks comes from complexity of electronic interactions in such a structure which can only be analyzed using costly modified quantum mechanical methods. We introduce a hybrid quantum/molecular dynamics computational framework to deal with different diversities of synthesized perovskite layers. We use powerful reactive force field interatomic potentials for relaxing the organic part including the van der Waals effect and interactively get electronic structure using the DFT-1/2 approach. All the procedure is verified and may be modified by the accurate hybrid functional methods. Couple of potential inorganic cations with various combination of halides are considered via this approach. This let us to find best candidate among large number of combinations. Furthermore we could predict a modified fractional distribution and doping elements for some introduced mixed cation perovskites in the literature.

HL 50.4 Wed 15:45 POT 251

Spatially elucidating the role of defects in the photophysics of mixed halide perovskites — •David O. Tiede[1], Juan F. Galisteo-López[2], Mauricio E. Calvo[2], and Hernán Míguez[2] — [1]University of Münster, Institute of Physics, Münster, Germany — [2]Instituto de Ciencia de Materiales de Sevilla (CSIC-US), Seville, Spain

Light-induced structural changes in mixed halide perovskites are among the most critical instabilities of this material that hamper their future commercialization. In particular, reversible light-induced phase segregation and its corresponding spectral cha ges in emission is a major drawback in precise bandgap tuning, which is crucial for both efficient light harvesting in tandem solar cells and modifying the spectral output of LEDs. Over the past years, various reports have pointed towards the critical role of defects in this process and a strong dependency on environmental effects. However, the exact mechanism of the migration of halides is still under debate.

In this work we have carried out a spectrally-resolved microphotoluminescence experiments, employing a confocal microscope, to study the formation of iodine-rich domains in CH3NH3PbBrxI3-x thin films. With macroscopic measurements we verify that defects account for a dominant role on phase segregation and cause the formation of iodine-rich domains in minor parts of the material. By modifying the atmospheric conditions and changing the stoichiometry of halide components during the synthesis, we clarify the impact of vacancies and interstitials on the photophysics of these materials.

30 min. break

HL 50.5 Wed 16:30 POT 251

Study of photon recycling in perovskite optoelectronics — •Changsoon Cho[1,2,3,4], Baodan Zhao[1], Gregory Tainter[1],

Frederik Nehm[2], Karl Leo[2], Jung-Yong Lee[3], Richard Friend[1], Dawei Di[1,4], Felix Deschler[1], and Neil Greenham[1] — [1]Cavendish Laboratory, Department of Physics, University of Cambridge, J.J. Thomson Avenue, Cambridge CB3 0HE, UK — [2]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Technische Universität Dresden, Dresden 01187, Germany — [3]School of Electrical Engineering, Korea Advanced Institute of Science and Technology (KAIST), Daejeon 34141, Republic of Korea — [4]State Key Laboratory of Morden Optical Instrumentation, College of Optical Science and Engineering, Zhejiang University, Hangzhou 310027, China

Photon recycling (PR), consisting of successive light re-absorption and re-emission processes, is a key mechanism to understand the distinct optical properties of perovskite light-emitting diodes (PeLEDs). Here we verify the existence of PR effect via the measurement of spatially-resolved photoluminescence (PL) and electroluminescence (EL). To quantify the PR effect in PeLEDs, we propose an optical modelling method taking photon re-absorption and re-emission into account. According to the optical analysis of currently reported state-of-the-art devices, PR is shown to be able to contribute to more than 70% of the EQEs. Finally, we introduce various optical designs of PeLEDs, to maximize PR effect and enhance the quantity and property of light emission.

HL 50.6 Wed 16:45 POT 251

On the Radiative Recombination Efficiency and Carrier Lifetime in Halide Perovskite Solar Cell Materials — •Thomas Unold[1], Martin Stolterfoht[2], Jose Marquez-Prieto[1], Dieter Neher[2], and Thomas Kirchartz[3] — [1]Helmholtz-Zentrum Berlin — [2]Institute of Physics and Astronomy, Universität Potsdam — [3]Forschungszentrum Juelich GmbH

The open-circuit voltage, which is currently considered the main performance limitation of halide perovskite solar cells, is determined by bulk and interface recombination processes in the solar cell.[1] Under ideal conditions the open-circuit voltage approaches the internal quasi-Fermi level splitting (QFLS), which may be estimated by the measurement of the external photoluminescence quantum yield (PLQY) and the absorption properties.[2] The photoluminescence quantum yield and quasi-Fermi level splitting can also be estimated by measurement of the time-resolved photoluminescence (TRPL), if the radiative recombination constants and photon recycling are taking into account properly.[3] A survey of the literature shows that the reported PLQY for measured open-circuit voltages sometimes vary by orders of magnitude, which is difficult to understand from the point of theory. In this contribution we show that careful consideration of the above points leads to a consistent picture of the interrelation of the QFLS, PLQY and TRPL lifetime, and discusses possible sources of error in the analysis. [1] Stolterfoht et al., Nature Energy 3 (2018) 847 [2] Liu et al., ACS Energy Lett. 4 (2019) 110 [3] Staub et al., Phys. Rev. Appl. 6 (2016) 044017

HL 50.7 Wed 17:00 POT 251

Carrier Diffusion in Bulk and Nanocrystalline Halide Perovskites — •Michael Lichtenegger and Alexander Urban — Nanospectroscopy Group, Nano-Institute Munich, Department of Physics, Ludwig-Maximilians-Universität München, Königinstr.10, 80539 Munich, Germany

Carrier injection, transport and extraction are crucial physical properties for optoelectronic applications such as solar cells and light-emitting diodes (LEDs). Depending on the magnitude of the exciton binding energy in a material, electron-hole pairs can exist as free carriers or can form a bound state, so-called excitons. Large binding energies appear especially for systems where at least one spatial dimension is confined, e.g. in nanocubes, 2D nanoplatelets 1D nanowires or 0D quantum dots. Consequently, carrier transport will be very different depending on the nature of the material.

Our goal is to investigate and understand carrier diffusion in large perovskite crystals and assemblies of nanocrystals. For this we have realized a contactless photoluminescence (PL) and confocal time-correlated single photon counting (TCSPC) setup. We use this to measure the diffusion length for bulk perovskite films, and thin films of nanocrystals. We modify the perovskite compositions, geometries and passivating ligands to investigate the nature of the transport processes and determine critical parameters such as diffusion lengths and diffusion coefficients.

HL 50.8 Wed 17:15 POT 251

Temperature-dependent high spatial-resolution spectroscopy to investigate NCs in single micelles — •Markus Schoger, Carola Lampe, Moritz Gramlich, and Alexander Urban — Nanospectroscopy Group, Department of Physics, Ludwig-Maximilians-Universität, Munich, Germany

Halide perovskite nanocrystals (NCs) have shown outstanding potential for light-emitting applications with high quantum yields and an emission wavelength tunable throughout the visible spectrum. Despite these impressive advances, they still suffer from several issues, which currently impede widespread commercialization. To enhance their stability, we recently introduced a colloidal synthesis, wherein the NCs are grown inside diblock copolymer micelles.1 These nanoreactors additionally provide a protective shell, limiting degradation and ion migration. In order to maximize their potential and enable optoelectronic integration, an in-depth understanding of the nanostructure structure and resulting properties on a single micelle level is critical. Here, we present temperature-dependent high spatial-resolution spectroscopy to investigate single micelle-encapsulated perovskite NCs in temperature intervals from 4 K up to room temperature to gain insight into their fundamental properties.

1 V. A. Hintermayr, C. Lampe, M. Low, J. Roemer, W. Vanderlinden, M. Gramlich, A. X. Bohm, C. Sattler, B. Nickel, T. Lohmuller, and A. S. Urban, Nano Lett. 19 (8), 4928 (2019).

HL 51: Semiconductor lasers I

Time: Wednesday 15:00–18:00 Location: POT 51

HL 51.1 Wed 15:00 POT 51

Direct Band-Gap Emission from Hexagonal SiGe: Towards a SiGe Nanolaser — •Claudia Rödl, Jens Renè Suckert, Jürgen Furthmüller, Friedhelm Bechstedt, and Silvana Botti — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Incorporation of microelectronics and optoelectronics is expected to revolutionize various fields of technology, such as communication, sensing, and imaging. A Si-compatible nanolaser would be the key to achieve integrated silicon photonics. However, Si as well as Ge in their diamond-structure equilibrium phases are known to be optically inactive due to the indirect nature of their band gaps. The hexagonal allotropes of Si and Ge in the lonsdaleite phase, which can now be grown in good quality, may overcome this limitation. Hexagonal Si is still indirect, whereas hexagonal Ge is a direct semiconductor. Unfortunately, the dipole matrix elements of the lowest optical transitions are almost zero. Here, we show that it is possible to enhance the optical oscillator strengths of hexagonal Ge by applying tensile uniaxial strain or alloying it with Si. Upon structural modification, the two lowest conduction bands change order and the lowest optical transitions become strongly dipole active. We compare our results to recent data from our experimental collaborators. Using first-principles density-functional theory with hybrid functionals and the MBJLDA meta-GGA, we calculate structural and electronic properties and show how the absorption and emission spectra are affected by strain and alloying, respectively.

HL 51.2 Wed 15:15 POT 51

Thresholdless transition to coherent emission at telecom wavelength from metallic cavity nanolasers — •Frederik Lohof[1], Sören Kreinberg[2], Kaisa Laiho[2], William Hayenga[3], Paweł Holewa[2], Mercedeh Khajavikhan[3], Stephan Reitzenstein[2], and Christopher Gies[1] — [1]Institute for Theoretical Physics, University of Bremen — [2]Institute for Solid State Physics, Technical University Berlin — [3]CREOL, Univerity of Central Florida

The miniaturization of semiconductor nanolasers has created an avenue to (near) thresholdless devices with small footprints for applications in photonics and quantum information. In this regime, the onset of coherent emission, i.e. the threshold, must be determined from a change in

the photon statistics of the emission, as output intensity and linewidth provide ambiguous information. We present results from theoretical and experimental studies of telecom wavelength, thresholdless coaxial nanolasers using metallic cavities. These cavities allow to confine light on length scales below the diffraction limit, leading to high field intensities and large light-matter interactions. Our theoretical modeling gives access to time-resolved photoluminescence and fingerprints of the emission's photon statistics, given by photon-correlation functions. In modeling of the experimentally obtained data, we demonstrate a clear onset of coherent emission at finite pump powers. Our combination of experimental and theoretical techniques results in a comprehensive picture of the device dynamics, verifying its lasing operation and providing directions for future experimental designs of nanolasers.

HL 51.3 Wed 15:30 POT 51

Characteristics of red MECSEL with a quantum dot active region — •Ana Ćutuk[1], Roman Bek[2], Michael Jetter[1], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integraed Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart — [2]Twenty-One Semiconductors GmbH, Kiefernweg 4, 72654 Neckartenzlingen

Quantum dots (QDs) as active region for a laser are very attractive due to their promising properties e.g. higher differential gain, lower threshold, better temperature stability and wavelength versatility. We choose a membrane approach as it is realized by a membrane external-cavity surface-emitting laser (MECSEL) for improved thermal budget. Therefore we realized a semiconductor membrane structure consisting of an AlGaInP/InP QD active region deposited on GaAs substrate in the Stranski-Krastanow growth mode by metal-organic vapor-phase epitaxy (MOVPE) with emission in the red spectral range. Our usual processing technique implies a membrane release from the substrate with capillary bonding between two heat spreaders. However, the internal strain makes this approach rather difficult, which is why also wafer-bonding of the semiconductor structure to one heat spreader and further processing of the membrane including bonding the second heat spreader was performed. In this contribution we present our newest results on the QD-based MECSEL. Ongoing characterization includes comparison of the two bonding approaches in terms of laser output in order to learn more about the influence of the internal strain.

HL 51.4 Wed 15:45 POT 51

Miniaturized lasers for picosecond ultrasonics — •Michal Kobecki — Experimentelle Physik 2, Technische Universität Dortmund, D-44221 Dortmund, Germany

There is a great desire to extend ultrasonic techniques for imaging and characterization of nanoobjects. This may be achieved by picosecond ultrasonics, where using ultrafast lasers it is possible to generate and detect acoustic wave with the frequencies up to terahertz and wavelength down to nanometers. In our work we present the picosecond ultrasonics setup based on miniaturezed mode-locked semiconductor lasers, which are appropriate to obtain necessary power, pulse duration and repetition rate.

Project was focused on generation and detection of the strain pulses in thin metal films (Al,Pt,Cr,Au) deposited on GaAs substrates. The used mode locked laser diode (MLLD) based on AlGaInAs/InP quantum-well active media was manufactured at Glasgow University. Invastigated device emits 1-ps duration laser pulses with repetition rate of 20 GHz and average power of 50mW at 930nm wavelength.In experiments we have used standard pump-probe scheme. Detected signal reflects an ultra-short strain pulse generated in a film and its echo arriving back to the surface. Observed signals are in perfect agreement with the data obtained by means of conventional set-ups, which gives motivation for further development in the field and pursuing more ambitious goals.

HL 51.5 Wed 16:00 POT 51

Monolithic passively mode-locked quantum well lasers — •Christoph Weber[1], Andreas Klehr[2], Andrea Knigge[2], and Stefan Breuer[1] — [1]Institute of Applied Physics, Technische Universität Darmstadt, 64289 Darmstadt, Germany — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Gustav-Kirchhoff-Straße 4, 12489 Berlin, Germany

Monolithic passively mode-locked quantum well lasers emitting at wavelength around 1070 nm are ideal sources of picosecond short optical pulses at high repetition rates for novel data transmission systems or multi-photon imaging applications. For 2 mm long narrow ridge waveguide lasers with an absorber to total length ratio of 10 % emission of 2 ps short optical pulses with high pulse train stability has been reported [Weber et al, IEEE J. Quantum Electron. 54 (3), 2000609 (2018)]. In this contribution we study monolithic semiconductor lasers with different lengths, different absorber to total length ratios and different ridge widths and gain material based on InAs/InGaAs quantum wells. We analyze the pulse generation and the pulse train timing stability in dependence on the different laser cavity designs.

30 min. break

HL 51.6 Wed 16:45 POT 51

Optical and quantum optical characterization of silver-coated InP-based nanolasers on silicon — •Aris Koulas-Simos[1], Kaisa Laiho[1], Jianxing Zhang[2], Cun-Zheng Ning[2], and Stephan Reitzenstein[1] — [1]Institute of Solid State Physics, Technische Universität Berlin, Berlin Germany — [2]Tsinghua University, Department of Electronic Engineering, Beijing, China

A nanolaser is an optical laser device with a design close to the size limit of the cubic light wavelength. In comparison to conventional lasers, nanolasers possess very low-threshold powers for few-photon operation and may exhibit even a "thresholdless" input-output behavior thanks to the high β-factors close to unity, where the β-factor describes the coupling efficiency of the spontaneous emission to the lasing mode. Here, we investigate at first the conventional optical properties such as the LL-curve and the linewidth narrowing of silver-coated bulk InP nanolasers emitting at telecom wavelengths. More importantly, to confirm lasing of a device, the knowledge of the photon statistics is required. We verify that by observing the transition from thermal to coherent emission in excitation-dependent second order correlation measurements.

HL 51.7 Wed 17:00 POT 51

Development towards AlGaInP based electrically pumped VECSELs for the red spectral range — •Michael Zimmer, Zhihua Huang, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart.

In recent years, electrically pumped vertical external-cavity surface-emitting lasers (EP-VECSELs) have been studied extensively due to their potential for miniaturization and integration applications. Based on their good beam quality and compact device size EP-VECSELs are excellent candidates for a new generation of light sources. However, in the red wavelength regime EP-VECSELs have not been realized yet. Here we present the design of an AlGaInP based EP-VECSEL aiming at an emission around 670 nm. To realize an EP-VECSEL, a homogeneous charge carrier distribution within the active region of the device and the avoidance of heat at the same place need to be targeted. Thus, we apply a combination of bottom disk contacts and a thick current spreading layer for current confinement. Growth of our proposed EP-VECSEL structure takes place by metal-organic vapor-phase epitaxy (MOVPE) on a GaAs substrate. For device fabrication, a flip-chip process including dry and wet chemical etching steps as well as the complete removal of the GaAs substrate is performed. Electroluminescence profile measurements indicate promising results of an enlarged emission area with quasi-homogenous current density distribution and tens of micrometers in diameter.

HL 51.8 Wed 17:15 POT 51

Scalable networks of quantum dot micropillar lasers — Louis Andreoli[1], Javier Porte[1], Maxime Jacquot[1], Stephan Reitzenstein[2], Laurent Larger[1], and •Daniel Brunner[1] — [1]Institut FEMTO-ST, Université Bourgogne Franche-Comté CNRS UMR 6174, Besançon, France — [2]Technische Universität Berlin, Berlin, Germany

Large scale networks of semiconductor lasers are a long shought after technology. Since the demonstration of semiconductor lasers they have been heavily involved in investigating nonlinear dynamics and chaos. However, scalable networks with the potential for hosting 100s of such lasers have never been achieved. We will demonstrate individual and addressable single mode pumping of densely packed, homogenized arrays of quantum dot micropillar lasers. We are able to pump more than 50 devices and realize all-optical nearest neighbor coupling. It is the first time such large semiconductor laser networks have been demonstrated, and our concept is scalable in principle until over 100.000

lasers. Our experiment opens new avenus for fundamental nonlinear dynamics experiments and high profile applications such as novel neuromorphic computing concepts and material processing.

HL 51.9 Wed 17:30 POT 51

Stabilization of an optical frequency comb interband cascade laser at 3.3 micrometer by time-delayed optical self-injection — •Dominik Auth[1], Mahmood Bagheri[2], Clifford Frez[2], Chadwick L. Canedy[3], Igor Vurgaftman[3], Jerry R. Meyer[3], and Stefan Breuer[1] — [1]Institute of Applied Physics, Technische Universität Darmstadt, 64289 Darmstadt, Germany — [2]Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA, 91109, USA — [3]Naval Research Laboratory, Washington, DC, 20375, USA

Interband cascade lasers emitting optical frequency combs in the mid-wave infrared at wavelengths around 3.3 micrometer are promising sources for applications like dual comb spectroscopy probing strong fundamental absorption lines of numerous chemical and biological agents [Bagheri et. al. Sci. Rep. 8(1) (2018), 3322]. In this contribution, the intermode beat frequency (IBF) tuning range and IBF line width of an 4 mm long optical frequency comb interband cascade laser subject to single cavity optical self-injection is investigated experimentally and by modelling [Drzewietzki et al., Opt. Express 21 (2013), 16142].

HL 51.10 Wed 17:45 POT 51

Lasing of an artificial, topological defect in a 1D, linear Su-Schrieffer-Heeger chain — •Philipp Gagel[1], Tristan Harder[1], Monika Emmerling[1], Sebastian Klembt[1], Christian Schneider[1], and Sven Höfling[1,2] — [1]Technische Physik and Wilhelm-Conrad-Röntgen-Research Center for Complex Material Systems, Julius-Maximilians-Universität Würzburg, Würzburg, Germany — [2]SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, UK

The concept of topology has been adapted to categorize states of matter by topological invariants: Quantities which persist under adiabatic deformation. One of the various distinct features is the appearance of edge- and corner states between areas with different topological invariants, that are immune to external perturbations. Here we demonstrate lasing from an artificially created topological defect in a one-dimensional, linear Su-Schrieffer-Heeger chain of coupled photonic cavities by non-resonant optical pumping. The stability against distortions in combination with the intrinsic energy gap of the system provides a source for stable single mode lasing that is well suited for the next generation of optoelectronic devices, which can potentially be operated under electrical pumping and at ambient conditions.

HL 52: Focus Session: Functional Metal Oxides for Novel Applications and Devices I (joint session HL/DS)

Metal oxides exhibit a myriad of fascinating physical properties that enable a large variety of potential applications such as sensors and detectors, solar energy harvesting, transparent and potentially bendable electronics, power electronics, high-electron-mobility transisitors, memristors, topological quantum computation and so on. These functionalities typically require homo- or heteroepitaxial layers of high crystallinity with bendable amorphous semiconducting oxides as an exception. This session sets a focus on growth of bulk and thin films, experimental and theoretical investigation of their physical properties as well as fabrication and characterization of demonstrator devices.

Organizers: Oliver Bierwagen (Paul-Drude-Institut für Festkörperelektronik, Berlin), Holger Eisele (TU Berlin), Jutta Schwarzkopf (Leibniz-Institut für Kristallzüchtung, Berlin) and Holger von Wenckstern (Universität Leipzig).

Time: Wednesday 15:00–18:15 Location: POT 81

Invited Talk HL 52.1 Wed 15:00 POT 81

Modulation Doping in High-Mobility Alkaline-Earth Stannates — •Bharat Jalan — Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN 55455, U.S.A.

Interfaces between perovskite oxides have created tremendous excitement because of the potential for emergent phenomena and novel field-effect devices. The vast majority of these papers focus on the $LaAlO_3/SrTiO_3$ (LAO/STO) interfaces including some on Al_2O_3/STO and $ReTiO_3$/STO (Re refers to the rare-earth elements) interfaces among others. Amazingly, all these heterostructures involve the use of STO as an active layer where electron transport occurs. Attempts to synthesize non-STO based *modulation-doped* heterostructure have been unsuccessful so far despite theoretical predictions. Nor has any appreciable level of control been gained over the electron density at the interface, which is critical to device applications.

In this talk, we will report the *first* demonstration of true *modulation doping in a wider bandgap perovskite oxides without the use of STO*. We show that the La-doped $SrSnO_3/BaSnO_3$ system precisely fulfills the theoretical criteria for electron doping in $BaSnO_3$ using electrons from La-doped $SrSnO_3$, and we demonstrate how rearrangement of electrons can be used to control the insulator-to-metal transition in these heterostructure. We further show the use of angle-resolved HAXPES as a non-destructive approach to not only determine the location of electrons at the interface but also to quantify the width of electron distribution in $BaSnO_3$. The transport results are in good agreement with the results of self-consistent solution to one-dimensional Poisson and Schrödinger equations.

HL 52.2 Wed 15:30 POT 81

Two-dimensional electron (hole) gas in $BaSnO_3/LaInO_3$ heterostructures: A first-principles study — •Wahib Aggoune, Dmitrii Nabok, and Claudia Draxl — Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

We investigate the structural and electronic properties of heterostructures formed by the nonpolar $BaSnO_3$ (BSO) and polar $LaInO_3$ (LIO) perovskites, employing density functional theory. Focusing on the impact of thickness and surface termination of the LIO side, we analyze the electronic properties of the interface. For the stoichiometric LIO film, an internal electric field is induced due to the different terminations of its two sides. Increasing the LIO thickness, this field causes an upward shift of the valence band maximum (VBM). Reaching a thickness of 6 LIO unit cells, the VBM crosses the Fermi level, leading to partial occupation of the conduction band minimum (CBM). Consequently, a two-dimensional electron gas (2DEG) forms at the BSO side of the interface, confined within three unit cells. A high electron mobility is expected due to the *s*-character of the CBM. The corresponding hole gas (2DHG) forms at the LIO side, confined within one unit cell. As a result, this combination gives rise to the formation of a conducting interface starting from the insulating BSO and LIO components. We also present its results for interfaces with non-stoichiometric LIO. Depending on the surface termination, either a 2DEG or a 2DHG forms at the interface. In this case, the 2D charge confinement is mainly attributed to the spontaneous polarization induced at the interface.

HL 52.3 Wed 15:45 POT 81

Epitaxial growth of Lanthanum doped BaSnO3 thin films by PLD — •Reshma Ravindran, Daniel Pfützenreuter, Julian Stöver, Klaus Irmscher, and Jutta Schwarzkopf — Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2 12489 Berlin

Barium stannate (BaSnO3) has gained a lot of attention during the last few years due to its high charge carrier mobility, which is higher than for most transparent conducting oxides and the highest reported

for perovskite materials [1]. This makes BaSnO3 especially interesting for the use in electronic applications, e.g. field effect transistors. For single crystals, a mobility of 320 cm2/Vs at room temperature has been published. However, the mobility in epitaxial films is in the range of 70-100 cm2/Vs. This has initiated research efforts to improve structural and electrical properties of BaSnO3 thin films.

In our study, we report on epitaxially grown La-doped BaSnO3 (La concentration was 4 wt.-%) thin films on SrTiO3 substrates by pulsed laser deposition (PLD). We will show that PLD parameters like substrate temperature, target-to-substrate distance and laser spot size have to be carefully adjusted in order to obtain the formation of phase pure BaSnO3 thin films. Hall measurements will indicate that the charge carrier mobility is critically correlated with the structural quality of the epitaxial films analyzed by atomic force microscopy and x-ray diffraction. [1] H. J. Kim et al. Phys. Rev. B 86, 165205 (2012)

HL 52.4 Wed 16:00 POT 81

Epitaxial growth of La doped $BaSnO_3$ thin films by Plasma-assisted molecular beam epitaxy — •Georg Hoffmann[1], Martina Zupancic[2], Martin Albrecht[2], Zbigniew Galazka[2], and Oliver Bierwagen[1] — [1]Paul-Drude-Institut für Festkörperelektronik Leibniz-Institut im Forschungsverbund Berlin e.V. — [2]Leibniz-Institut für Kristallzüchtung

For oxide molecular beam epitaxy (MBE), the use of suboxides is an essential part for the growth of complex oxides, e.g. SnO for $BaSnO_3$ (BSO). However, the conventional approach of BSO growth using SnO suboxide from a SnO_2 charge ($SnO + Ba + 2O \rightarrow BaSnO_3$) requires high cell temperatures and adds a parasitic oxygen background due to the reaction $SnO_2 \rightarrow SnO + 1/2\ O_2$. Using a SnO_2 + Sn mixture as a charge can address both issues, first: the suppression of the parasitic oxygen due to the reaction $SnO_2 + Sn \rightarrow 2\ SnO$ and second: providing higher fluxes at lower temperatures.

Using this new approach, smooth BSO films were grown by plasma-assisted MBE on $SrTiO_3$ (STO) substrates. The crystal quality was analyzed in-situ by reflective high energy electron diffraction. Ex-situ, morphology and structural parameters were determined by atomic force microscopy, X-ray diffraction, and high resolution transmission electron microscopy images.

The results reveal an increased BSO growth-temperature window with decreasing SnO/Ba flux ratio. Further, the influence of the STO miscut angle, as well as the STO orientation will be discussed, and electrical properties of La doped BSO films are pointed out.

30 min. break

Invited Talk HL 52.5 Wed 16:45 POT 81

Engineering of LiNbO3 films for next generation acoustic and energy harvesting applications — •Ausrine Bartasyte, Samuel Margueron, Vincent Astié, Giacomo Clementi, Mihaea Ivan, and Merieme Oubahaz — FEMTO-ST Institute, University of Franche-Comté, Besançon, France

The next generation of high frequency wide-band RF filters or frequency-agile filters are urgently needed for the development of 5G infrastructures/networks/communications. Today, LiNbO3 and LiTaO3 single crystals are key materials in electro-optics and RF acoustic filters. This motivates further development of acoustic wave devices based on highly electromechanically coupled LiNbO3 thin films, adapted to the high-frequency applications. The challenges and the achievements in the epitaxial growth of LiNbO3 films and their integration with Si technology and to acoustic devices will be discussed in detail. The deposition techniques enabling the control of film composition/ nonstoichiometry of volatile alkali metal oxides & the methods of compositional analysis will be presented. We have demonstrated an extremely high acoustical performance compatible with filter applications for SAW devices, based on epitaxial LiNbO3 films, operating in the frequency range around 5 GHz. Moreover, it was demonstrated that the power density of 9.62 mW .cm-3 (comparable to present performance of lead-based piezoelectric harvester) can be harvested by vibrational energy transducer based on thick LiNbO3 films.

Invited Talk HL 52.6 Wed 17:15 POT 81

Oxide Memristors for unified data storage and data processing — •Heidemarie Schmidt — Leibniz-IPHT Jena — IFK, FSU Jena — Fraunhofer ENAS Chemnitz

In the future, new hardware components will determine the power and strength of artificial intelligence and manchine learning. These components are called memristors [1]. The first memristor with unified analog data storage and information processing is the BiFeO3 (BFO) memristor. BFO is an electroforming-free, bipolar memristor and its potential has been shown in in-memory information processing [2], neuromorphic computing [3], and hardware cryptography [4]. Another electroforming-free memristor is the unipolar memristor YMnO3 (YMO). In order to develop memristor technology and applications further, it is more than ever necessary to understand the underlying resistive switching mechanisms when a write voltage is applied. We discuss results from quasi-static test measurements on BFO [5] and from temperature dependent transport measurements on YMO [6]. [1] Leon Chua, IEEE Transactions on Circuit Theory 18, 507, 1971 [2] T. You et al., Adv. Funct. Mat. 24, 3357-3365, 2014. [3] N. Du et al., Front. Neurosci. 9, 227, 2015. [4] N. Du et al., J. Appl. Phys. 115, 124501, 2014. [5] N. Du et al., Phys. Rev. Applied 10, 054025, 2018. [6] V.R. Rayapati et al., J. Appl. Phys. 124, 144102, 2018

HL 52.7 Wed 17:45 POT 81

Investigations on leakage current in epitaxial K0.5Na0.5NbO3 thin films grown by PLD — •Daniel Pfützenreuter, Julian Stöver, Klaus Irmscher, Jens Martin, and Jutta Schwarzkopf — Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin

KxNa1-xNbO3 is a lead-free, ferro- and piezoelectric compound, which offers a high potential for memory applications and sensors in thin films form. However, KxNa1-xNbO3 thin films often suffer from a high leakage current. This is assumed to be mainly attributed to the high volatility of the alkaline components at high temperatures, but also interface effects have to be regarded. Pulsed laser deposition (PLD) represents a suitable method for the epitaxial growth of K0.5Na0.5NbO3 films. In this study the impact of strain, film thickness and bottom electrode on vertical electric behaviour of epitaxially grown K0.5Na0.5NbO3 films is investigated. For this purpose, K0.5Na0.5NbO3 films were grown on SrRuO3 and La0.67Sr0.33MnO3 covered SrTiO3 and DyScO3 substrates as well as directly on SrTiO3:Nb substrates with a film thickness between 20 and 200 nm. While for small film thicknesses Ohmic charge transport is observed in I-V-measurements, the charge transport mechanism changes to pronounced Schottky like behaviour at thicker films. This transition is investigated in more detail by comparing the measured I-V curves with calculated ones for different mechanisms of current flow. Furthermore, we find a strong correlation between the lattice strain in the films and the kind of charge transport mechanism.

HL 52.8 Wed 18:00 POT 81

Tuning the composition properties of SrTiO3 thin films grown by metal-organic vapor phase epitaxy (MOVPE) — •Aykut Baki, Julian Stöver, Toni Markurt, Carsten Richter, Klaus Irmscher, Martin Albrecht, and Jutta Schwarzkopf — Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2 12489 Berlin

SrTiO3 represents a prototype cubic perovskite and has several of interesting physical properties as for instance a high dielectric constant at room temperature and resistive switching behavior. MOVPE is employed as deposition method since it provides film growth close to the thermodynamic equilibrium and thus stoichiometric, defect-poor thin films with smooth surfaces and interfaces. In this study, epitaxial SrTiO3 films were successfully grown on 0.5 wt.% Nb-doped SrTiO3 substrates by using the metal-organic precursors Sr(tmdh)2-tetraglyme and Ti(iso-propoxid)2(tmdh)2 solved in dry toluene. It has been shown that the phase formation of phase-pure SrTiO3 is achieved by adjusting the substrate temperature to a range of 675 °C < TC < 725 °C. By varying the Sr/Ti ratio in the gas phase, the cation ratio in the SrTiO3 thin films has been precisely controlled. The structural quality of the grown films has been proved by high-resolution x-ray diffraction, atomic force microscopy and transmission electron microscopy. The insulating films have been tested for their dielectric properties by a Pt/SrTiO3/SrTiO3:Nb test-structure for temperatures between 20 K and 300 K. IV-curves have shown strong forming-less resistive switching.

HL 53: Hybrid Perovskite and Photovoltaics II (joint session CPP/HL)

Time: Wednesday 15:00–16:15 Location: ZEU 260

HL 53.1 Wed 15:00 ZEU 260

The Efficiency Potential of Neat Perovskite Films — •Martin Stolterfoht — Uni Potsdam

Perovskite photovoltaic (PV) cells have demonstrated power conversion efficiencies (PCE) that are close to those of monocrystalline silicon (m-Si) cells, however, in contrast to silicon PV, perovskites are not limited by Auger recombination. Nevertheless, compared to GaAs and m-Si devices, perovskite cells stand out by their significantly lower fill factors (FFs) which is due to a combination of resistive and non-radiative recombination losses. This necessitates a deeper understanding of the underlying loss mechanism and in particular the ideality factor of the cell. Here, by measuring the intensity (I) dependence of the external (V_OC) and internal voltage (i.e. the quasi-Fermi level splitting, QFLS), we can quantify the transport resistance-free efficiency of the complete cell as well as the efficiency potential of any neat perovskite films with and without attached transport layers (TLs). Moreover, QFLS(I) measurements on different perovskite compositions allow to disentangle the impact of the interfaces and the perovskite surface on the non-radiative FF and V_OC loss. We find that potassium passivated quadruple cation perovskite films stand out by their exceptionally high implied PCEs of above 28% which could be readily achieved if charge collection losses and energy alignment issues are overcome. Finally, strategies are presented to reduce both the ideality factor and transport losses to push the FF to the thermodynamic limits.

HL 53.2 Wed 15:15 ZEU 260

Shallow Nano-Textures for Light Management in Solution-Processed Perovskite Solar Cells — •Philipp Tockhorn[1], Johannes Sutter[1], Klaus Jäger[1], Amran Al-Ashouri[1], Christiane Becker[1], and Steve Albrecht[1,2] — [1]Helmholtz Zentrum Berlin - 12489 Berlin — [2]Technische Universität Berlin - 10623 Berlin

Metal halide perovskites have led to highly efficient thin-film solar cells in the past decade. Here, we report enhanced PCEs achieved by light management in spin-coated perovskite single junction solar cells on shallow nano-textures. For this, sinusoidal nano-textures with a period of 750 nm and a texture height of 380 nm are employed. In our p-i-n devices, the nano-textured substrate is coated with a bottom contact comprising ITO and a self-assembling monolayer as well as a spincoated perovskite, while the top contact is realised by evaporation. With this design, we obtain a PCE of 18.9%, which marks an increase of 3% with respect to its planar reference. This efficiency gain is mostly achieved by an increase in short circuit current density (Jsc), achieved through enhanced light scattering by the sinusoidal nano-textures. External quantum efficiency and reflectance measurements on these devices confirm the observed increase in Jsc of about +1 mA/cm2 promoted by the improved light in-coupling. Furthermore, we observe a systematic reduction of 10-20 mV in open-circuit voltage on the nano-textured devices. Therefore, we investigate the influence of the nano-textures on the electronic quality of the perovskite itself and its interfaces to charge selective contacts with absolute photoluminescence measurements as well as electrical simulations.

HL 53.3 Wed 15:30 ZEU 260

Electronic structure nonionic surfactant-mixed PEDOT:PSS and its effects on perovskite solar cells — •Dongguen Shin[1,2,3], Donghee Kang[3], Na Eun Jung[3], and Yeonjin Yi[3] — [1]Institut für Physik & IRIS Adelershof, Humboldt-Universität zu Berlin, Brook-Taylor Straße 6, 12489 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Albert-Einstein-Straße 15, 12489 Berlin, Germany — [3]Institute of Physics and Applied Physics, Yonsei University, 50 Yonsei-ro, Seodaemoon-Gu, Seoul 03722, Republic of Korea

PEDOT:PSS, generally used hole transport layer, has the limitation of increasing the performance of perovskite solar cells (PSCs) due to its semi-metallic properties. One of the manners of tailoring the electronic properties of PEDOT:PSS is mixing of the nonionic surfactant (e.g. Triton X-100 (TX)) into PEDOT:PSS, which supposedly get the affirmative impact on the charge extraction and exciton quenching at the interface. In this work, we explore the electronic structure of PEDOT:PSS with nonionic surfactant TX mixture by using the X-ray and ultraviolet photoelectron spectroscopy (XPS, UPS) measurement, and investigate the power conversion efficiency (PCE) enhancement of perovskite solar cells (PSCs) by using the mixture of PEDOT:PSS and TX surfactant in PSCs. we reveal that it led to the prevention of interfacial recombination as the insulating tunneling layer without energetic junction loss at the interface MAPbI3 with PEDOT:PSS. Consequently, we establish an efficient charge extraction condition without the interfacial recombination on PSCs.

HL 53.4 Wed 15:45 ZEU 260

In-situ study of slot-die printed titania films for up-scale fabrication of all-solid-state dye-sensitized solar cells — •Nian Li[1], Wei Chen[1], Manuel Scheel[1], Volker Körstgens[1], Matthias Schwartzkopf[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1,3] — [1]Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany. — [2]Deutsches Elektronen-Synchrotron DESY Notkestrasse 85, D-22603 Hamburg, Germany. — [3]Heinz Maier-Leibnitz Zentrum (MLZ) Technische Universität München Lichtenbergstr. 1, D-85748 Garching, Germany.

Printing, a simple and low-cost technique, is employed to fabricate mesoporous titania films as electron-transporting layers for upscaling all-solid-state dye-sensitized solar cells (DSSCs). The deposition methods strongly affect the final titania morphology, and further solar cell efficiency. Therefore, a detailed understanding of structure formation is of crucial importance for optimizing the industrial coating films. In the present work, we provide insights into the structure evolution of slot-die printed films via in situ grazing-incidence small-angle X-ray scattering (GISAXS). The printing-solution synthesis is performed by sol-gel chemistry and a structure-directing template polystyrene-block-polyethylene oxide (PS-b-PEO) to achieve the structure tailoring. The evolution of nanostructure length scales of the titania/PS-b-PEO composite film is revealed in real-time and in situ during slot-die printing. The resulting mesoporous titania films with highly ordered structures serve as photoanodes of all-solid-state DSSCs.

HL 53.5 Wed 16:00 ZEU 260

The role of anchors for the efficiency of p-type dye-sensitized solar cells — •Miftahussurur Hamidi Putra and Axel Gross — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

In recent years, p-type dye-sensitized solar cells (pDSSC) have attracted a lot of attention as an alternative to conventional solar cells. However, the efficiency of this solar cell is still below 10% which hampers their utilization. One of the promising type of dyes for p-DSSC solar cells are ruthenium-based complexes $[Ru(bpy)_3]^{2+}$ [1]. The efficiency of p-DSSCs is critically influenced by the anchors through which they are bound to a semiconductor substrate such as NiO. First-principles electronic calculations based on time-dependent density functional theory (TDDFT) have been performed in order to evaluate the performance of various candidates for anchoring $[Ru(bpy)_3]^{2+}$ complexes. Results will be presented and discussed with respect to properties that are related to the efficiency of p-DSSC solar cells, such as injection free energy (ΔG_{inj}), light harvesting efficiency (LHE), hole injecting efficiency (HJE), regeneration free energy (ΔG_{reg}) and the excited state lifetime (τ) [1,2].

[1] Y. Pellegrin, L. Le Pleux, E. Blart, A. Renaud, B. Chavillon, N. Szuwarski, M. Boujtita, L. Cario, S. Jobic, D. Jacquemin, and F. Odobel, J. Photochem. Photobiol. A: Chem. **219**, 235 (2011).
[2] A. Sen and A. Groß, Int. J. Quantum Chem. **119**, e25963 (2019).

HL 54: Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions IV (joint session O/CPP/DS/HL)

Time: Wednesday 15:00–17:30 Location: GER 38

Invited Talk HL 54.1 Wed 15:00 GER 38

Electron-phonon interactions in realistic materials — •Fabio Caruso — Institut für Physik und IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

Functional materials used in actual devices are typically doped, they operate at finite temperature, and they may be subject to perturbations such as, *e.g.*, external fields and light pulses. These aspects may alter profoundly the electron-phonon interaction (EPI), its influence on the electronic properties of solids, and even lead to the manifestation of novel emergent phenomena absent in perfect crystals.

We conducted a first-principles investigation of the EPI in functional materials at realistic operational conditions based on many-body perturbation theory. Our work reveals that: (i) n-type doping of polar oxides, such as EuO and TiO_2, allows one to trigger and control the formation of polarons (electrons dressed by a phonon cloud) [1]; (ii) in the record-breaking thermoelectric material SnSe, temperature may lead to a five-fold suppression of carrier lifetimes due to enhanced phonon emission [2]. Overall, the striking sensitivity to doping, temperature, and external fields, makes the EPI a powerful tool to tailor the optoelectronic properties of quantum materials. Possible strategies to extend the many-body theory of the EPI to the study of time-dependent phenomena will further be discussed [3].

[1] J. Riley, F. Caruso, C. Verdi, *et al.*, Nature Commun. **9** (1), 2305 (2018). [2] F. Caruso, M. Troppenz, S. Rigamonti, C. Draxl, Phys. Rev. B **99** (8), 081104 (2019). [3] F. Caruso, D. Novko, C. Draxl, arXiv:1909.06549v (2019).

HL 54.2 Wed 15:30 GER 38

Fully Anharmonic, Non-Perturbative First-Principles Theory of Electronic-Vibrational Coupling in Solids — Marios Zacharias, Matthias Scheffler, and •Christian Carbogno — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

The coupling between nuclear vibrations and the electronic structure plays a pivotal role for many material properties, including optical absorption and electronic transport. In this regard, however, today's state-of-the-art methodologies rely on two approximations [1]: the harmonic (phonon) approximation for the nuclear motion and the linear response description of the electronic structure with respect to harmonic displacements. In this work, we overcome ***both*** these approximations by performing fully anharmonic *ab initio* molecular dynamics (*ai*MD) calculations and by accounting for the non-perturbative, self-consistent response of the wave functions along the *ai*MD trajectory. By this means, we obtain fully anharmonic, vibronically renormalized spectral functions, from which macroscopic material properties like temperature-dependent band gaps and electronic transport coefficients are obtained. We validate our approach using silicon as an example, for which the traditional electron-phonon coupling formalism is recovered. Using cubic $SrTiO_3$ as example, we further demonstrate that anharmonic electronic-vibrational coupling effects are not captured in traditional formalisms, but they play a decisive role here and in other complex materials like perovskites.

[1] F. Giustino, *Rev. Mod. Phys.* **89**, 015003 (2017).

HL 54.3 Wed 15:45 GER 38

Thermal conductivity of highly-doped Si: Role of electron-phonon and point-defect phonon scattering — •Bonny Dongre[1], Jesús Carrete[1], Shihao Wen[2], Jinlong Ma[2], Wu Li[2], Natalio Mingo[3], and Georg KH Madsen[1] — [1]Institute of Materials Chemistry, TU Wien, A-1060 Vienna, Austria. — [2]Institute for Advanced Study, Shenzhen University, Shenzhen 518060, China — [3]LITEN, CEA-Grenoble, 17 rue des Martyrs, 38054 Grenoble Cedex 9, France.

Theoretical investigation of the thermal conductivity reduction in highly-doped Si is an area of active research. Recently, first-principles electron-phonon scattering was found to produce a significant reduction in the thermal conductivity of highly-doped Si. However, the study could not reproduce the experimental results.

In the present work, we calculate the first-principles phonon scattering rates by electrons and point defects, and use them to calculate the thermal conductivity of highly-P- and B-doped Si for a range of temperatures and concentrations. We find that the phonon scattering by electrons dominates at carrier concentrations below 10^{19} cm^{-3} and is enough to reproduce the experimental thermal conductivity reduction at all temperatures. However, at higher defect concentrations point-defect phonon scattering contributes substantially to the thermal conductivity reduction even at room temperature. With a combined treatment of the phonon scattering by electrons as well as phonons, an excellent agreement is obtained with the experimental values at all temperatures.

HL 54.4 Wed 16:00 GER 38

Precise yet Fast High-Throughput Search for Thermal Insulators — •Florian Knoop, Thomas A.R. Purcell, Matthias Scheffler, and Christian Carbogno — Fritz-Haber-Institut der Max-Planck-Gesellschaft

We present a systematic and numerically precise computational search for thermal insulators in material space performed with the *FHI-vibes* high-throughput framework [1]. *FHI-vibes* employs a robust metric that quantifies the degree of anharmonicity in the nuclear dynamics via the statistical comparison of first-principles forces with those forces that would act in the harmonic approximation. This enables us to efficiently scan over many materials, including complex oxides and chalcogenides as well as ternary structures like perovskites. By this means, we single out strongly anharmonic systems, for which we perform *ab initio* Green-Kubo simulations to assess their thermal conductivities, thereby naturally including all anharmonic effects [2]. Our strategy allows to avoid redundant calculations and to achieve a much higher quality of information than traditional high-thoughput studies. Besides validating the performed search and analyzing its results, we discuss how big-data analytics techniques can be utilized to further accelerate and guide this search.

[1] https://vibes.fhi-berlin.mpg.de
[2] C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901 (2017)

HL 54.5 Wed 16:15 GER 38

Ambivalent Impact of Electron-Phonon Interaction on Electronic and Transport Properties of Organic Semiconductors — •Frank Ortmann — Center for Advancing Electronics Dresden, Technische Universität Dresden, Germany

Vibrations are omnipresent in molecules and of great importance in Organic Semiconductors due to the softness of the materials and the strong electron-phonon coupling. One possibility to investigate this interaction is to study the low-energy edge of optical absorption spectra, which lacks an in-depth understanding for organic materials. We have recently observed a strong dependence of low-energy excitonic features on the molecular building blocks in organic films, which we associated to molecular flexibility and polaron deformation. We will discuss implications of low-frequency molecular vibrations on the polaronic and excitonic density of states in donor-acceptor mixtures featuring charge-transfer excitons. We will also discuss how a distinguished treatment of strong-coupling molecular vibrations of different energies leads to an improved description of charge carrier transport in organic materials.

HL 54.6 Wed 16:30 GER 38

Quantum Nuclear Effects in Thermal Transport of Semiconductors and Insulators — •Hagen-Henrik Kowalski[1], Mariana Rossi[1,2], Matthias Scheffler[1], and Christian Carbogno[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]MPI for Structure and Dynamics of Matter, Hamburg, Germany

To date, the computation of thermal conductivities relies on either perturbation theory or (*ab initio*) molecular dynamics (MD) [1]. While perturbative approaches include quantum-nuclear effects (QNE), they typically neglect higher orders of anharmonicity. Conversely, classical MD includes all orders of anharmonicity, but neglects QNEs. To overcome these limitations, we have developed a formalism that accounts for ***both*** quantum-nuclear effects and all orders of anharmonicity. For this purpose, the nuclear dynamics are assessed via Thermostatted Ring Polymer MD (TRPMD) [2] and the thermal conductivity is obtained via the Green-Kubo formalism using a newly proposed TRPMD based heat-flux estimator. Using solid Argon and Silicon as model systems, we discuss the influence of QNEs on thermal transport by com-

paring velocity, energy, and heat-flux autocorrelation spectra. This allows to rationalize the impact of QNEs on vibrational frequencies, lifetimes, and on the thermal conductivity in different temperature regimes.

[1] C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901, (2017).
[2] M. Rossi, M. Ceriotti, D. Manolopoulos, *J. Chem. Phys.* **140**, 234116 (2014).

HL 54.7 Wed 16:45 GER 38

Speeding-up *ab initio* molecular dynamics with hybrid functionals using adaptively compressed exchange operator based multiple time stepping — •Sagarmoy Mandal and Nisanth N. Nair — Department of Chemistry, Indian Institute of Technology Kanpur, India

Ab initio molecular dynamics (AIMD) with hybrid density functionals and a plane wave basis is known to predict the structural and dynamical properties of condensed matter systems accurately. However, such hybrid functional based AIMD simulations are not routinely used due to the high computational cost associated with the application of the Hartree-Fock exchange operator. We propose a strategy [1] to combine the Adaptively Compressed Exchange (ACE) operator formulation [2] and a multiple time step integration scheme to reduce the computational cost significantly. We also show that computing the ACE operator with localized orbitals can further improve the computational efficiency. Finally, we use this method in combination with the Well-Sliced Metadynamics approach to compute the free energy barrier of chemical reactions in systems containing hundreds of atoms.

[1] S. Mandal, N.N. Nair, J. Chem. Phys. **151** (2019) 151102.
[2] Lin Lin, J. Chem. Theory Comput. **12** (2016) 2242.

HL 54.8 Wed 17:00 GER 38

Calculation of current-induced heating and vibrational instabilities in single molecule circuits — Giuseppe Foti and •Hector Vazquez — Inst. of Physics, Academy of Sciences of the Czech Rep., CZ

Current-induced heating in molecular wires arises from the interaction between tunneling electrons and localized vibrations. Vibrational instabilities occur when excitation of molecular vibrations is not balanced by dissipation mechanisms, and can lead to the breakdown of the junction. In this talk I will address predictions for vibrational instabilities in single molecule junctions with separated unoccupied resonances. We use DFT-NEGF to study the electronic structure of the junction under an applied bias, while rates of absorption and emission of vibrations are calculated using kinetic equations [1,2]. We find and characterize several unstable modes. These results are then generalized using model calculations to generate a stability diagram of the junction under bias [3]. The talk will discuss the effect of a self-consistent treatment of electron-vibration interaction, and highlight the role played by the structure of the electron-vibration coupling matrix. Our work reveals the interplay of electronic structure and electron-vibration coupling in a broad class of molecular wires.

[1] J-T Lü, P. Hedegaard and M. Brandbyge, Phys. Rev. Lett. 107, 046801 (2011).
[2] G. Foti and H. Vázquez, J. Phys. Chem. C 121, 1082 (2017).
[3] G. Foti and H. Vázquez, J. Phys. Chem. Lett. 9, 2791 (2018).

HL 54.9 Wed 17:15 GER 38

***Ab Initio* Green-Kubo Approach of Charge Transport in Crystalline Solids** — •Zhen-Kun Yuan, Marios Zacharias, Matthias Scheffler, and Christian Carbogno — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

State-of-the-art approaches for calculating the charge transport coefficients in crystalline materials rely on a harmonic description of the lattice vibrations and a perturbative treatment of electron-phonon couplings (EPCs) [1]. For materials featuring sizable anharmonic lattice vibrations and/or strong EPCs, such approaches are, however, not applicable. Here, we present an *ab initio* approach based on the Green-Kubo theory of linear response [2] that does neither rely on the harmonic approximation nor on a perturbative treatment of EPCs, thus overcoming these issues. The electrical conductivity is obtained from the time correlations of the electric charge flux, which is computed along fully anharmonic *ab initio* molecular dynamics trajectories. We demonstrate our approach by calculating the electrical conductivity of the harmonic material Si and the anharmonic $SrTiO_3$. We carefully check the convergence behavior of the calculated results with respect to supercell size and examine possible strategies to overcome finite-size effects [3].

[1] F. Giustino, *Rev. Mod. Phys.* **89**, 015003 (2017).
[2] R. Kubo, M. Yokota, and S. Nakajima, *J. Phys. Soc. Jpn.* **12**, 1203 (1957).
[3] C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901 (2017).

HL 55: Superconducting Electronics: SQUIDs, Qubits, Circuit QED, Quantum Coherence and Quantum Information Systems 2 (jointly with MA, HL) (joint session TT/HL)

Time: Thursday 9:30–12:30 Location: HSZ 03

HL 55.1 Thu 9:30 HSZ 03

Waveguide Bandgap Engineering with an Array of Superconducting Qubits — •Jan David Brehm[1], Alexander N. Poddubny[2], Alexander Stehli[1], Tim Wolz[1], Hannes Rotzinger[1,3], and Alexey V. Ustinov[1,4,5] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, Karlsruhe, Germany — [2]Ioffe Institute, St. Petersburg, Russia — [3]Institut für Festkörperphysik, Karlsruher Institut für Technologie, Karlsruhe, Germany — [4]National University of Science and Technology MISIS, Moscow, Russia — [5]Russian Quantum Center, Skolkovo, Moscow, Russia

In one dimension the interaction of qubits with free space instead of a cavity gives rise to an effective qubit-qubit coupling which is of infinite range and can be tuned by varying the qubit separation. In this work, we experimentally study an array of eight superconducting transmon qubits with local frequency control, which are all coupled to the mode continuum of a superconducting waveguide. The spacing between adjacent qubits is substantially smaller than the wavelength corresponding to their excitation frequency, eliminating almost completely the coherent exchange type interaction between qubits. By consecutively tuning the qubits to a common resonance frequency we observe the formation of super- and subradiant states as well as the emergence of a bandgap. Furthermore, we study the nonlinear saturation of the collective modes with increasing photon number and electromagnetically induce a transparency window in the bandgap region of the ensemble.

HL 55.2 Thu 9:45 HSZ 03

Employing a real-time processor for experiments with superconducting qubits — •Richard Gebauer[1], Nick Karcher[1], Alexey V. Ustinov[2,3], Martin Weides[2,4], Marc Weber[1], and Oliver Sander[1] — [1]Institute for Data Processing and Electronics, KIT, Karlsruhe, Germany — [2]Physikalisches Institut, KIT, Karlsruhe, Germany — [3]Russian Quantum Center, National University of Science and Technology MISIS, Moscow, Russia — [4]School of Engineering, University of Glasgow, Glasgow, United Kingdom

The control of superconducting quantum bits (qubits) relies on the ability to read out their state with high precision and apply custom pulses on the nanosecond timescale. As the field progresses, experiment schemes tend to get more complicated once the number of pulses increases, complex parameter changes are necessary and further data processing is needed. Conventional setups consisting of arbitrary waveform generators and digitizers connected to a measurement computer are not ideally suited to cope with this increased complexity.

A faster and more flexible solution is FPGA-based electronics. It not only dramatically reduces costs and space requirements but also simplifies measurements and enables customized control schemes like quantum feedback. Combined with a real-time processor, complex experiment flows and online data processing render possible.

We will present our platform to control and readout superconducting qubits with a focus on the real-time processing subsystem. Furthermore, we will show multiple experimental applications where the real-time processor is utilized, like evaluating correlation functions.

HL 55.3 Thu 10:00 HSZ 03

High power dispersive qubit readout and state preparation without parametric amplifier — •Martin Spiecker[1], Daria Gusenkova[1], Richard Gebauer[2], Lukas Grünhaupt[1], Patrick Winkel[1], Francesco Valenti[1,2], Ivan Takmakov[1,2,3], Dennis Rieger[1], Alexey V. Ustinov[1,4], Wolfgang Wernsdorfer[1,3,5], Oliver Sander[2], and Ioan M. Pop[1,3] — [1]Physikalisches Institut, KIT, Germany — [2]Institute for Data Processing and Electronics, KIT, Germany — [3]Institute of Nanotechnology, KIT, Germany — [4]Russian Quantum Center, MISIS, Moscow, Russia — [5]Institute Neel, CNRS, Grenoble, France

High-fidelity qubit readout is an essential requirement for fault-tolerant quantum algorithms. In theory, within the dispersive readout scheme, the state discrimination can be improved significantly if the resonator's photon population increases [1]. However, in practice the optimal photon number does usually not exceed 2.5 photons [2], and parametric amplifiers are needed to achieve a substantial signal-to-noise ratio.
In order to investigate the limitations of the readout fidelity we used a fluxonium qubit with a granular aluminum superinductance [3] having the advantage of reduced nonlinearity in comparison to previously used Josephson junction arrays. We demonstrate qubit measurements without a parametric amplifier at readout powers corresponding up to 200 photons in the resonator.
[1] A. Blais et al., PRA 69(6), 062320 (2004)
[2] T. Walter et al., PRA 7.5, 054020 (2017)
[3] L. Grünhaupt and M. Spiecker et al., Nat. Mater. 18, 816-819 (2019)

HL 55.4 Thu 10:15 HSZ 03

Experimental violation of the standard quantum limit for parametric amplification of broadband signals — •K. Fedorov[1,2], M. Renger[1,2], S. Pogorzalek[1,2], C. Scheuer[1,2], Q. Chen[1,2], Y. Nojiri[1,2], M. Partanen[1], A. Marx[1], F. Deppe[1,2,3], and R. Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 Munich, Germany

Phase-preserving amplification is a crucial part of many protocols in microwave quantum information processing, such as quantum teleportation, remote state preparation [1], or dispersive qubit readout. Josephson parametric amplifiers (JPAs) allow amplification close to the standard quantum limit (SQL), implying a fundamental bound of 50 % for the maximal quantum efficiency η for amplification of narrowband input signals. We demonstrate that the SQL does not hold for broadband input signals and experimentally find $\eta = 70\,\%$ with an amplification chain consisting of a JPA and a cryogenic HEMT amplifier. We show that η can reach 100 % and experimentally is limited by the Poissonian fluctuations in the JPA pump line.
We acknowledge support by Germany's Excellence Strategy EXC-2111-390814868, Elite Network of Bavaria through the program ExQM, and the European Union via the Quantum Flagship project QMiCS (GrantNo.820505).
[1] S. Pogorzalek *et al.*, Nat. Commun. **10**, 2604 (2019).

HL 55.5 Thu 10:30 HSZ 03

Optimal control of a compact 3D quantum memory — Julia Lamprich[1,2], Stephan Trattnig[1,2], •Yuki Nojiri[1,2,3], Qiming Chen[1,2,3], Stephan Pogozarek[1,2], Michael Renger[1,2,3], Kirill Fedorov[1,2,3], Achim Marx[1,3], Matti Partanen[1,3], Frank Deppe[1,2,3], and Rudolf Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Walther-Meißner-Strasse 8, D-85748 Garching, Germany — [2]Physik-Department, Technische Universität München, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 Munich, Germany

Quantum memories are of high relevance in the context of quantum computing and communication. For building scalable architectures based on superconducting quantum circuits, 3D cavities are promising candidates for a quantum memory. Recently, a compact layout exploiting the multimode structure of a rectangular 3D cavity has been demonstrated [1]. In that work, the fidelity of the transfer process was also limited by state leakage. This can be overcome by pulse shaping using optimal control strategies [2]. Henceforth, we implement a search algorithm (CMA-ES) to find optimized pulses promising higher gate fidelities, and present first experimental results.

We acknowledge support by the Germany's Excellence Strategy EXC-2111-390814868, Elite Network of Bavaria through the program ExQM, and the European Union via the Quantum Flagship project QMiCS (Grant No. 820505).
[1] E. Xie et al., Appl. Phys. Lett. 112, 202601 (2018).
[2] Shai Machnes et al., Phys. Rev. Lett. 120, 150401 (2018)

HL 55.6 Thu 10:45 HSZ 03

Quasiclassical Green's Function Approach to Normal-Metal Quasiparticle Traps — •Raphael Schmit and Frank Wilhelm — Saarland University, Theoretical Physics Department

Superconducting qubits, such as the charge or the flux qubit, are thought to store the information needed for quantum information processing. However, unwanted interactions with the qubit's environment lead to decoherence of the qubit and thus information loss. In addition to these extrinsic sources for decoherence, there is also an intrinsic one: the coupling between the qubit and the non-equilibrium quasiparticle excitations in the superconductor the qubit is made of. Decoherence is due to quasiparticle tunneling through a Josephson junction, but there is also an inhomogeneous broadening caused by changes in the occupations of Andreev states in the junction. Both mechanisms are highly depending on the location of the quasiparticles: quasiparticles far away from junctions have much less contribution to decoherence than the ones close to it. While it is difficult to prevent the generation of quasiparticles, trapping them in less active regions of the device seems to provide a practicable way to improve the device performance.

We are aiming to establish a quantitative theory of normal-metal traps simply consisting of an island of normal metal which is in good metallic contact with the superconductor. To do so, we are applying a Green's function formalism - the Keldysh technique in the dirty limit with a quasiclassical approximation - to investigate the properties of non-equilibrium quasiparticles in mesoscopic devices.

HL 55.7 Thu 11:00 HSZ 03

Transmission spectra of an ultrastrongly coupled qubit-dissipative resonator system — •Luca Magazzù and Milena Grifoni — Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

We calculate the transmission spectra of a flux qubit coupled to a dissipative resonator in the ultrastrong coupling regime. Such a qubit-oscillator system constitutes the building block of superconducting circuit QED platforms. The calculated transmission of a weak probe field quantifies the response of the qubit, in frequency domain, under the sole influence of the oscillator and of its dissipative environment, an Ohmic heat bath. We find the distinctive features of the qubit-resonator system, namely two-dip structures in the calculated transmission, modified by the presence of the dissipative environment. The relative magnitude, positions, and broadening of the dips are determined by the interplay among qubit-oscillator detuning, the strength of their coupling, and the interaction with the heat bath.
[1] L. Magazzù and M. Grifoni, J. Stat. Mech. 104002 (2019).

15 min. break.

HL 55.8 Thu 11:30 HSZ 03

Diagrammatic Resummation Theory Approach to Few-Photon Scattering and Dynamics in Waveguide QED — •Kiryl Piasotski and Mikhail Pletyukhov — RWTH Aachen University, Germany

In the present talk, the diagrammatic resummation theory approach to the problems of multi-photon scattering and dynamics in the single-qubit waveguide QED is presented. It is shown that within the rotating wave approximation, irrespectively of the number of radiation channels, dispersion of the modes they are supporting, and the nature of the radiation-qubit coupling, the determination of both scattering and dynamical observables in the subspace of the fixed excitation number, is reducible to a solution of the closed finite system of linear integral equations. Further, the above described theoretical machinery is showcased on the number of problems regarding the systems with delayed coherent quantum feedback, namely it is shown how the formalism could be applied to determine the coherence functions of radiation within the scattering setup, as well as the determination of certain dynamical characteristics of non-Markovian waveguide QED systems.

HL 55.9 Thu 11:45 HSZ 03

Josephson-Photonics Devices as a Source of Entangled Mi-

crowave Photons — •Björn Kubala[1], Ambroise Peugeot[2], Simon Dambach[1,3], Juha Leppäkangas[4], Marc Westig[2], Gerbold Menard[2], Yuri Mukharsky[2], Carles Altimiras[2], Patrice Roche[2], Philippe Joyez[2], Denis Vion[2], Daniel Esteve[2], Fabien Portier[2], and Joachim Ankerhold[1] — [1]ICQ and IQST, Ulm University, Germany — [2]SPEC, CEA Paris-Saclay, France — [3]School of Physics and Astronomy, University of Nottingham, UK — [4]Physikalisches Institut, Karlsruhe Institute of Technology, Germany

The realization and characterization of efficient sources of entangled microwave photons is of paramount importance for many future applications of quantum technology. Josephson-photonics devices are very promising candidates for this task since they allow one to create a broad range of different entangled states in a surprisingly simple and robust way. Such devices consist of a dc-voltage-biased Josephson junction which is placed in series to several microwave cavities. Steady states with multifaceted entanglement properties then appear in steady state resulting from the interplay of multiphoton creation processes associated with the inelastic tunneling of Cooper pairs and subsequent individual photon leakage from the cavities. In this talk, we present a detailed theoretical study of the bipartite entanglement between photon pairs in the output transmission lines. Numerical simulations, taking into account low-frequency fluctuations of the bias voltage and the finite bandwidth of microwave signal detectors, show excellent agreement with recent experimental data.

HL 55.10 Thu 12:00 HSZ 03

Theory of injection locking for the Josephson laser — •Ciprian Padurariu, Lukas Danner, Björn Kubala, and Joachim Ankerhold — Institute for Complex Quantum Systems and IQST, Ulm University, 89069 Ulm, Germany

An intriguing recent experiment [1] has observed features of lasing in the microwave emission of a cavity driven by inelastic Cooper pair tunneling across a dc-voltage biased Josephson junction. A successful theory was developed explaining the emission in the lasing regime [2], however, the theory of injection locking remained unexplained.
Here, we provide the theory for injection locking in Josephson photonic devices. Specifically, we provide an analytical derivation of the phenomenological Adler equation for a large class of Josephson devices. We extract detailed guidelines for designing circuits capable of locking the phase against noises and estimate the rate of thermal and quantum phase slips that limit the locking precision.
The work aims at providing the missing ingredient, phase-stabilized Josephson oscillations, required to demonstrate the quantum entanglement of the emitted microwave light.
[1] M.C. Cassidy et al., Science 355, 939 (2017).
[2] S. Simon and N. Cooper, Phys. Rev. Lett. **121**, 027004 (2018).

HL 55.11 Thu 12:15 HSZ 03

Electron transport and spin qubit manipulation with surface acoustic waves — •Mikel Olano[1] and Geza Giedke[1,2] — [1]Donostia International Physics Center, Donostia, Spain — [2]Ikerbasque Foundation for Science, Bilbao, Spain

Spin qubits in quantum dots are among the most promising systems for the implementation of quantum computation. While coherence times and gate operation times have become very competitive, the realization of long-range interactions to enable more flexible quantum gates remains a challenge.

Here we investigate theoretically an approach to tackle this problem using a moving electrons trapped in the potential of a surface acoustic wave, that serves as an intermediary between distant stationary quantum dots.

We analyse the coherent transport and transfer of spin qubits between stationary and moving dots and quantum gates between two interacting spin qubits. Applications for the generation of multipartite entanglement and joint measurement of several qubits are discussed. The talk will highlight the parameters to be taken into account if these processes are to be optimized. The impact of the main sources of decoherence and non-adiabatic behaviour due to the time-dependence of the potential are discussed.

HL 56: 2D Materials and their Heterostructures II (joint session DS/O/HL)

Time: Thursday 9:30–10:45 Location: CHE 89

HL 56.1 Thu 9:30 CHE 89

Longitudinal Nonlinear Spin Sensitive Response in two-dimensional Materials — •Dominik Kreil, Mario Graml, and Helga M. Böhm — Institute of Theoretical Physics, Johannes Kepler University Linz, Altenbergerstr. 69, A-4040 Linz, Austria

Future spin- and valleytronic devices will demand a deeper understanding of electronic systems. [1] With increasing intenstitys of state of the art terahertz lasers linear approximations become more imprecise. Nonlinear plasmonic effects arising from coherent oscillations of free charge carriers in metals or highly doped semiconductors serve to enhance optical processes. The underlying dynamics of electrons (or holes) was successfully treated semi-classically [2] in three-dimensional (3D) nanostructures; quantum expressions for up to the third order of the longitudinal nonlinear polarizabilities of the 3D, 2D and 1D homogeneous electron gases as well as graphene are also known. We here present a general discussion of higher order response functions resulting from time-dependent perturbation theory. Using the random phase approximation as in Ref. [3] we also derive a closed formula for longitudinal nonlinear spin sensitive response functions in arbitrary order. It holds for all the above listed systems and for imbalanced spin- or valley-polarizations. An application to the 2D spin-polarized electron gas with parabolic dispersion and in graphene [4,5] is presented.
References: [1] Vitale et al., Small 14, 1801483 (2018). [2] Krasavinet al., Laser & Photonics Reviews 12, 1700082 (2018). [3] Mikhailov, Phys. Rev. B. 93, 085403 (2016). [4] D. Kreil et al., Phys. Rev. B. 92, 085403 (2015). [5] D. Kreil et al., Lithuanian J. Phys. 59, 35 (2019).

HL 56.2 Thu 9:45 CHE 89

Predicting Exfoliability of MAX Phases into MXenes Using Ab-initio Thermodynamics — •Ali Muhammad Malik, Delwin Perera, Jochen Rohrer, and Karsten Albe — Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany

In recent years, research on 2D MAX-derived MXenes has expanded significantly due to their potential application in energy storage systems, electromagnetic interface shielding, electrocatalysis and gas detection. Almost 40 MAX phases have been predicted to be exfoliable based on force constant calculations and exfoliation energies. However, in experiment only 21 have so far been chemically exfoliated. In this work, we present a descriptor that combines calculated reaction energies and surface stabilities under experimentally relevant conditions. In agreement with experiments, we show that this descriptor is indeed capable of predicting the exfoliability of MXenes from Ti-based MAX phases in HF, whereas Cr-based MAX phases are predicted to decompose into Cr_3C_2 (carbide). We suggest that this descriptor is capable to guide experimental synthesis efforts in particular with respect to the choice of etchant and concentration.

HL 56.3 Thu 10:00 CHE 89

Characterization and Stability of Janus TiXY (X/Y= S, Se, and Te) Monolayers — Aybey Mogulkoc[1], Yesim Mogulkoc[1], Seymur Jahangirov[2], and •Engin Durgun[2] — [1]Department of Physics, Ankara University, 06100, Ankara, Turkey — [2]UNAM and Institute of Materials Science and Nanotechnology, Bilkent University, 06800, Ankara, Turkey

The addition of third element to binary 2D structures can lead to superior properties, hence extensive analyses on the characterization of such systems are required to reveal their full potential. In this study, we examine the structural, mechanical, electronic, thermal, and optical properties of TiXY (X/Y= S, Se, and Te) monolayers by using first-principles techniques. The stability of 1T and 2H-phases are revealed by phonon spectrum analysis and molecular dynamics simulations. Following the investigation of the mechanical response, electronic structures are examined together with partial density of states analysis. While monolayers of 1T-TiXY are found to be semimetals, monolayers of 2H-TiXY are semiconductors with indirect band gap. The optical spectrum is obtained by calculating the imaginary dielectric function and is correlated with the electronic structure. The variation of heat capacity with temperature is investigated and low/high temperature response is shown. Finally, possible structural distortions

are also taken into account and charge density wave transition in 1T-TiSeS due to Peierls instability is demonstrated. Our results not only reveal the stable Janus monolayers of TiXY but they also point out these systems as promising candidates for nanoscale applications.

HL 56.4 Thu 10:15 CHE 89

Semiconducting defect-free polymorph of borophene: Peierls distortion in two dimensions — Semran Ipek[2], Aybey Mogulkoc[1], •Seymur Cahangirov[2], and Engin Durgun[2] — [1]Department of Physics, Ankara University, 06100, Ankara, Turkey — [2]UNAM and Institute of Materials Science and Nanotechnology, Bilkent University, 06800, Ankara, Turkey

In contrast to the well-defined lattices of various two-dimensional (2D) systems, the atomic structure of borophene is sensitive to growth conditions and type of the substrate which results in rich polymorphism. By employing ab initio methods, we reveal a thermodynamically stable borophene polymorph without vacancies which is a semiconductor unlike the other known boron sheets, in the form of an asymmetric centered-washboard structure. Our results indicate that asymmetric distortion is induced due to Peierls instability which transforms a symmetric metallic system into a semiconductor. We also show that applying uniaxial or biaxial strain gradually lowers the obtained band gap and the symmetric configuration is restored following the closure of the band gap. Furthermore, while the Poisson's ratio is calculated to be high and positive in the semiconducting regime, it switches to negative once the metallicity is retrieved. The realization of semiconducting borophene polymorphs without defects and tunability of its electronic and mechanical response can extend the usage of boron sheets in a variety of nanoelectronic applications

HL 56.5 Thu 10:30 CHE 89

First-principles study of hydrogenation on bilayer GaN — •Anh Khoa Augustin Lu[1], Tetsuya Morishita[1,2], Tomoe Yayama[3], and Takeshi Nakanishi[1,2] — [1]MathAM-OIL, AIST, Sendai, Japan — [2]CD-FMat, AIST, Tsukuba, Japan — [3]Department of Applied Physics, Kogakuin University, Tokyo, Japan

In the last decade, a large number of two-dimensional materials has been discovered. In recent years, two-dimensional III-V materials have arisen with the experimental demonstration of two-dimensional GaN. Here, we focus on the case of bilayer GaN. While the atomic structure of pristine bilayer GaN is relatively well understood, the impact that hydrogenation remains unclear since unlike transition metal dichalcogenides, pristine GaN has dangling bonds. In that respect, the present work focuses on the atomic structure, stability and electronic properties of bilayer GaN passivated by hydrogen atoms, with a large range of hydrogen coverage. First-principles calculations based on the density functional theory were performed to identify the structures with the lowest energy. While previous studies have focused on structures oriented along the c-plane, our results reveal that depending on the hydrogen concentration, the plane orientation of the most stable structure (c-, m-, or a-plane) is different. In particular, at high hydrogen concentration, structures oriented along the m- and a-planes have the lowest energy. Their stability is confirmed by first-principles molecular dynamics simulations performed at finite (room) temperature. By modulating the hydrogen concentration, one can therefore tailor the atomic structure and properties of bilayer GaN.

HL 57: Thin Oxides and Oxide Layers I (joint session DS/HL/O)

Time: Thursday 9:30–10:45 Location: CHE 91

HL 57.1 Thu 9:30 CHE 91

Atomically sharp epitaxial interface between Ba_2SiO_4 and Si(001) — •Julian Koch and Herbert Pfnür — Leibniz Universität Hannover, Institut für Festkörperphysik

Epitaxial growth of Ba_2SiO_4 on Si(001) is a challenge, since neither crystal symmetry nor lattice constants match in a simple manner, but as we show, it has the potential to become the first high quality crystalline high-k gate dielectric. We combined X-ray photoelectron spectroscopy (XPS), low energy electron diffraction (LEED) and aberration-corrected scanning transmission electron microscopy (STEM) in order to optimize the epitaxial growth by molecular beam epitaxy. The films were grown by a co-deposition method that requires no diffusion of Si from the substrate. While 400 °C turned out to be sufficient to form chemically homogeneous films, crystalline films required an annealing step to $670-690$ °C with the break-up of interfacial Si-O bonds as crucial step. STEM confirms that the interface is atomically sharp and that a single layer of the silicate is changed to a (2×3) structure at the interface from the (2×1.5) bulk structure. Electrical measurements on MOS-diodes with this material show small hysteresis in CV-curves, low interface trap densities ($< 6 \times 10^{10}$ cm^2eV^{-1}) and low leakage currents.

HL 57.2 Thu 9:45 CHE 91

Nano-scale spectroscopic analysis of $LaAlO_3/SrTiO_3$ interfaces using scattering-type Scanning Near-field Optical Microscopy — •Yigong Luan[1], Julian Barnett[1], Marc Rose[2], Felix Gunkel[2], Martin Lewin[1], and Thomas Taubner[1] — [1]Institute of Physics (IA) RWTH Aachen — [2]PGI-3, Forschungszentrum Jülich

In the group of functional oxide materials, the interface of bulk insulators $LaAlO_3$ and $SrTiO_3$ (LAO/STO) attracts attention due to its highly confined and conductive two-dimensional electron gas (2DEGs), which could be interesting for high-electron-mobility transistors. 2DEGs at oxide interfaces result from electronic reconstruction, which is highly dependent on the local structure [1]. The extraction of their electronic properties is difficult for far-field spectroscopy and conventional nano-resolved microscopy (e.g. STM), as the conducting layer is highly confined and buried below an insulating layer (LAO). We overcome these limitations by using scattering-type Scanning Near-field Optical Microscopy for a quantitative extraction of electron properties from "phonon-enhanced spectroscopy", as the presence of free charge carriers leads to significant changes to the phonon resonance due to plasmon-phonon coupling [2]. We use an improved model (Finite Dipole Model) combining with Transfer Matrix Method to interpret the experimental results, investigating the influence of both LAO layer and 2DEGs on the STO phonon near-field resonance in detail, which allows us to extract the local electronic properties.

[1] A. Ohtomo et al., Nature 427, 423 (2004)
[2] M. Lewin et al., Adv. Funct. Mater, 28. 1802834 (2018)

HL 57.3 Thu 10:00 CHE 91

Optoelectrical properties of VO_2 ultra-thin films — •Maximilian Obst[1], Laura Rodríguez[2], Gustau Catalan[2,3], Susanne C. Kehr[1], and Lukas M. Eng[1,4] — [1]Institute of Applied Physics, Technische Universität Dresden, Germany — [2]Institut Catalá de Nanociéncia i Nanotecnologia and The Barcelona Institute of Nanoscience and Technology, Campus UAB, Barcelona, Catalonia — [3]ICREA-Institució Catalana de Recerca i Estudis Avançats, Barcelona, Catalonia — [4]ct.qmat: Dresden-Würzburg Cluster of Excellence - EXC 2147, Technische Universität Dresden, Germany

Vanadium dioxide (VO_2) is a material that is in the central research focus due to its metal-to-insulator phase transition (MIT) at room temperature. Experimentally, this temperature-regime is easily accessible, and hence allows profound MIT-studies while dreaming of interesting applications, such as phase-change memories. Although thicker VO_2 films are intensively investigated, the properties and physical behavior of ultrathin VO_2 layers are far from being understood.

In this work, an epitaxial VO_2-film of 10 nm grown on a rutile(001) single-crystal is explored, applying a broad set of electrical and optical methods. While Raman-spectroscopy revealed no structural phase transition of the film, electrical transport measurements as well as spectrally-resolved (UV to mid-IR) reflectivity measurements clearly show the MIT at ∼300 K. In conclusion, the structural and electrical phase transition seems to be completely disentangled in these ultrathin films. However, thin VO_2-films might easily oxidize to V_2O_5, as was indicated by measuring the vanadium $2p_{3/2}$-peak using XPS.

HL 57.4 Thu 10:15 CHE 91

Towards quasi two-dimensional β-Ga2O3 — •Constance Schmidt, Mahfujur Rahaman, and Dietrich R. T. Zahn — Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany

β-Ga2O3 is a transparent oxide semiconductor with outstanding properties due to its wide bandgap (Eg = 4.9 eV). It is already intensively

studied in its bulk and thin film form. Studies on ultrathin films or even quasi-2D films are less common. Nevertheless, for nano electronics quasi-2D β-Ga2O3 can be beneficial as semiconductor or insulator, depending on layer thickness and doping [1]. β-Ga2O3 is not a van-der-Waals material, which makes conventional exfoliation challenging. Attempts show that layer thicknesses below 60 nm are not yet possible by exfoliating β-Ga2O3 [2]. To overcome this difficulty, we use a van-der-Waals material (GaSe), exfoliate thin flakes on Si with 300 nm SiO2, HOPG and Mica substrates, and oxidize these flakes by thermal annealing ((600 - 1000)°C, 30 min, in air) to obtain quasi 2D β-Ga2O3. In this work, we show the preparation of Se free quasi-2D β-Ga2O3 by annealing using temperatures higher than 700°C. The thin flakes obtained have thicknesses in the range of (0.5 - 50) nm as measured with atomic force microscopy. Energy dispersive X-ray spectra reveal the chemical composition of the 2D flakes and most importantly the absence of Se. Raman spectroscopy (excitation: 325 nm) verifies the β-Ga2O3 phase.

[1] J. Su, et al., J. Phys. Chem. C 122 43 24592-24599 (2018) [2] Y. Kwon, et al., APPLIED PHYSICS LETTERS 110 131901 (2017)

HL 57.5 Thu 10:30 CHE 91

Thermal phase transformations through iron oxides/ oxide substrates interfaces — •Mai Hussein Hamed[1,2], David N. Mueller[1], Tomáš Duchoň[1], Ronja Hinz[1], Claus M. Schneider[1,3], and Martina Müller[1,4] — [1]Peter-Grünberg-Institut (PGI-6), Forschungszentrum Jülich GmbH, Germany — [2]Faculty of Science, Helwan University, Cairo, Egypt — [3]Fakultät für Physik, Duisburg-Essen Universität , Germany — [4]Experimentelle Physik I, Technische Universität Dortmund, Germany

Oxide heterostructures possess a wide range of electrical and magnetic properties arising, in particular, vie interactions across their interfaces. Therefore, our primary goal is understanding, controlling and tuning the interface properties. In this study, using hard X-ray photoelectron spectroscopy (HAXPES), we demonstrate phase transformations from Fe_3O_4 to either γ-Fe_2O_3 or FeO through active redox reactions across three relevant interfaces, i.e. (1) the outside atmosphere/Fe_xO_y film interface, (2) the interface between phase-transformed Fe_xO_y/Fe_xO_y intralayers and (3) the Fe_xO_y/oxide substrate interface. We find that the "active" oxide substrates ($SrTiO_3$ or YSZ) play an important role as an additional oxygen supplier or scavenger. This leads to a clear alteration of the standard temperature-pressure phase diagram of iron oxides. Accordingly, we calculate the effective oxygen pressure through the interfaces and adjust the phase diagram. Our findings allow us not only to control the interfaces but more importantly, to tune their physical functionalities by a controlled thermal phase design, giving access to far from equilibrium phases.

HL 58: Nitrides: Preparation and characterization I

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

HL 58.1 Thu 9:30 POT 112

MOVPE growth of (11-22) AlGaN/AlN on m-plane sapphire — •Humberto Foronda[1,2], Sarina Graupeter[1], Valeria Bonito-Oliva[2], Mike Pietsch[2], Priti Gupta[1], Norman Susilo[1], Frank Mehnke[1], Johannes Enslin[1], Tobias Schulz[2], Tim Wernicke[1], Klaus Irmscher[2], Martin Albrecht[2], and Michael Kneissl[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Berlin — [2]Leibniz-Institut für Kristallzüchtung,Berlin

The efficiency of UVC-LEDs emitting below 240 nm drops with decreasing wavelength on (0001) grown $Al_xGa_{1-x}N$. One reason is a change in the optical polarization of the emitted light leading to a reduced light extraction efficiency (LEE). LEDs on semipolar planes, i.e. (11-22), overcome poor LEE due to a rotation of the wurtzite unit cell while decreasing the polarization fields. (11-22) $Al_xGa_{1-x}N$/AlN by metalorganic vapor phase epitaxy (MOVPE) was investigated for realizing UVC-LEDs on this orientation. When growing $Al_xGa_{1-x}N$ on (10-10) sapphire, layers with (11-22) orientation were achieved, but a deterioration of the surface morphology due to misoriented grains was observed. The protrusion and density of these grains was reduced by tailoring growth and nitridation conditions on sapphire such that a grain-free planar (11-22) surface was achieved. A reduced growth rate suppressed grains at the surface as well as increasing the pressure during nitridation. (11-22) $Al_{0.65}Ga_{1-0.65}N$:Si layers with different silicon concentrations were grown, where a minimum resistivity of 0.024 Ω cm was achieved, comparable to results on (0001). AlGaN multiquantum wells revealed 240 nm photoluminescence emission.

HL 58.2 Thu 9:45 POT 112

Optoelectronic Characterization of GaN Nanowires on SiC-6H — •Andrea Wieland[1,2], Theresa Hoffmann[1], and Martin Stutzmann[1] — [1]Walter Schottky Institut and Physics Department, Technische Universität München, Garching, Germany — [2]Ludwig-Maximilians-Universität München, Munich, Germany

Gallium nitride (GaN) nanowires (NWs) have gained interest for device fabrication due to their large surface-to-volume ratio, high crystal quality and optical waveguide characteristics. [1] As the polarity of GaN NWs influences the electronic properties at the heterointerfaces of the NWs and the substrate, polarity determination and control of the GaN NWs are key requirements to achieve desired NW-based device properties.

We have established the growth of GaN NWs on both polarities of hexagonal silicon carbide (SiC-6H) substrates by molecular beam epitaxy. Selective area growth of GaN NWs allows the variation of the NW dimensions and positions. To obtain optimal growth results the substrate temperature has been varied. Photoluminescence spectroscopy measurements at low temperatures have been performed for optical characterization of the GaN NW. Furthermore, the influence of the SiC-6H substrate polarity on the GaN NWs polarity has been investigated by means of KOH etching and contact potential difference measurements via Kelvin Probe Force Microscopy.

[1] J. Winnerl et al., J. Appl. Phys. 123, 203104 (2018)

HL 58.3 Thu 10:00 POT 112

Growth of AlN on Si(111) by reactive pulsed sputtering — •Florian Hörich, Jürgen Bläsing, Armin Dadgar, and André Strittmatter — Otto-von-Guericke University Magdeburg

Efficient, nitride-based UV light emitting diodes demand for AlN buffer structures with well-aligned crystallographic planes both in growth as well as in in-plane direction to enable low-defect densities within the subsequent layer stack. Currently, best crystallographic qualities are reported for sputtered AlN layers on sapphire substrates which are thermally annealed at temperatures up to 1700°C . This technique cannot be used with silicon substrates because of the lower melting temperature of Si. Thus, sputtering of AlN layers must be optimized to obtain low-defect density buffer structures on Si. We present our work on the growth of AlN on Si(111) by reactive pulsed sputtering, where growth temperatures below 800°C are used. The low growth temperature aims at reducing thermal stress in the epitaxial layer. We examine the effect of an Al seed layer and the impact of the nitrogen source for the crystalline quality. The thickness of the Al seed layer is critical and an optimum for a deposition time of 4 s (would correspond to a 0.2 nm Al layer) is found. Ammonia as nitrogen source is not favourable during growth of AlN directly onto the Si substrate. Since NH3 reacts with the Si surface forming SiN the growth of AlN is limited. With N2 as nitrogen source these limiting chemical reactions are not observed enabling AlN growth on top of the Al seed layer. For an AlN layer thickness of 40 nm the FWHM values of the XRD rocking curves are 0.65° (0002) and 1.35° (10-10).

HL 58.4 Thu 10:15 POT 112

Room temperature excitonic recombination processes in GaInN/GaN quantum wells at studied via carrier density dependent time-resolved photoluminescence — •S. Müllner[1,2], P. Henning[1,2], P. Horenburg[1], H. Bremers[1,2], U. Rossow[1], and A. Hangleiter[1,2] — [1]Institute of Applied Physics, Technische Universität Braunschweig, Germany — [2]Laboratory for Emerging Nanometrology, Braunschweig, Germany

Our experimental results indicate excitonic recombination processes in nonpolar *m*-plane GaInN/GaN quantum wells (QW) even at high carrier densities. This follow-up study from polar *c*-plane GaInN/GaN, where a similar trend has been reported, was realized by time-resolved photoluminescence experiments at room temperature in which the

excess carrier density, δn, is tuned by the laser fluence. Of particular interest is the regime of high carrier densities. Here, we find that the nonradiative lifetime $\tau_{nr} \sim 1/\delta n$, evidencing excitonic Auger recombination. In addition, we observe a constant radiative lifetime, τ_r, with δn. In the model of free charge carrier recombination, this is expected for the low injection regime in which the background carrier density $n_0 \gg \delta n$, however, for the high injection regime, a $\tau_r \sim 1/\delta n$ dependence is predicted. Assuming excitonic recombination, $\tau_r(\delta n)$ is constant for high carrier densities, as we observe it, even further underlying excitonic recombination. We assure that we are in the high carrier density regime by comparing $\tau_{nr}(\delta n)$, where the transition between the low and high injection regime is signatured by an increase of τ_{nr}, associated with defect recombination.

HL 58.5 Thu 10:30 POT 112

STEM and STEBIC analysis of screw dislocations in GaN to investigate structural and electronic properties — •Tobias Westphal[1], Sevastian V. Shapenkov[2], Oleg S. Vyvenko[2], and Michael Seibt[1] — [1]University of Goettingen, IV. Physical Institute, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Faculty of Physics and IRC Nanotechnology Research Park, St. Petersburg State University, Ulyanovskaya 1, 198504, St. Petersburg, Russia

As GaN has a quite high grown-in dislocation density, in the order of $10^6\,cm^{-2}$ - $10^8\,cm^{-2}$ depending on the growth technique, investigating the electronic and optical properties of dislocations is of particular interest. Freshly introduced a-screw dislocations produced by indentations perpendicular to the basal (0001) plane of specially undoped low-resistance GaN show an intense dislocation related luminescence (DRL) with an energy peak at around 3.18 eV [1]. This red shift of about 300 meV with respect to the band gap can be explained by a dissociated dislocation, where the stacking fault ribbon forms a quantum well. Therefore, structural investigations of the dislocation core with high spatial resolution are of tremendous interest.

In this contribution, we report about STEM and scanning transmission electron beam induced current (STEBIC) measurements of dislocations in GaN. Measuring EBIC inside the TEM increases the spatial resolution compared to EBIC in the SEM, as the generation volume inside the sample is much smaller, which allows us to investigate single dislocations near the indentation prick.

[1] O. Medvedev et al., J. Appl. Phys. 123, 161427 (2018)

30 min. break.

HL 58.6 Thu 11:15 POT 112

Investigations on the defect luminescence in high aluminum containing AlGaN heterostructures — •Marcel Schilling, Norman Susilo, Tim Wernicke, and Michael Kneissl — Technische Universität Berlin, Institute of Solid State Physics, Hardenbergstraße 36, 10623 Berlin, Germany

The realization of deep ultraviolet light emitting diodes (DUV-LEDs) with emission wavelength near 232 nm is very challenging as the photon energy is very close to the band gap of AlN, i.e. AlGaN layers with extremley high Al mole fraction are required. One problem is, that during metal organic vapor phase epitaxy of AlGaN crystalline point defects like vacancies or impurities are incorporated. Deep levels in the energy band gap associated to these point defects result in non-radiative carrier recombination decreasing the internal quantum efficiency (IQE) of DUV-LEDs. Therefore the understanding of the generation of point defects during the growth in high aluminum containing AlGaN layers is crucial for the development of efficient DUV-LEDs. In this study the defect luminescence of AlGaN layers is investigated by photoluminescence spectroscopy. The origin of the defect luminescence is determined by comparing defect luminescence spectra with transition energies for different defects and defect complexes reported in literature. Furthermore, the AlGaN layer quality is improved by optimizing the growth conditions in the reactor in correlation with the purity of the photoluminescence spectra. For example the defect luminescence in a 72% AlGaN layer near a wavelength of 442 nm, is investigated and most probably assigned to a V_{Al}^{3-} vacancy.

HL 58.7 Thu 11:30 POT 112

Indium rich cubic group III Nitrides fabricated with molecular beam epitaxy — •Falco Meier, Dirk Reuter, and Donat J. As — Department of physics, Paderborn University

Indium Nitride (InN) and Indium Gallium Nitride (InGaN) are one of the most important semiconductor materials with a wide variety of applications, such as infrared LEDs, high-frequency and high temperature electronic devices. InN synthesized in the metastable cubic phase (c-InN) has received intensive attention because of its high electron mobility, the low phonon scattering, and the small direct band gap. Due to the high degree of symmetry in c-InN strong build-in electric fields are avoided. However, it is difficult to grow high-crystalline-quality InN because of its low dissociation temperature and the lack of lattice matched substrates. In this work we use a c-GaN buffer layer on a pseudo-substrate of 3C-SiC(001)/Si(001) for the growth of cubic InN and In-rich InGaN with plasma assisted molecular beam epitaxy. A set of parameters for the growth of phase-pure c-InN with a thickness of about 100 nm is determined. A smoothening of the Surface where the e-Beam of the reflection high-energy electron diffraction hits the Sample was verified with Atomic Force Microscopy. High resolution x-ray diffraction indicates that phase pure c-InN grow fully relaxed on the c-GaN buffer layers. The hexagonal phase content was below 5%. In-rich c-InGaN with nominal 10% and 20% Ga contents are also grown. Post growth characterization show that only a part of the nominal offered Ga content are incorporated into the c-InGaN compound indicating spinodal decomposition at the low growth temperatures.

HL 58.8 Thu 11:45 POT 112

Capacitance-Voltage spectroscopy at room temperature of self-assembled GaN quantum dot ensembles under illumination — •Carlo Alberto Sgroi[1], Julien Brault[2], Jean-Yves Duboz[2], Peter Conrad[1], Arne Ludwig[1], and Andreas D. Wieck[1] — [1]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]CNRS - CRHEA, Rue Bernard Grégory, 06560 Valbonne, France

We present capacitance voltage (CV) measurements under illumination at room temperature of charge-tunable self-assembled wurtzite GaN quantum dots (QDs) in an $Al_xGa_{1-x}N$ matrix grown by MBE.

GaN and its alloys have excellent properties such as their thermal stability, high thermal conductivity and wide bandgap energies which make them an ideal candidate for next-generation GaN-based power devices and QD storage devices. Due to polarization and strain effects in wurtzite $GaN/Al_xGa_{1-x}N$ heterostructure layers, the band structure is different where QDs and wetting layer (WL) are, respectively. Large electric fields and phonon processes promote charge transfer through the WL.

Performing CV spectroscopy on an AlGaN-Schottky diode structure with embedded GaN QDs, we observe a hysteresis effect in the charging and discharging of the QDs at room temperature. Under illumination of 395 nm, bandgap excitation of the QDs, we change the electron exchange mechanism and are able to remove the hysteresis effect completely.

HL 58.9 Thu 12:00 POT 112

Effect of low temperature GaN underlayers on the carrier lifetimes in GaInN/GaN quantum wells — •Philipp Horenburg[1], Philipp Henning[1], Savutjan Sidik[1], Uwe Rossow[1], Heiko Bremers[1,2], and Andreas Hangleiter[1,2] — [1]Institute of Applied Physics, Technische Universität Braunschweig, Germany — [2]Laboratory for Emerging Nanometrology, Braunschweig, Germany

We demonstrate the impact of low temperature GaN underlayers (UL) grown under various conditions on the carrier lifetimes and the radiative efficiency and in GaInN/GaN quantum well (QW) structures. Since nonradiative recombination is associated with crystal defects in close proximity to the QW, the material grown underneath has a substantial influence on the carriers in QW. As the recombination dynamics can be significantly affected by changes in the density of defects and background carriers, the QW is not least susceptible to the growth conditions of this UL. We have grown a series of c-plane QW structures by low-pressure MOVPE on sapphire substrates. While GaInN is widely used an UL material, we chose a pure GaN UL grown at low temperature. Power and temperature dependent measurements show a strong increase of the internal quantum efficiency by two orders of magnitude compared to structures without a low temperature UL. Time-resolved photoluminescence measurements reveal that, with increasing thickness of the UL, not only the nonradiative lifetime increases, but also the radiative lifetime is affected just as for GaInN UL. These observations suggest that not the composition, but particularly the growth conditions affect the recombination dynamics in the QW structure.

HL 58.10 Thu 12:15 POT 112

Luminescence of GaN quantum dots on highly reflective deep UV Bragg mirrors — •Hannes Schürmann[1], Christoph

Berger[1], Gao Kang[2], Gordon Schmidt[1], Peter Veit[1], Frank Bertram[1], Sebastian Metzner[1], Armin Dadgar[1], Jürgen Bläsing[1], André Strittmatter[1], Mark Holmes[2], and Jürgen Christen[1] — [1]Institute of Physics, Otto-von-Guericke-University Magdeburg, Germany — [2]Institute of Industrial Science, The University of Tokyo, Japan

Towards the realization of room temperature stable and efficient single photon emitters, we present the structural and optical properties of GaN quantum dots (QDs) embedded in an AlGaN semi-microcavity with deep UV Bragg reflectors (DBR).

The structure was grown by MOVPE on AlGaN/sapphire template. Embedded in an AlGaN λ-cavity, the GaN QDs result from a 2 nm GaN layer with growth interruption. The DBR consists of 50 AlN/AlGaN pairs with 99.7 % reflectivity. Mesa structures were produced by reactive ion etching to investigate individual QDs.

Quasiresonantly excited QDs exhibit narrow emission lines between 269 - 273 nm with FWHM down to 0.9 meV at 8 K. Autocorrelation measurements reveal a clear antibunching with $g^{(2)}(0)$ values down to 0.34, which proofs single photon statistics of QD emission matching the DBR stopband.

HL 59: THz and MIR physics in semiconductors

Time: Thursday 9:30–12:30 Location: POT 151

HL 59.1 Thu 9:30 POT 151

Light impact ionization in HgTe quantum wells close to critical thickness — •Stefan Hubmann[1], Grigory Budkin[2], Michael Urban[1], Vasily Bel'kov[2], Eugenius Ivchenko[2], Alexander Dmitriev[2], Johannes Ziegler[1], Dimitriy Kozlov[3], Nikolay Mikhailov[3], Sergey Dvoretsky[3], Ze-Don Kvon[3], Dieter Weiss[1], and Sergey Ganichev[1] — [1]Terahertz Center, University of Regensburg, 93040 Regensburg, Germany — [2]Ioffe Institute, 194021 St. Petersburg, Russia — [3]Rzhanov Institute of Semiconductor Physics, 630090 Novosibirsk, Russia

We report on the observation of terahertz radiation induced band-to-band impact ionization in HgTe quantum well structures close to critical thickness characterized by a nearly linear energy dispersion. This carrier multiplication process is detected for frequencies from 0.6 to 1.07 THz and in a temperature range from 4 to 90 K. Furthermore, the product of the angular radiation frequency ω and the momentum relaxation time τ is close to unity denoting a transition between the quasi-static regime $\omega\tau \ll 1$ and the high-frequency regime $\omega\tau \gg 1$. We developed a microscopic theory of light impact ionization for both regimes in HgTe quantum wells with nearly linear energy dispersion. We show that the probability of impact ionization in the transition regime is proportional to $\exp(-E_0^2/E^2)$, of the radiation electric field amplitude E and the characteristic field parameter E_0, where E_0 is strongly dependent on the radiation frequency.

HL 59.2 Thu 9:45 POT 151

Towards plasmonic tunnel gaps by on-chip laser ablation for on-chip THZ applications — •Michael Zartenar[1], Philipp Zimmermann[1,2], Alexander Höttger[1], Noelia Fernandez[1], Anna Nolinder[1], Kai Müller[1], Jonathan Finley[1,2], and Alexander Holleitner[1,2] — [1]Walter Schottky Institute and Physics Department, Technical University of Munich, Am Coulombwall 4a, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 Munich, Germany

We demonstrate that prestructured metal plasmonic nanogaps can be shaped on-chip to below 10 nm by femtosecond laser ablation. We explore the plasmonic properties and the nonlinear photocurrent characteristics of such formed tunnel junctions. The photocurrent can be tuned from multiphoton absorption toward the laser-induced strong-field tunneling regime in the nanogaps, and gives rise to a field emission of ballistic hot electrons propagating across the nanoscale junctions. We show that a unipolar current of hot electrons is achieved by designing the plasmonic enhancement factors in the junctions to be asymmetric, which allows ultrafast electronics on the nanometer scale. We particularly demonstrate that femtosecond optical pulses in the near-infrared (NIR) applied to such nanogaps can drive electronic circuits with a prospective bandwidth of up to 10 THz. We thank the DFG for funding via the Cluster of Excellence e-conversion.

HL 59.3 Thu 10:00 POT 151

Modeling of the Hot Carrier Dynamics in Graphene THz Magneto Plasmons — •Florian Stawitzki[1], Sebastian Matschy[1], Stephan Winnerl[2], Matt Chin[3,4], Thomas E. Murphy[4], and Martin Mittendorff[1] — [1]Universität Duisburg-Essen, Duisburg, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]US Army Research Laboratory — [4]University of Maryland, College Park, MD, US

Patterning graphene in plasmonic structures leads to resonant absorption and an increased light-matter interaction that also results in enhanced THz non-linear absorption. The charge carriers in graphene can be heated efficiently, leading to a decrease in chemical potential. This causes an ultrafast redshift of the plasmon frequency, and thus a strong increase in transmission at the resonance frequency. Here we study the dynamics of THz plasmons in an array of micrometer sized discs of bilayer graphene on SiC. These plasmons hybridize with the cyclotron motion in strong magnetic fields leading to splitting of the plasmon resonance into two branches that can be distinguished with circularly polarized radiation. We experimentally and theoretically investigate the nonlinear absorption in magnetic fields of up to 10T. A two-temperature model is used to simulate the time dependent temperature of the charge carriers. The results are in good agreement with pump-probe measurements performed at the free-electron laser FELBE at HZDR.

We thank the German Research Foundation for funding through CRC 1242.

HL 59.4 Thu 10:15 POT 151

Mid-infrared induced transparency in boron-doped diamond — •Alexander Paarmann[1], Sergey Pavlov[2], Andreas Pohl[3], Martin Wolf[1], and Heinz-Wilhelm Hübers[2,3] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Institute of Optical Sensor Systems, German Aerospace Center (DLR), Berlin, Germany — [3]Humboldt University Berlin, Berlin, Germany

The properties of deep impurity levels in elemental semiconductors have important implications for many applications, ranging from electronic and optoelectronic devices to superconductivity. Remarkably, boron dopants implanted into high-quality diamond single crystals result in exceptionally large binding energies leading to impurity state transitions around 350 meV, i.e., in the mid-infrared spectral range.

Facilitated by the localized nature of the electronic impurity levels, such systems typically show very strong nonlinear-optical interactions. This can be used, for instance, to probe the ultrafast dynamics to elucidate the relaxation mechanism of photo-excited states with pump-probe spectroscopy [1]. Moreover, as we show here, the bleaching of the fundamental impurity transition also leads to a dramatic fluence dependence of the transmission. This opens up many possibilities for using boron-doped diamond for nonlinear-optical applications.

[1] S.G. Pavlov, et al., Diamond & Related Materials 92, 259 (2019)

HL 59.5 Thu 10:30 POT 151

Anisotropic nonlinear THz response of bilayer graphene — •Angelika Seidl[1,2], Peter Richter[3], Thomas Seyller[3], Harald Schneider[1], Manfred Helm[1,2], and Stephan Winnerl[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf — [2]Technische Universität Dresden, Dresden — [3]Technische Universität Chemnitz, Chemnitz

The intraband absorption of doped graphene is utilized in novel devices for the THz frequency range, in particular for detectors and modulators. In many cases the nonlinear THz response can be understood as a hot carrier effect, i.e. by modelling the response of an isotropic hot Fermi-Dirac distribution of carriers [1]. We have performed degenerate pump-probe experiments at 2 THz on quasi-freestanding bilayer graphene (QFBLG) on SiC utilizing the free-electron laser FELBE.We find a pump-induced transmission, corresponding to a reduced Drude absorption of hot carriers. The induced transmission is about two times lager for the case of co-polarized pump and probe beam as compared to the cross-polarized case, which clearly indicates an anisotropic distribution of carriers after intraband excitation. The fluence dependence

of this phenomenon is discussed for fluences up to 10 $\mu J/cm^2$.

[1] H. A. Hafez, S. Kovalev, J.-C. Deinert, Z. Mics, B. Green, N. Awari, M. Chen, S. Germanskiy, U. Lehnert, J. Teichert, Z. Wang, K.-J. Tielrooij, Z. Liu, Z. Chen, A. Narita, K. Müllen, M. Bonn, M. Gensch and D. Turchinovich, Nature textbf561, 507 (2018).

30 min. break

HL 59.6 Thu 11:15 POT 151

Symmetry breaking and circular photogalvanic effect in epitaxial $Cd_xHg_{1-x}Te$ films — Stefan Hubmann[1], Grigory Budkin[2], •Maximilian Otteneder[1], Dmitro But[3], Daniel Sacré[1], Ivan Yahniuk[3], Kilian Diendorfer[1], Vasily Bel'kov[2], Dmitry Kozlov[4], Nikolay Mikhailov[4], Sergey Dvoretsky[4], Vasily Varavin[4], Vladimir Remesnik[4], Sergey Tarasenko[2], Wojciech Knap[3], and Sergey Ganichev[1] — [1]Terahertz Center, University of Regensburg, Regensburg, Germany — [2]Ioffe Institute, St. Petersburg, Russia — [3]International Research Centre CENTERA, Institute of High Pressure Physics, Warsaw, Poland — [4]Rzhanov Institute of Semiconductor Physics, Novosibirsk, Russia

We report on the observation of symmetry breaking and the circular photogalvanic effect (CPGE) in $Cd_xHg_{1-x}Te$ alloys. We demonstrate that irradiation of bulk epitaxial films with circularly polarized terahertz radiation leads to the CPGE yielding a photocurrent whose direction reverses upon switching the photon helicity. This effect is forbidden in bulk zinc-blende crystals by symmetry arguments and, therefore, its observation indicates either symmetry reduction of the bulk material or that photocurrents are excited in topological surface states formed in alloys with low cadmium concentration. Bulk states play a crucial role since the CPGE is also clearly detected in samples with non-inverted band structure and therefore we suggest that strain is a reason of the symmetry reduction. We develop a theory of the CPGE showing that it results from quantum interference of different pathways contributing to the free-carrier absorption of radiation.

HL 59.7 Thu 11:30 POT 151

Nonlinear charge transport in GaAs/InGaAs core/shell nanowires at terahertz frequencies — •Rakesh Rana[1], Leila Balaghi[1,2], Ivan Fotev[1,2], Harald Schneider[1], Manfred Helm[1,2], Emmanouil Dimakis[1], and Alexej Pashkin[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Center for advancing electronics Dresden (cfaed), Technische Universität Dresden, 01062 Dresden, Germany

We report the high-field transport and the plasmonic response of GaAs/InGaAs core/shell nanowires (NWs) by employing optical pump - terahertz probe spectroscopy with peak electric fields up to 2 MV/cm. The plasmon mode experiences a systematic redshift and a suppression of the spectral weight with the increase of the driving THz field. The electron mobility exhibits a threshold-like behavior and starts to decrease for peak electric fields above 0.7MV/cm. This phenomenon is assigned to the increase of the effective mass due to the intervalley scattering in InGaAs. Our analysis shows the absence of the carrier multiplication in NWs even for fields beyond 1 MV/cm, in contrast to bulk InGaAs. Remarkably, the linear dependence between the plasmon spectral weight and the square of its frequency breaks down in the high field regime. Our theoretical modeling demonstrates that this behavior stems from a non-uniform distribution of the local electric field inside the NW leading to intervalley scattering mainly in its middle part. The discovered properties prove the potential of NWs for terahertz band nanoelectronics.

HL 59.8 Thu 11:45 POT 151

μJ -level picosecond far-infrared pulses generated via difference frequency mixing in organic DSTMS crystal — •Jiang Li[1,3], Rakesh Rana[1], Alexej Pashkin[1], Manfred Helm[1,2], and Harald Schneider[1] — [1]Institute of Ion Beam Physics and Material Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Institute of Applied Physics, Technische Universität Dresden, Dresden, Germany — [3]Institute of Fluid Physics, CAEP, Mianyang, Sichuan, China

We report on the generation of narrowband far-infrared pulses with energies up to 3 μJ. The technique relies on difference-frequency generation in the organic nonlinear crystal DSTMS from two linearly chirped near-infrared pulses. The tunability of the difference frequency ranging from 9 to 24 THz is achieved by tuning the frequency of the pump pulses. The measured output power was observed to increase monotonically with frequency. Our simulation based on a 1-D nonlinear wave equation model reproduces this behavior and attributes it mainly to the frequency-dependent far-infrared absorption in DSTMS. As the two near-infrared pulses are derived from the signal outputs of two optical parametric amplifiers pumped by the same Ti: sapphire femtosecond amplifier, the generated THz transient is envelop-phase stable and can be accurately sampled using an electro-optic detection scheme. This THz source provides many attractive possibilities for selective excitation of low-energy transitions or high-harmonic generation in condensed matter.

HL 59.9 Thu 12:00 POT 151

Interband Cascade Photodetectors for Light Detection in the mid Infrared — •Andreas Bader[1], Anne Schade[1], Florian Rothmayr[2], Caroline Kistner[2], Johannes Koeth[2], Fabian Hartmann[1], and Sven Höfling[1] — [1]Technische Physik, Physikalisches Institut, Julius-Maximilians-Universität Würzburg — [2]nanoplus Nanosystems and Technologies GmbH, Gerbrunn

Interband cascade photodetectors (ICD) [1] based on InAs/GaSb type-II superlattice (SL) absorbers present a novel type of photodetectors for applications in the infrared spectral region. By adjusting the period of the SL, the cut-off wavelength can be tailored in a wide range from SWIR (1-3μm) up to VLWIR ($>$ 14μm) [2]. Cascading multiple discrete absorbers in series allows for high absorption while mitigating internal losses in the absorber within the carrier diffusion length. Furthermore, cascading reduces the overall noise leading to a higher detectivity [3]. These properties allow for the use of ICDs in multiple possible applications like gas sensing, thermal imaging and medical diagnostics. We present our work on a five-stage ICD for gas sensing applications in the MIR. A responsivity of 0.24 A/W was achieved in photovoltaic operation at room temperature. The ICD shows a cut-off wavelength of 4.7μm. The absorption of gaseous H_2O and CO_2 was investigated and clear absorption lines were resolved.

[1] Li et al, APL, 86, 10 (2005)
[2] Christol et al, Proc. of SPIE, 10563, 204 (2017)
[3] Hinkey et al, 114, 104506 (2013)

HL 59.10 Thu 12:15 POT 151

MBE-growth of p-doped InAs on undoped GaSb terahertz emitter — •Cyril Sadia-Salang[1], Rommel Jagus[1], Gerald Angelo Catindig[2], Alexander De Los Reyes[2], Armando Somintac[2], Arnel Salvador[2], and Elmer Estacio[2] — [1]Materials Science and Engineering Program, University of the Philippines Diliman, Quezon City 1101, The Philippines — [2]Condensed Matter Physics Laboratory, National Institute of Physics, University of the Philippines Diliman, Quezon City 1101, The Philippines

In this contribution, a terahertz (THz) wave surface emitter consists of a thin epitaxial layer of p-type InAs grown via molecular beam epitaxy on an undoped GaSb substrate. Multilayer buffer structures were grown prior to forming the p-InAs epilayer. These structures include 3 periods of 20-nm undoped GaAs and 260-nm undoped InAs, and 10 periods of InGaAs(3 nm)/GaAs(3 nm) superlattice as a way of minimizing surface roughness. The first 2 min of deposition of each GaAs buffer and InAs buffer proceeded with application of growth interruption. The second sample was capped with an n-doped GaAs to contribute to surface smoothening. The THz emission efficiency of p-InAs epilayers was evaluated using 1.55 μm femtosecond laser excitation in reflection geometry. The THz signal strength of the p-InAs epilayer is comparable to that of an InGaAs-based emitter. Additional improvement should be obtained by using thin InAs layer on GaSb in the transmission geometry.

HL 60: Perovskite and photovoltaics V (joint session HL/CPP)

Time: Thursday 9:30–12:00 Location: POT 251

HL 60.1 Thu 9:30 POT 251

Surface Properties of $FA_xCs_{1-x}Pb(I_yBr_{1-y})_3$ — •Julian Gebhardt[1], Daniel Urban[1], and Christian Elsässer[1,2] — [1]Fraunhofer IWM, Wöhlerstraße 11, D-79108 Freiburg — [2]FMF Universität Freiburg, Stefan-Meier-Straße 21 D-79104 Freiburg

Since the rise of hybrid perovskites as promising material for photovoltaic applications inspired by $MAPbI_3$ ($MA=CH_3NH_3^+$), many research efforts have been directed towards overcoming practical issues of such light absorbing layers. Apart from replacing silicon as absorber in single-junction solar cells, a promising route is to combine perovskites with established materials in multi-junction tandem cells. For these applications, hybrid perovskite design, i.e., mixing inorganic and organic ions in order to balance stability and light absorbing properties, changes in terms of target properties. This search temporarily concluded in materials of the type $FA_xCs_{1-x}Pb(I_yBr_{1-y})_3$ ($FA=HC(NH_2)_2^+$), with $x \approx 0.8$ and $y \approx 0.7$. During the extensive search for perovskite based absorber materials, theoretical understanding has proven vital to navigate the huge combinatorial space. Naturally, such investigations focused on bulk properties. This neglects the important step from lab scale absorber materials design towards working devices that require contacting and possibly passivation.

We present an investigation of surface properties of the $FA_xCs_{1-x}Pb(I_yBr_{1-y})_3$ family by electronic-structure theory to guide future interface optimization for these and other absorber materials. Focusing on non-polar surfaces, we investigate the stability and effects on the electronic-structure.

HL 60.2 Thu 9:45 POT 251

Theoretical analysis of ultrathin Cu(In,Ga)Se2 solar cells with Zn(O,S) buffer layer — •gabin landry mbopda tcheum[1,3], ariel teyou ngoupo[1], narngar guirdjebaye[1], soumaila ouedraogo[2], and jean-marie b. ndjaka[1] — [1]University of Yaounde I, Yaounde, Cameroon — [2]Université Joseph Ki-ZERBO, Ouagadougou, Burkina Faso — [3]Friedrich-Schiller-Universität, Jena, Germany

The optimisation of Cd-free buffer layer, for CIGS based solar cells, appears as an ingenious way to reduce the absorber thickness without compromising the solar cell*s performance. Therefore, we discuss and present simulated electrical properties of CIGS solar cells with Zn(O,S) buffer layers. We present the electrical performance of this type of thin films solar cells with ultra thin absorber and buffer layers. However, as ultra thin absorber leads to increasing recombinations at the back contact, we introduced SnSe and a highly doped CIGS layer (known as p+-CIGS layer) as back surface field between the Mo layer and CIGS absorber. Here, we discussed their impact on the cell*s efficiency and on the band alignment.

HL 60.3 Thu 10:00 POT 251

A comprehensive argument for the defect tolerance of metal-halide perovskite solar absorbers — •Anoop Chandran, Irene Aguilera, Christoph Friedrich, Thomas Kirchartz, Uwe Rau, and Stefan Blügel — PGI-1, IAS-1 and IEK-5, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Charge transport and recombination probabilities are related to the defects in a semiconductor. Reduction of scattering centres is essential to preserve the optoelectronic properties of solar absorbers. The ability of semiconductors to retain its properties in the presence of defects or the elimination of defects by a self-reorganisation mechanism is collectively known as defect tolerance.

Defect states formation is dictated by the bonding behaviour of the band extremes. Compression or dilation of lattice from its equilibrium configuration results in the change of energy levels. Rate of this change can be used to measure the deformation potential and thereby defect tolerance of materials. We develop a turn-key solution for the automated computing of the deformation potential combining the FLEUR codes[1] with the open science platform AiiDA[2] to study metal-halide perovskites using density-functional-theory(DFT).

[1] www.flapw.de

[2] G. Pizzi et al. Comp. Mat. Sci. 111, 218-230 (2016)

We acknowledge the Center of Excellence MaX-Materials Science at the Exascale (EU H2020-INFRAEDI-2018) and the Jülich Supercomputing Center, (project CJPGI10) for support.

HL 60.4 Thu 10:15 POT 251

Differences between vacuum deposition and solution processing of lead halide perovskites — •Martin Kroll, Ran Ji, Zongbao Zhang, Tim Schramm, Changsoon Cho, Frederik Nehm, Yana Vaynzof, and Karl Leo — TU Dresden, IAPP, Nöthnitzer Straße 61, 01187 Dresden

Vacuum deposition is the preparation technique of choice for large scale production of organic thin film solar cells, due to the superior control it offers over film formation and deposition of multilayers. It is also possible to deposit perovskite materials by thermal evaporation, however motivated by its simplicity and low associated costs, most research groups focus on solution processed perovskites. Nevertheless, recent reports show that power conversion efficiencies of vacuum deposited perovskite solar cells surpassed 20%, making them comparable to solution processed devices. The fabrication of perovskite thin films by thermal evaporation in vacuum faces different challenges that solution processing and often results in different film properties. We compare the properties and performance of perovskites fabricated by the two methods and report on the deviations we observe in morphology, stability and photovoltaic device performance. We discuss the influence of processing conditions during vacuum and solution processing on the properties of the perovskites films as well as their effect on the device performance, stability and reproducibility.

30 min. break

HL 60.5 Thu 11:00 POT 251

Tuning the Grain Size and Porosity of MAPbI3 Perovskite films for High Efficiency Solar Cells — •Qingzhi An[1,2], Fabian Paulus[1,2], and Yana Vaynzof[1,2] — [1]Integrated Center for Applied Photophysics and Photonic Materials, TU Dresden, Germany — [2]Center For Advancing Electronics Dresden (cfaed), TU Dresden, Germany

In this work, a facile approach to control perovskite grain size and porosity is introduced. By slightly tuning the amount of H3PO2 (HPA) in the perovskite precursor solution, we demonstrate that the average perovskite grain size can be enlarged by one magnitude regardless of the underlying charge extraction layer. We correlate these microstructural changes to the photovoltaic performance of devices and demonstrate that optimal HPA concentration leads to open circuit voltages of 1.16 V and a power conversion efficiency of 19 %. We also demonstrate that further increase in the HPA amount in perovskite precursor solution results in the formation of a regular, porous perovskite networks with highly degree of crystalline orientation. Such porous structures can be of great interest to application in light-emitting diodes or semi-transparent photovoltaic devices. This work demonstrates that tuning the fraction of HPA in perovskite precursor solution is an effective method to control the perovskite grain size and layer topology.

HL 60.6 Thu 11:15 POT 251

Charge Carrier Transport in Halide Perovskites Investigated by Optical-Pump Terahertz-Probe Spectroscopy — Hannes Hempel[1], •Andrei Petsiuk[1], Martin Stolterfoht[2], Pascal Becker[1], Dieter Neher[2], Rainer Eichberger[1], and Thomas Unold[1] — [1]Helmholtz Zentrum Berlin für Materialien und Energie GmbH — [2]Institute of Physics and Astronomy, Universität Potsdam

Metal-halide hybrid perovskites exhibit excellent optoelectronic properties except for their rather moderate charge carrier mobilities. The origin of these moderate mobilities has been attributed to several (contradicting) effects, such as the formation of large and small polarons, dynamic disorder due to the soft nature of these materials, slow rotational modes of the organic molecules, as well as to the confinement of charge carriers in grains, ferroelectric domains or nanostructures. To clarify the nature of the charge carrier transport, we probed different hybrid and inorganic halide perovskites thin films and nano-crystals by temperature dependent Optical-Pump Terahertz-Probe (OPTP) spectroscopy. We find a strongly increasing mobilities with lower temperature, thus excluding small polaron formation and hopping transport. Instead, this behavior can be modeled by conventional large polaron theory and Fröhlich-type electron-phonon scattering.

HL 60.7 Thu 11:30 POT 251

Singlet Fission Processes in Hybrid Organo-Metal Halide Perovskites Semiconductors — •Karunanantharajah Prashanthan[1,2], Klaus Lips[1], Simone Raoux[1], and Rowan MacQueen[1] — [1]Institute for Nanospectroscopy, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH — [2]Department of Physics, University of Jaffna, Jaffna, Sri Lanka

Solar cells made from Organo-Metal Halide Perovskites show power conversion efficiency very close to the record efficiency of commercially available thin film technologies. Looking to the future of these devices, there exists promising approaches to push the efficiency beyond the Shockley-Queisser single junction thermodynamic limit. Singlet fission is a quantum mechanical process which occurs in various organic molecules, whereby a photogenerated high-energy singlet exciton spontaneously splits into two lower-energy triplet excitons. In this work, we present the possible routes and challenges involved in combining singlet fission materials with low bandgap hybrid metal halide perovskite solar cells. Using time-resolved photoluminescence spectroscopy we investigate the dynamic processes involved in singlet fission and the subsequent injection of energy and charge into the perovskite layer. The objective is to form augmented photovoltaic devices which can efficiently harvest triplets from a singlet fission layer, substantially reducing the energy loss to carrier thermalization.

HL 60.8 Thu 11:45 POT 251

Manganese Doping Induced Quantum Confinement in the Perovskite Nanocrystals via Ruddlesden-Popper Defects — •Kavya Reddy Dudipala, Sharmistha Paul, Tushar Debnath, Jochen Feldmann, and Lakshminarayana Polavarapu — Chair for Photonics and Optoelectronics, Nano-Institute Munich and Department of Physics, Ludwig-Maximilians-Universität (LMU), Königinstr. 10, 80539 Munich, Germany

The concept of doping manganese ions (Mn^{2+}) into II-VI semiconductor nanocrystals (NCs) has recently been extended to perovskite NCs. The transfer of the exciton energy from a semiconductor host to Mn^{2+} dopants leads to orange emission from a spin-forbidden 4T1-6A1 Mn d-d transition. To date, most studies on Mn^{2+} doped NCs focused on enhancing the emission related to the Mn^{2+} dopant via an energy transfer mechanism. Here, we show that the doping of Mn^{2+} ions into $CsPbCl_3$ NCs not only results in a Mn^{2+}-related orange emission, but also strongly influences the excitonic properties of the host NCs. We observe for the first time that Mn^{2+} doping leads to the formation of Ruddlesden-Popper defects and thus induces quantum confinement in host perovskite NCs. We find that a slight doping with Mn^{2+} ions improves the size distribution of the NCs, which results in a prominent excitonic peak. However, with increasing the Mn^{2+} concentration, the number of Ruddlesden-Popper planes increases leading to smaller single crystal domains. The enhanced confinement and crystal inhomogeneity cause a gradual blue shift and broadening of the excitonic transition.

HL 61: Focus Session: Tailored Nonlinear Photonics I

The research field of nonlinear photonics is driven by the tailoring and control of nonlinear light-matter interactions and by the application of nonlinear concepts for advanced light management. Current research activities are driven by concepts from quantum optics, coherent optics, and solid-state physics. The progress in the field strongly benefits from advanced solid-state materials, nanostructures, and photonic structures, as well as from extremely intense and efficient ps and fs laser sources. The application of new concepts paves technically viable routes towards advanced nonlinear photonic devices, which are indispensable for the implementation of efficient frequency conversion, conditional photonic functionalities, and photonic quantum technologies.

Organizers: Artur Zrenner (Universität Paderborn), Thomas Zentgraf (Universität Paderborn) and Manfred Bayer (TU Dortmund)

Time: Thursday 9:30–13:00 Location: POT 51

Invited Talk HL 61.1 Thu 9:30 POT 51

Supercontinuum second-harmonic generation spectroscopy of 2D semiconductors — •Steffen Michaelis de Vasconcellos — Institute of Physics and Center for Nanotechnology, University of Münster, Germany

Two-dimensional semiconductors such as MoS_2 or WS_2 and their heterostructures have recently emerged as promising material systems for novel optoelectronic devices due to their unique electrical, mechanical, and optical properties. Several of these atomically thin materials are particularly suited for nonlinear light-matter interactions. Their strong optical nonlinearity, broadband and tunable optical absorption, and ultrafast response have been successfully employed in all-optical modulators, lasers, wavelength converters, and optical limiters. The prototypical nonlinear process second-harmonic generation is a powerful tool to gain insight into nanoscale materials, because of its dependence on the crystal symmetry and electronic structure. We have developed a new method to perform ultra-broadband SHG spectroscopy, which provides access to the frequency-dependent nonlinear susceptibility $\chi^{(2)}$ of atomically thin materials and allows for the identification of excitonic resonances.

Invited Talk HL 61.2 Thu 10:00 POT 51

Quasi-instantaneous switch-off of deep-strong light-matter coupling — •Christoph Lange[1], Maike Halbhuber[1], Joshua Mornhinweg[1], Viola Zeller[1], Cristiano Ciuti[2], Dominique Bougeard[1], and Rupert Huber[1] — [1]University of Regensburg, Germany — [2]Université de Paris, France

Optical microresonators facilitate custom-tailored quantum states of matter by dressing electronic excitations with virtual cavity photons. Once the rate of energy exchange between light and matter modes exceeds the carrier frequency of light itself, 'deep-strong coupling' emerges, and the vacuum ground state is profoundly modified, giving rise to novel phenomena including cavity-mediated superconductivity and other phase transitions. While the exploration of the equilibrium properties of deep-strong coupling has just started, yet more unusual quantum dynamics are expected on subcycle scales. Here, we explore the intriguing dynamics that arises when deep-strong light-matter coupling is switched off quasi-instantly. The experiments employ custom-tailored THz nanoresonators coupled to cyclotron resonances of two-dimensional electron gases. Femtosecond photoexcitation of an integrated switch element extinguishes the fundamental cavity mode and decouples it from the cyclotron resonance, more than an order of magnitude faster than the oscillation cycle of light. The quasi-instantaneous extinction of the polariton states is hallmarked by sub-polariton-cycle oscillations of the transmission as confirmed by a quantum model.

HL 61.3 Thu 10:30 POT 51

Nonlinear optical susceptibility of potassium titanyl phosphate — •Agnieszka Kozub, Sergej Neufeld, Adriana Bocchini, Uwe Gerstmann, Arno Schindlmayr, and Wolf Gero Schmidt — Department Physik, Universität Paderborn, Paderborn, Germany

$KTiOPO_4$ (KTP) is a very important nonlinear optical material. Due to its high conversion efficiency, non-hygroscopicity, and cost-efficiency it is widely used for second harmonic generation (SHG). However, only very few experimental measurements on its SHG efficiency are available. In particular, its photon energy dependence has not been systematically studied. Previous theoretical works [1-3] focus mainly on the linear optical properties of KTP. Our present work aims at closing this gap.

Based on the Berry-phase formulation of the dynamical polariza-

tion [4] the second-order nonlinear optical susceptibility tensor $\chi^{(2)}$ is calculated and compared with the available experimental data. Particular attention is paid to the influence of non-stoichiometry and point defects on the KTP optical response.

[1] A. H. Reshak, I. V. Kityk, and S. Auluck, J. Phys. Chem. B 114, 16705 (2010).

[2] M. Ghoohestani, A. Arab, S. J. Hashemifar, and H. Sadeghi, J. Appl. Phys 123, 015702 (2018).

[3] S. Neufeld, A. Bocchini, U. Gerstmann, A. Schindlmayr, and W. G. Schmidt, J. Phys. Mater. 2, 045003 (2019).

[4] C. Attaccalite, M. Grüning, Phys. Rev. B 88, 235113(2013).

HL 61.4 Thu 10:45 POT 51

Systematic Investigation of the Nondegenerate Two-Photon Absorption Coefficient in ZnSe — •Laura Krauss-Kodytek, Claudia Ruppert, and Markus Betz — Experimentelle Physik 2, Technische Universität Dortmund, Otto-Hahn-Straße 4a, 44227 Dortmund, Germany

The two-photon absorption (TPA) coefficient β_{TPA} is strongly enhanced in case of extremely nondegenerate photon pairs ($\hbar\omega_1 \neq \hbar\omega_2$) when compared to the degenerate case ($\hbar\omega_1 = \hbar\omega_2$) [1]. However, a systematic study of the TPA strength as a function of the involved photon pair's energy ratio ω_1/ω_2 remains elusive.

To investigate this dependence we use an optical parametrical amplifier which provides photon pairs within energy ratios from unity to 3.5. The photon pair's sum energy of 3.1 eV slightly exceeds the bandgap of ZnSe ($E_{\mathrm{g}} = 2.7$ eV at room temperature). The ZnSe samples have a thickness of 40 μm and a (100)- or (110)-orientation.

The setup is designed in a pump-probe fashion and the peak signals at time overlap reflect the TPA strength β_{TPA}. We observe an enormous increase of the nondegenerate TPA strength compared to the degenerate one. Further, the measured trend of the β_{TPA} as a function of the energy ratio is well in line with the theoretical predictions [2].

[1] D. Fishman et al., Nature Photonics **5**, 561-565 (2011)

[2] W.-R. Hannes and T. Meier, Physical Review B **99**, 125301 (2019)

30 min. break

Invited Talk HL 61.5 Thu 11:30 POT 51

Watching plasmonic skyrmions spin using ultrafast two-photon photoelectron spectroscopy — •Harald Giessen[1], Tim Davis[1,2], Bettina Frank[1], Pascal Dreher[3], David Janoschka[3], and Frank Meyer zu Heringdorf[3] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart — [2]University of Melbourne — [3]CENIDE, University of Duisburg Essen

Plasmonic skyrmions are topological defects in the electromagnetic near-field on thin metal films, recently observed using scanning near-field optical microscopy. However, only one spatial component of the electric field was measured and one of the most intriguing features of skyrmions, namely their dynamics, was not assessed. Here we introduce a new technique, time-resolved vector microscopy, that enables us to compose entire movies on a sub-femtosecond time scale and a 10 nm spatial scale of the electric field vectors of surface plasmon polaritons. Specifically, we image complete time sequences of propagating surface plasmons as well as plasmonic skyrmions on atomically flat single crystalline gold films that have been patterned using gold ion beam lithography. This allows us to unambiguously resolve all vector components of the electric field as well as their time dynamics, enabling the retrieval of the experimental time-dependent skyrmion number, and indicating the periodic transformation from skyrmions to anti-skyrmions and back.

HL 61.6 Thu 12:00 POT 51

Quasiparticle and excitonic effects in the lithium niobate polaron optical absorption — •Falko Schmidt, Wolf Gero Schmidt, Arno Schindlmayr, and Uwe Gerstmann — Department Physik, Universität Paderborn, 33095 Paderborn, Germany

Lithium niobate ($LiNbO_3$), a perovskite-structure ferroelectric, is widely employed in nonlinear optical applications. The material employed in technical applications is usually grown from a congruent melt and therefore characterized by a high concentration of intrinsic defects which influence its optical properties. The latter are usually interpreted within the polaron concept [1]. Polarons tend to localize at crystal defects, especially at positively charged impurities, due to the attractive Coulomb potential and the additional lattice distortion. In the present study we perform many-body perturbation theory calculations in order to determine the influence of electron quasiparticle and electron-hole attraction effects on the polaron optical absorption. By means of comparison between simulated spectra and measured data [1] we are able to propose detailed atomic structures giving rise to both polarons and bipolarons.

[1] OF Schirmer, M Imlau, C Merschjann, B Schoke, J. Phys.: Condens. Matter **21**, 123201 (2009).

HL 61.7 Thu 12:15 POT 51

PSF-analysis of ferroelectric domain-walls in waveguide structures — •Peter Mackwitz, Laura Padberg, Christof Eigner, Christine Silberhorn, Gerhard Berth, and Artur Zrenner — Universität Paderborn, Warburger Straße 100, 33098 Paderborn, Germany

The occurring nonlinear contrast mechanism of periodically poled waveguide structures in $LiNbO_3$ and $KTiOPO_4$ is examined via a combined experimental and numerical approach. The numerical calculation is based on a vectorial model, whereby the experimental access is realized by a direct imaging technique which records the spatial distribution of the second-harmonic signal in the back focal plane. As the model depends on the optical properties of the material, different scenarios of contrast mechanisms can be simulated and compared to the experimental data. It turns out that many features of the nonlinear signatures arise from destructive interference of phase-shifted wavelets at the domain walls as well as the waveguide boundaries. The phase is acquired due to the interaction of the focus with differentially poled domains, whose susceptibility tensor appears rotated by 180°. Another ingredient for the contrast are new tensor elements which do only occur at the domain walls. With this work a comprehensive explanation for the contrast mechanism in the coherent surface near regime is given.

HL 61.8 Thu 12:30 POT 51

All-optical switching of exciton polariton vortices — Xuekai Ma[1], •Bernd Berger[2], Marc Assmann[2], Rodislav Driben[1], Torsten Meier[1], Christian Schneider[3], Sven Höfling[3,4], and Stefan Schumacher[1,5] — [1]Department of Physics and Center for Optoelectronics and Photonics Paderborn (CeOPP), Universität Paderborn, Warburger Strasse 100, 33098 Paderborn, Germany — [2]Experimentelle Physik 2, Technische Universität Dortmund, 44227 Dortmund, Germany — [3]Technische Physik, Universität Würzburg, Am Hubland, 97074, Würzburg, Germany — [4]SUPA, School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, United Kingdom — [5]College of Optical Sciences, University of Arizona, Tucson, AZ 85721, USA

Vortices are elementary excitations in exciton polariton condensates that consist of a $2\pi\cdot$m radial phase shift of the polariton wavefunction, where m is the topological charge of the vortex. This topological charge translates into the orbital angular momentum (OAM) state of the emitted light field, which we detect by application of a dedicated OAM spectroscopy technique. This technique gives us the opportunity to study the temporal dynamics of vortices in exciton polariton condensates without using complex interferometric techniques that also always require a phase reference. Here, we theoretically and experimentally demonstrate the switching of the charge of a localized vortex in a microcavity polariton condensate.

HL 61.9 Thu 12:45 POT 51

Semiclassical theory of multi-photon absorption in bulk zinc-blende type semiconductors — •Wolf-Rüdiger Hannes and Torsten Meier — Department of Physics and CeOPP, University of Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany

Multi-photon absorption coefficients of zinc-blende type semiconductors are studied in the independent-electron approximation. Our theory is based on a gauge-invariant form of the semiconductor Bloch equations including inter- and intraband excitations. Extending our initial analysis [1,2] we use a GaAs bandstructure and complex dipole moments obtained from k·p theory. Considering a pump-probe scheme, the nonlinear-optical response is analyzed for varying excitation parameters, such as pulse frequencies, propagation directions, and polarization angles. Analytical solutions are obtained for near half-gap excitation in the cw-limit using a simplified multiband model valid in the vicinity of the Γ-point. We also investigate multi-photon absorption in a non-perturbative regime, where it shows Rabi-like oscillations as a function of the light intensity.

[1] W.-R. Hannes and T. Meier, Phys. Rev. B **99**, 125301 (2019).

[2] W.-R. Hannes, L. Krauß-Kodytek, C. Ruppert, M. Betz, and T. Meier, Proceedings of the SPIE **10916**, 109160O (2019).

HL 62: Focus Session: Functional Metal Oxides for Novel Applications and Devices II (joint session HL/DS)

Metal oxides exhibit a myriad of fascinating physical properties that enable a large variety of potential applications such as sensors and detectors, solar energy harvesting, transparent and potentially bendable electronics, power electronics, high-electron-mobility transisitors, memristors, topological quantum computation and so on. These functionalities typically require homo- or heteroepitaxial layers of high crystallinity with bendable amorphous semiconducting oxides as an exception. This session sets a focus on growth of bulk and thin films, experimental and theoretical investigation of their physical properties as well as fabrication and characterization of demonstrator devices.

Organizers: Oliver Bierwagen (Paul-Drude-Institut für Festkörperelektronik, Berlin), Holger Eisele (TU Berlin), Jutta Schwarzkopf (Leibniz-Institut für Kristallzüchtung, Berlin) and Holger von Wenckstern (Universität Leipzig).

Time: Thursday 9:30–13:00 Location: POT 81

Invited Talk HL 62.1 Thu 9:30 POT 81

Basics of Gas Sensing with Semiconducting Metal Oxides — •Nicolae Barsan — University of Tuebingen, Tuebingen, Germany

This contribution will present the basic knowledge needed to understand gas sensing with semiconducting metal oxides. It will explain how the interaction with atmospheric gases changes both surface charge and free charge carriers concentration and will descrice that in terms of reception and transduction functions. The body of essential data needed for the understanding of sensing for the case of two representative oxides, namely SnO2 and WO3 will be presented together with the description of the most relevant operando investigation techniques, namely Kelvin probe work function changes measurements and Diffuse Reflectance Infrared Fourier Transform Spectroscopy.The example of CO detection in the presence of humidity will be in the focus. It will be shown how this knowledge can be formalized with the help of the quasi-chemical reactions. Furthermore it will be explained how the charging of the surface changes the properties of the oxide and how this can be quantified with the help of the Poisson and electro-neutrality equations for both n and p-type materials.

HL 62.2 Thu 10:00 POT 81

Optical and photocatalytic properties of gallium-zinc-oxynitrides thin films grown by molecular beam epitaxy — •Elise Sirotti, Max Kraut, Florian Pantle, and Martin Stutzmann — Walter Schottky Institut and Physics Department, Technische Universität München, Am Coulomwall 4, 85748 Garching, Germany

GaN and ZnO are two well-studied materials with favorable energy positions of their band edges with respect to the redox levels of many electro-chemical reactions. However, their large band gap limits the use for simultaneous efficient solar light absorption and photocatalytic activity. By forming an alloy of both materials, the band gap can be reduced by more than 1 eV, while the energetic position of the conduction band stays almost constant. We present the growth of GZNO thin films by means of plasma-assisted MBE on c-plane sapphire. The quality and composition of the quaternary compound have been optimized by varying the temperature, metal fluxes and nitrogen-to-oxygen ratio during deposition. We performed photo-thermal deflection spectroscopy, valence band XPS and EDX measurements to investigate the influence of the composition on the electronic properties. As a result, the influence of the different components on the energetic positions of the conduction band and valence band has been clarified. With electrochemical measurements, we gain insights into the photo-catalytic activity and stability of the thin films. The high flexibility gained by MBE growth allows us to acquire additional knowledge about the fundamental principles of the band gap narrowing process.

HL 62.3 Thu 10:15 POT 81

Surface Stability of β-Ga_2O_3 at Realistic Temperature and Pressure Conditions from First Principles — •Konstantin Lion[1,2], Sergey V. Levchenko[3,2], Matthias Scheffler[2,1], and Claudia Draxl[1,2] — [1]Humboldt-Universität zu Berlin, Berlin, DE — [2]Fritz-Haber-Institut der MPG, Berlin, DE — [3]Skolkovo Institute of Science and Technology, Moscow, RU

The surface properties of a material play a vital role in epitaxial growth and electrical contacts. Depending on the miscut direction on off-oriented (100) β-Ga_2O_3 substrates, homoepitaxially grown layers show distinct surface morphologies, i.e., the formation of $(\bar{2}01)$ facets [1]. In a first-principles approach, it is important to account for the experimental growth conditions, since they can influence surface stability and thus surface faceting. In this work, we study the stability of all symmetrically inequivalent low-index surfaces of β-Ga_2O_3 at realistic conditions using *ab initio* atomistic thermodynamics. In the calculation of the phase diagrams of all surfaces, we include vibrational contributions to the surface free energy. We find that $(\bar{2}01)$ faceting on (100) substrates is thermodynamically favored at $T = 825\,^{\circ}\mathrm{C}$ and an oxygen partial pressure of 1 mbar, the conditions during homoepitaxial growth. This shows that thermal equilibrium has been reached during growth. Also, we find that the (001) surface is stabilized at higher oxygen chemical potentials, which explains its role as a cleavage plane at ambient conditions.

[1] R. Schewski *et al.*, APL Materials **7**, 022515 (2019)

HL 62.4 Thu 10:30 POT 81

Investigations of β-Ga_2O_3(100) cleavage surfaces by scanning tunneling microscopy and spectroscopy — •Celina Seraphin Schulze[1], Jonathan Hofmann[1], Christian Bruckmann[1], Martin Franz[1], Zbigniew Galazka[2], Wjatscheslav Martyanov[1], and Holger Eisele[1] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung (IKZ), Berlin, Germany

We present surface investigations of three differently doped β-Ga_2O_3 crystals by scanning tunneling microscopy and spectroscopy. One sample is unintentionally doped, while both others are doped by Si and Sn. All the bulk β-Ga_2O_3 single crystals were grown from the melt by the Czochralski method [1,2] and cleaved *in situ* under a base pressure below 1×10^{-8} Pa for experimental investigation. On the flat β-Ga_2O_3(100) cleavage surfaces of each sample dark contrasts occur that can be partially assigned to unintentional background doping by Si. By low energy electron diffraction measurements on the β-Ga_2O_3(100) surfaces we observed an unreconstructed surface with a 1×1 diffraction pattern. Scanning tunneling spectra show intrinsic electronic states within the band gap, induced most likely by oxygen vacancies. This project was supported by the Leibniz Association, Leibniz Science Campus GraFOx, project C2-3.

[1] Z. Galazka *et al.*, ECS J. Solid State Sci. Technol. 6, Q3007 (2017)

[2] Z. Galazka *et al.*, J. Crystal Growth 529, 125297 (2020)

HL 62.5 Thu 10:45 POT 81

Growth and characterization of Si delta-doped β-Ga_2O_3 layers by MOVPE — •Saud Bin Anooz, Raimund Grüneberg, Robert Schewski, Martin Albrecht, Andreas Fiedler, Klaus Irmscher, Zbigniew Galazka, Günter Wagner, and Andreas Popp — Leibniz-Institut für Kristallzüchtung (IKZ), Max-Born-Str. 2, 12489 Berlin, Germany

Si delta-doped β-Ga_2O_3 layers have been grown on (100) and (010) β-Ga_2O_3 substrates by MOVPE. AFM images of the grown layer on (010) oriented substrate show 2D island growth, while for layers grown on (100) with 6o miscut angle substrate step flow growth mode has been found resulting in a lower surface roughness for the (100) surface compared to (010). The amount of Si incorporated into the grown layers as well as the shape of the interface were studied by secondary ion mass spectrometry (SIMS). The SIMS depth profile for the Si delta-doped layer grown on a (010) substrate shows a gradual transition

from the high Si doped to the unintentionally doped regime. However, the Si depth profile of the layer grown on (100) 6° off substrate shows sharp interfaces between the high and low doped regions, a clear advantage with regard to later devices. This could be explained by the surface morphology of the grown layers on (010) and (100) substrates.

30 min. break

Invited Talk HL 62.6 Thu 11:30 POT 81

Ultra-thin oxides on InGaN nanowires: Passivation layers for nanostructured photoelectrodes and optical analysis of chemical processes — Paula Neuderth[2], Mariona Coll[3], Jörg Schörmann[2], Christian Reitz[6], Jordi Arbiol[4], Roland Marschall[5], and •Martin Eickhoff[1,2] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]Institute of Experimental Physics I Justus Liebig University Giessen Germany — [3]Institut de Ciencia de Materials de Barcelona ICMAB-CSIC, Spain — [4]ICREA Pg. Lluís Companys 23 08010 Barcelona, Spain — [5]Physical Chemistry III, University of Bayreuth, Germany — [6]Institute of Nanotechnology (INT), Karlsruhe Institute of Technology, Germany

We demonstrate an experimental strategy for systematically assessing the influence of surface passivation layers on the photocatalytic properties of InGaN nanowire (NW) photoanodes by combining photocurrent analysis, photoluminescence spectroscopy and high resolution transmission electron microscopy. We apply this approach to separate the influence of different mechanisms recombination and transport processes of photogenerated carriers and to compare the effect of TiO2, CeO2 and Al2O3 coatings deposited by atomic layer deposition. Due to efficient charge transfer from the InGaN NW core a stable TiO2-covered photoanode with visible light excitation is realized. As a second application we demonstrate that due to the sensitivity of the InGaN NW photoluminescence to surface adsorbed oxygen the optical analysis of oxygen diffusion in ultrathin ceria coatings deposited by atomic layer deposition is possible.

HL 62.7 Thu 12:00 POT 81

Growth Window, Solubility Limit and Material Properties of κ-$(Al_xGa_{1-x})_2O_3$ PLD thin films — •A. Hassa[1], C. Wouters[2], M. Kneiss[1], P. Storm[1], H. von Wenckstern[1], D. Splith[1], C. Sturm[1], M. Albrecht[2], and M. Grundmann[1] — [1]Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Linnéstraße 5, 04103 Leipzig, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, D-12489 Berlin, Germany

The orthorhombic polymorph of Ga_2O_3, namely κ, is of increasing interest because of its predicted large polarization of $23\,\mu C/cm^2$ [1] rendering it well suited for possible usage e.g. in HEMT's. The high bandgap of about 5 eV [2] can be enlarged by alloying with Al_2O_3 enabling such heterostructure-based devices. We present κ-$(Al_xGa_{1-x})_2O_3$ thin films grown on (00.1)Al_2O_3 by tin-assisted pulsed laser deposition (PLD) [2]. For some thin films a homogeneous target with a defined composition and for an 2 inch in diameter thin film a two-fold PLD target consisting of Ga_2O_3/Al_2O_3 semicircular segments were utilized to grow a sample with laterally continuous composition spread [3]. Al content, growth rates and the occurrence of single phase κ-$(Al_xGa_{1-x})_2O_3$ depends systematically on growth conditions. Further, we present the dependence of structural and optical properties on alloy composition. The maximum observed Al incorporation in the κ-phase was $x = 0.46$ with a bandgap of 5.85 eV.

[1] M. B. Maccioni *et al.*, Appl. Phys. Express 9, 04102 (2016).
[2] M. Kneiß *et al.*, APL Materials 7, 022516 (2019).
[3] H. von Wenckstern *et al.*, CrystEngComm 15, 10020 (2013).

HL 62.8 Thu 12:15 POT 81

Epitaxy of κ-$(Al,Ga)_2O_3$ heterostructures and superlattices by VCCS-PLD — •Philipp Storm[1], Max Kneiss[1], Thorsten Schultz[2], Daniel Splith[1], Holger von Wenckstern[1], Norbert Koch[2], Michael Lorenz[1], and Marius Grundmann[1] — [1]Universität Leipzig, Felix-Bloch Institut für Festkörperphysik — [2]Humboldt Universität zu Berlin, Institut für Physik

Ga_2O_3 is a wide band gap semiconductor with pronounced polymorphism. The thermodynamically stable and therefore most often investigated polymorph is the monoclinic β-phase. However, the metastable, orthorhombic κ-phase gained significant interest due to its high predicted spontaneous polarization of $23\,\mu C/cm^2$ [1]. Exploiting the polarization differences at κ-$Ga_2O_3/CaCO_3$ [2] or κ-Ga_2O_3/κ-$(Al,Ga)_2O_3$ heterointerfaces could allow for the formation of 2DEGs with high carrier densities, crucial for QWIP or HEMT devices. Nevertheless, only little is known about κ-$(Al,Ga)_2O_3$ heterostructures [3]. In this work, VCCS-PLD (vertical continuous composition spread pulsed laser deposition) [4] was utilized for the growth of κ-$(Al,Ga)_2O_3$ heterostructures and superlattices that were investigated regarding structural, morphological and optical properties to evaluate their potential for device applications.

[1] M. B. Maccioni *et al.* : Appl. Phys. Express 9, 041102 (2016)
[2] S. B. Cho *et al.* : Appl. Phys. Lett. 112, 162101 (2016)
[3] P. Storm *et al.* : APL Mater. 7, 111110 (2019)
[3] M. Kneiß *et al.* : ACS Comb. Sci. 20, 643 (2018)

HL 62.9 Thu 12:30 POT 81

Tin-assisted growth of κ-$(Al_xGa_{1-x})_2O_3/(In_xGa_{1-x})_2O_3$ superlattice heterostructures by pulsed laser deposition — •Max Kneiss, Philipp Storm, Anna Hassa, Daniel Splith, Chris Sturm, Holger von Wenckstern, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik

The orthorhombic κ-phase of Ga_2O_3 possesses a similarly high bandgap of 5 eV as the thermodynamically stable β-phase, but further is expected to exhibit a high spontaneous electrical polarization of $23\,\mu C/cm^2$ [1]. Polarization differences at interfaces of κ-phase heterostructures can be utilized for polarization doping to localize a 2DEG that typically features large carrier densities as well as high mobility. We present the coherent growth of κ-$(Al_xGa_{1-x})_2O_3/(In_xGa_{1-x})_2O_3$ quantum-well (QW) superlattices on c-sapphire substrates by pulsed laser deposition. Tin containing targets were necessary for the stabilization of the orthorhombic phase [2]. We found narrow superlattice oscillations up to the ninth order and up to $x \approx 0.5$ in XRD 2θ-ω scans as well as in reciprocal space maps for up to 15 layer pair superlattices confirming excellent crystal quality and abrupt interfaces. The evolution of superlattice oscillations as well as the optical properties will be evaluated in dependence on the QW and barrier width as well as on the composition of the QW and barrier layers. AFM measurements confirm smooth surface morphology for all samples. [1] Maccioni *et al.*, Appl. Phys. Expr. **9**, 041102 (2016) [2] Kneiß *et al.*, APL Materials **7**, 022516 (2019)

HL 62.10 Thu 12:45 POT 81

Band offsets at κ-$([Al,In]_xGa_{1-x})_2O_3/MgO$ interfaces — •Thorsten Schultz[1,2], Max Kneiss[3], Philipp Storm[3], Daniel Splith[3], Holger von Wenckstern[3], Marius Grundmann[3], and Norbert Koch[1,2] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Berlin, Germany — [2]Helmholtz-Zentrum für Energie und Materialien GmbH, Berlin, Germany — [3]Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Leipzig, Germany

Conduction and valence band offsets are amongst the most crucial material parameters for semiconductor heterostructure device design. Due to its expected high spontaneous electrical polarization and the possibility of polarization doping at heterointerfaces, the metastable orthorhombic κ-phase of Ga_2O_3 and its indium and aluminum alloy systems are an interesting material class. We report on valence and conduction band offsets of κ-$(Al_xGa_{1-x})_2O_3$ and κ-$(In_xGa_{1-x})_2O_3$ thin films to MgO as reference dielectric by X-ray photoelectron spectroscopy. The determined band alignments reveal the formation of a type I heterojunction to MgO for all compositions with conduction band offsets of at least 1.4 eV, providing excellent electron confinement. We further found that the conduction band offsets in the alloy system are mainly determined by the evolution of the bandgaps. Therefore, tunable conduction band offsets of up to 1.1 eV within the alloy system allow for subniveau transition energies in corresponding quantum wells from the IR to the visible regime, which are promising for application in, e.g., quantum-well infrared photodetectors.

HL 63: Focus: High-resolution Lithography and 3D Patterning (Part II) (joint session KFM/HL/CPP)

Chair: Robert Kirchner (TU Dresden)

Time: Thursday 9:30–12:20 Location: TOE 317

HL 63.1 Thu 9:30 TOE 317

Curvilinear Magnetism: Fabrication and characterization — •Denys Makarov — Helmholtz-Zentrum Dresden-Rossendorf e.V., Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany

Extending 2D structures into 3D space has become a general trend in multiple disciplines including electronics, photonics, and magnetics. This approach provides means to enrich conventional or to launch novel functionalities by tailoring curvature and 3D shape. We realize 3D curved magnetic thin films where new fundamental effects emerge from the interplay of the geometry of an object and topology of a magnetic sub-system [1]. The application potential of 3D magnetic architectures is explored for the realization of mechanically shapeable magnetoelectronics [2] for virtual and augmented reality appliances [3,4]. To advance in this research field, we develop novel theoretical methods [5-7], fabrication [1,8,9] and characterization techniques [8-11]. These topics will be addressed in the presentation.

[1] R. Streubel et al., J. Phys. D: Appl. Phys. 49, 363001 (2016). [2] D. Makarov et al., Appl. Phys. Rev. 3, 011101 (2016). [3] S. Cañón et al., Nature Electronics 1, 589 (2018) & Science Adv. 4, eaao2623 (2018). [4] J. Ge et al., Nature Comm. 10, 4405 (2019). [5] O. Volkov et al., PRL 123, 077201 (2019). [6] O. Volkov et al., Sci. Rep. 8, 866 (2018). [7] V. P. Kravchuk et al., PRL 120, 067201 (2018). [8] K. S. Das et al., Nano Let. 19, 6839 (2019). [9] M. Nord et al., Small 1904738 (2019). [10] R. Streubel et al., Nature Comm. 6, 7612 (2015). [11] T. Kosub et al., Nature Comm. 8, 13985 (2017).

HL 63.2 Thu 9:50 TOE 317

3D printing of complex submillimeter-sized wide angle objectives — •Zhen Wang[1], Ksenia Weber[1], Simon Thiele[2], Alois Herkommer[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Institute of Technical Optics and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 9, 70569 Stuttgart, Germany

Compact image sensors with a variety of focal lengths, fields of view, and other optical parameters, will be the enabling technology of integrated devices for industry 4.0. In order to miniaturize the imaging devices from currently several mm^3 to below 1 mm^3, and to achieve diameters of the optics below 1 mm, 3D printing with femtosecond laser pulses is the method of choice. Here, we present several multilens designs as well as printed objectives with fields of view that range from 60° to 95°, and focal lengths in the range of 200-300 μm, with diameters around 800 μm, which allow for wide-angle imaging. We characterize their performances and report how to overcome some issues when printing such challenging designs. In the future, those objectives can be directly printed onto CMOS imaging chips which will enable very compact image sensors.

HL 63.3 Thu 10:10 TOE 317

Additive technology for X-ray optical applications — •Adam Kubec, Frieder Koch, and Christian David — Paul Scherrer Institut

X-ray optics are used in many setups connected to materials analysis. Due to very different properties of X-rays as compared to visible light different challenges, have to be tackled in order to manufacture optics. The refractive index has only a small difference to unity. This results in a relatively small optical power. This makes it challenging to manufacture refractive lenses. A successful concentration of X-ray using refractive lenses could only been shown in 1996 using a set of individual refractive lenses.

Today refractive lenses for X-rays are commercially available and are widely used in many synchrotron radiation sources. However, it is still challenging to manufacture aberration free lenses for X-rays. Therefore, custom-made radially symmetric corrector phase plates are used to reduce the aberrations. Spiral phase plates can generate X-ray beams carrying orbital angular momentum of various topological charges.

Additive technology can now also used in order to manufacture refractive lenses directly. Due to the versatility of 3D printed geometries, it is possible to manufacture lenses adapted specifically to improve measuring techniques, such as Ptychography.

We will also see further applications of 3D printing for X-ray applications such as 3D resolution pattern (Siemens Star). These can be can be used to quantify the quality of X-ray tomography setups.

HL 63.4 Thu 10:30 TOE 317

Mass-producible microoptical elements by injection compression molding and focused ion beam structured titanium molding tools — •Simon Ristok[1], Marcel Röder[2], Simon Thiele[3], Mario Hentschel[1], Thomas Günther[2], André Zimmermann[2], Alois Herkommer[3], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [2]Hahn-Schickard, Stuttgart, Germany — [3]Institute of Applied Optics and Research Center SCoPE, University of Stuttgart, Germany

Injection molded polymer is the material of choice for micro-optics used in mass producible devices such as smartphones or optical sensors. For feature sizes on the micrometer scale the molding tools are usually fabricated by nickel electroplating on a silicon master, which was previously structured by electron beam lithography and subsequent etching. In total, two inversion steps are necessary to transfer the structure from the silicon master to a plastic polymer part. Here, we introduce an alternative method that requires only a single inversion step. An extremely robust titanium molding tool is directly structured with high precision by focused ion beam milling. We demonstrate the fabrication of Fresnel lenses with 100 μm diameter and a maximum structure height of 1 μm. The inverse Fresnel lens structured into the titanium is transferred to polymer by injection compression molding, enabling rapid mass replication. We show that the optical performance of the molded Fresnel lenses is in good agreement with simulations, rendering our approach suitable for applications which require compact and high quality optical elements in large numbers.

20 min. break

Invited Talk HL 63.5 Thu 11:10 TOE 317

3D Printing with Electrons - Advances and Opportunities — •Harald Plank — Institute of Electron Microscopy, Graz University of Technology, Graz, Austria

Since the advent of additive manufacturing, this technology class made tremendous progress. While achievable feature sizes continuously decreased from cm's over mm's towards the sub-micron range their 3D possibilities became increasingly powerful. Naturally, there is a strong interest to push 3D printing into the nano-scale, to take advantage of nanoscale effects. Within the small pool of relevant technologies at that scale, Focused Electron Beam Induced Deposition (FEBID) is a highly promising candidate, as it allows additive, direct-write manufacturing of even complex 3D architectures with feature sizes down to 20 nm on most materials and practically any given surface morphology. Together with an increasing availability of precursors with different functionalities, 3D-FEBID has advanced from a trial-and-error laboratory method to a predictable 3D nano-printing technology. In this talk, the audience is first introduced to the basic principles of 3D-FEBID, complemented by recent advances, which strongly increased precision, predictability and reliability. We then present software solutions for the comfortable upfront design of 3D objects and review several application examples, which strongly benefit from the here presented 3D nanofabrication appraoch. To highlight the industrial relevance of 3D-FEBID, we present concepts of advanced nano-probes for application in scanning probe microscopy. We close the talk with a view on current activities, remaining challenges and future opportunities.

HL 63.6 Thu 11:40 TOE 317

Perfluorinated amidinate compounds for focused electron beam induced deposition (FEBID) — •Katarzyna Madajska and Iwona Szymańska — Faculty of Chemistry, Nicolaus Copernicus University in Toruń, Gagarina 7, 87-100 Toruń, Poland

FEBID is a direct maskless nanolithography technique, based on the lo-

cal dissociation of adsorbates upon the irradiation with electrons.[1][2] Silver pentafluoropropionate was applied in the FEBID process yielding 2D and 3D deposits containing up to 70 at. % Ag. [3][4]

Here we report on our study of silver and copper complexes with perfluorinated amidines (CnF2n+1C(=NH)NH2), which are similar in structure to carboxylates but they differ in donor atoms (N,N-donor).

Thermal analysis, EI MS spectrometry, sublimation experiments and temperature variable infrared spectra analysis were carried out to determine the volatility of compounds and their thermal decomposition mechanism. The compounds selected, as based on the results of the volatility, were examined for their sensitivity to the electron beam, using an electron microscope (SEM, TEM).

[1] Utke and A. Gölzhäuser, Angewandte Chemie Int. Ed. 49 (2010) 9328-9330. [2] D. Belić, M. M. Shawrav, E. Bertagnolli, H. D. Wanzenboeck, Beilnstein J. Nanotechnol, 2017, 8, 2530-2543. [3] L. Berger, K. Madajska, I. B. Szymanska, K. Höflich, M. N. Polyakov, J. Jurczyk, C. Guerra-Nuñez, I. Utke, Beilstein J. Nanotechnol., 2018, 9, 224-232. [4] K. Höflich, J. M. Jurczyk, K. Madajska, M. Götz, L. Berger, C. Guerra-Nuñez, C. Haverkamp, I. Szymanska, I Utke, Beilstein J. Nanotechnol., 2018, 9, 842-849.

HL 63.7 Thu 12:00 TOE 317

Synthetic strategies towards FEBID precursors — •Iwona Szymańska and Katarzyna Madajska — Faculty of Chemistry, Nicolaus Copernicus University in Toruń, Gagarina 7, 87-100 Toruń, Poland

The choice of the precursor is crucial for the success of focus electron beam induced deposition (FEBID) because its physicochemical features determine the composition of the deposit.[1] The applied compounds should effectively generate volatile metal carriers, which can be transport over a surface substrate. In the next stage adsorbed molecules should clearly decompose upon electron beam irradiation forming nanostructures. Additionally, the FEBID precursors should be air stable, easy handling, low cost, and safe. Research was focused on the coordination compounds of copper(II) and copper(I), silver(I) and rhenium(III) with N- and O-donor ligands, which seems to be promising for a FEBID process. The influence of structural features such as: 1) the kind of the central atom and its oxidation state; 2) the coordination sphere composition, 3) the modifications of the ligand substituents by fluorination or branching, were observed. [2,3]

Acknowledgements: Nicolaus Copernicus University in Toruń (Statute Research no.103) for the financial support.

References [1] I. Utke et al., J. Vac. Sci. Technol. B, 2008, 26, 1197. [2] L. Berger et al., Beilstein J. Nanotechnol., 2018, 9, 842. [3] K. Höflich et al., Beilstein J. Nanotechnol., 2018, 9, 842.

HL 64: Poster II

This poster session includes contributions from the following topics: - Quantum dots and wires - Semiconductor lasers - Spin phenomena in semiconductors. - Focus Session: Integrated Quantum Photonics

Please put up your poster at the beginning of the sessions and remove the poster immediately after the session. The person peresenting the poster should attend it for at least half of the session duration (90 minutes) and indicate the time when to find him/her at the poster.

Time: Thursday 10:00–13:00 Location: P1A

HL 64.1 Thu 10:00 P1A

Unidirectional optical frequency comb injection of multi-section quantum well lasers — •Jan Lautenschläger[1], Christoph Weber[1], Dominik Auth[1], Andreas Klehr[2], Andrea Knigge[2], and Stefan Breuer[1] — [1]Institute of Applied Physics, Technische Universität Darmstadt, 64289 Darmstadt, Germany — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Gustav-Kirchhoff-Straße 4, 12489 Berlin, Germany

Unidirectional optical injection is a versatile concept to transfer optical properties from a master optical frequency comb laser into a slave optical frequency comb laser. Thereby the optical frequency comb stability of the slave device could be improved and the optical comb broadened. By studying optical injection of two similiar multi-section monolithic quantum-well lasers emitting at 1070 nm with different biasing schemes, an optical frequency comb generated by passive mode-locking is injected into a single-mode laser and the optical and radio-frequency properties of the light emitted by the slave laser are studied. We identify an optical frequency comb generation in the slave device and analyze regimes of injection locking.

HL 64.2 Thu 10:00 P1A

Continuous-wave room-temperature tunable THz-generating laser — •Ksenia Fedorova, Heyang Guoyu, Matthias Wichmann, Christian Kriso, Fan Zhang, Wolfgang Stolz, and Arash Rahimi-Iman — Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany

High-performance, room-temperature, continuous-wave (CW), tunable terahertz (THz) lasers are desirable sources for THz applications ranging from THz spectroscopy and imaging to safety and security applications. So far, THz-generation at room temperature has been mostly targeted by direct quantum cascade lasers. An alternative to that has been provided by THz-generating semiconductor disk lasers (SDLs) based on intracavity frequency conversion in periodically-poled nonlinear crystals. They can allow the demonstration of efficient THz emission in the 0.8-to-2-THz spectral window based on difference-frequency generation. Several studies have so far demonstrated non-tunable THz output from such SDL-based devices with remarkable beam quality. Here, a room-temperature, CW, tunable THz-generating SDL is demonstrated. We employ a dual-wavelength SDL with an intracavity aperiodically-poled lithium niobate crystal for difference-frequency generation in the 0.8-to-1.1 THz spectral window.

HL 64.3 Thu 10:00 P1A

Dispersion effects in passivley mode-locked lasers — •Jan Hausen[1], Christian Schelte[2,3], Julien Javaloyes[2], Svetlana V. Gurevich[2,3], and Kathy Lüdge[1] — [1]TU Berlin, Hardenbergstrasse 36, 10623 Berlin — [2]Universitat de les Illes Balears, Cra. de Valldemossa, km 7.5. Palma (Illes Balears) — [3]WWU Münster, Wilhelm-Klemm-Strasse 9, 48149 Münster

Haus master equation approaches have been utilized to unravel the dynamics of many different types of mode-locked lasers. Their key advantages are an intuitive understanding of the interplay of different effects such as gain and absorption as well as the fact that chromatic dispersion can be included much more easily than in the delay differential equations framework. However, to justify the validity of such Master equations for passively mode-locked lasers with an external cavity geometry that is neither in the long nor in the short cavity limit, a special set of dynamical boundary conditions is developed. The resulting system of coupled partial and ordinary differential equations allows for a uniform approach for studying instabilities either induced by dispersive effects or gain saturation in mode-locked laser irrespective of the cavity lengths.

HL 64.4 Thu 10:00 P1A

Voltage source control for passively mode-locked semiconductor lasers — •Pascal Sauer, Dominik Auth, Christoph Weber, and Stefan Breuer — Institute of Applied Physics, Technische Universität Darmstadt, 64289 Darmstadt, Germany

Monolithic passively mode-locked semiconductor lasers are compact versatile light sources emitting ultrashort optical pulses at high repetition rate. For pulse generation a forward biased gain section and a reverse biased saturable absorber section are implemented in one device. The negative voltage applied to the absorber does not need to be modulated, but is injected using a standard low-noise voltage source. In this contribution, we present a micro-controller based robot which can be interfaced by standard laboratory control software for automatic high-resolution mode-locking performance mapping using non-remote voltage sources.

HL 64.5 Thu 10:00 P1A

Nanowire lasers modified by electron irradiation — Gesine Theess, •Francesco Vitale, Maximilian Zapf, and Carsten Ronning — Institute of Solid State Physics, Friedrich Schiller Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Understanding the linear and nonlinear optical properties of semiconductor nanowires (NWs) is crucial for their envisaged integration into next-generation optoelectronic devices. In this work, the emission of optically pumped VLS-grown ZnO NW lasers was examined in situ in a cathodoluminescence apparatus as a function of the electron beam irradiation. A contrasting behavior between measurements in the spontaneous and stimulated emission regime was found: the spontaneous emission shows a distinct maximum after several minutes of irradiation, followed by a substantial decrease before saturation, while the stimulated emission decreases monotonically. In particular, the influence of defects was studied in relation to the modification of the optical and electronic properties induced by the electron beam.

HL 64.6 Thu 10:00 P1A

Electron pair charging in gate-defined quantum dots in indium antimonide nanowires — Felix Jekat[1], Benjamin Pestka[1], Sasa Gazibegovic[2,3], Diana Car[2,3], Sebastian Heedt[3], •Marcus Liebmann[1], Thomas Schäpers[4], Erik Bakkers[2,3], and Markus Morgenstern[1] — [1]II. Phys. Inst. B, RWTH Aachen Univ., Germany — [2]Dept. of Appl. Phys., Eindhoven Univ., The Netherlands — [3]Qutech and Kavli Inst. of Nanoscience, Delft, The Netherlands — [4]PGI-9, FZ Jülich, Germany

We investigate InSb nanowires placed on bottom gates with mechanically exfoliated hexagonal boron nitride (h-BN) as a dielectric. The sample consists of five 50 nm wide finger gates with a spacing of 30 nm. The h-BN is placed on top of the finger gates. The nanowires are then placed mechanically onto h-BN. We present transport measurements on gate-defined quantum dots at temperatures down to 300 mK. Due to the dielectric, the time stability of our device improved to around 5 μeV/h. The charge stability diagram shows Coulomb diamonds with a charging energy of 2.3 meV and an orbital energy of 0.3 meV. In a perpendicular magnetic field, the zero bias state splits at around 380 mT with a doubling of the gate-periodicity below and above the transition field. This splitting resembles the one reported on nanowires partially covered by superconductors. But since in our sample there is no superconductor involved, the doubling is of unknown origin. However, the change in periodicity implies a change of the pairing mechanism, possibly triggered by electron-electron interaction.

HL 64.7 Thu 10:00 P1A

Extended quasiparticle picture for quantum wires in the high-density limit — •Klaus Morawetz[1,2], Vinod Ashokan[3], Renu Bala[4], and Kare Narain Pathak[5] — [1]Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [2]International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil — [3]Department of Physics, Dr. B.R. Ambedkar NationalInstitute of Technology, Jalandhar (Punjab) - 144 011, India — [4]Centre for Advanced Study in Physics, Panjab University, 160014 Chandigarh, India — [5]Department of Physics, MCM DAV College for Women, 160036 Chandigarh, India

The high-density limit of quantum wires are considered and an extended quasiparticle picture is developed. This allows to calculate the reduced density, the pair correlation function and the effective mass. A non-universal behaviour of the Tan constant is reported for the Coulomb limit. The structure factor is obtained analytically which provides the exact correlation energy. [Eur. Phys. J. B 91 (2018) 29, Phys. Rev. B 97 (2018) 155147, arXiv:1909.09331]

HL 64.8 Thu 10:00 P1A

Characterization of the charge carrier transport in single GaN nanowire field-effect transistors — •Hannes Hergert[1,2], Patrick Uredat[1,2], Matthias T. Elm[1,2,3], and Peter J. Klar[1,2] — [1]Center for Materials Research, Justus Liebig University, 35392 Giessen, Germany — [2]Institute of Experimental Physics I, Justus Liebig University, 35392 Giessen, Germany — [3]Institute of Physical Chemistry, Justus Liebig University, 35392 Giessen, Germany

In the field of semiconductor technology the classical transistors are close to the limit of miniaturisation set by the laws of thermodynamics. For further optimisation new methods are necessary. Due to their high electron mobility and direct bandgap gallium nitride nanowires are a promising material system for future nanoelectronic applications, such as nanowire field-effect transistors (NWFETs). For the device realisation the electrical transport characteristics of such NWFETs need to be investigated. We prepared field-effect transistors of single nanowires by a combination of photo- and electron-beam lithography and characterized the transport properties of single GaN-nanowires. Their electrical resistance increases linearly with decreasing temperature, which is attributed to the high doping concentration and an associated activation energy. We determined the carrier concentration and the electron mobility from cryogenic temperatures to room temperature.

HL 64.9 Thu 10:00 P1A

Resolving the 1D subband structure of wurtzite GaAs wires by inelastic light scattering and PLE — •Sebastian Meier, Paulo de Faria Junior, Ferdinand Haas, Florian Dirnberger, Viola Zeller, Jaroslav Fabian, Dominique Bougeard, and Christian Schüller — Universität Regensburg, 93040 Regensburg, Germany

Resonant Raman scattering and photoluminescence excitation (PLE) measurements have been performed to measure the subband energies of wurtzite GaAs nanowires. Our wires were grown by MBE using the VLS method and have a GaAs core of down to 25 nm thickness which is protected by an AlGaAs shell. For laser excitation, we use a Ti:Sapphire laser, which can be tuned continuously in the energy region of the band gap.

In our Raman experiment, we find a number of peaks which are resonantly enhanced at different excitation energies. According to selection rules and resonance behaviour we interpret the peaks to stem from intersubband excitations of photoexcited electrons. Furthermore, we are able to identify the first excited absorption peak by PLE. Finally, we provide a theoretical account of the measured peaks considering realistic k·p calculations for the nanowire band structure.

HL 64.10 Thu 10:00 P1A

Fabrication and electrical characterization of top-gated RFETs — •Sayantan Ghosh, Muhammad Bilal Khan, Artur Erbe, and Yordan M. Georgiev — Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Following Moore's Law, the idea of "Beyond CMOS" came into picture, which incorporated emerging research and technology. One such idea is the reconfigurable field effect transistor (RFET). An RFET can be dynamically programmed to p or n polarity by the application of electrostatic potential. This is a silicon nanowire (SiNW) based transistor with two gates - one is used to tune the device polarity while the other modulates the flow of charges. In this work, SiNWs were fabricated using electron beam lithography and inductively coupled plasma etching. Subsequently, optimization of oxide shell/gate dielectric around the nanowires was carried out for better control over the conduction of charge carriers. Afterwards, nickel was deposited at both ends of the nanowire and flash lamp annealing was performed to create $NiSi_2$-Si-$NiSi_2$ Schottky junctions. In the next step, two top gates will be fabricated on the junctions followed by electrical characterization of device parameters. Such novel devices have the prospect of establishing efficient circuits and systems.

HL 64.11 Thu 10:00 P1A

Photoluminescence (PL) spectroscopy of a droplet self-assembled quantum dot (SAQD) coupled to a quantum well — •Christine Barthelmes[1], David Ficker[1], Zheng Zeng[1], Hendrik Bluhm[2], and Kardynal Beata[1] — [1]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, Germany — [2]JARA-Institute for Quantum Information, RWTH Aachen University, Germany

Realisation of the full potential of quantum networks depends on the ability to send photon qubits between quantum processors separated by long distances. One of the challenges of such a network is interfacing scalable qubits with photonic qubits. A viable protocol to transfer a quantum state between a photonic qubit and electrically controlled spin qubit in a GaAs/AlGaAs heterostructure has been recently proposed. In the protocol a GaAs/AlGaAs gate-defined double quantum (GDQD) hosts the spin qubit and it is tunnel coupled to a SAQD, which serves as a photon qubit receiver. Here, we present the results of optimization of the electron transfer process between the SAQD grown using droplet epitaxy and the quantum well (QW) in which the GDQD is to be defined. We tune the relative energies of electronic states in the In(Ga)As QD and the QW to achieve electron tunneling between them. Based on the time-energy uncertainty principle, we measure the competing processes of radiative recombination and carrier tunneling escape from the homogenous linewidth in PL of selected

SAQDs. Furthermore, we explore this effect for different spacer distances between the SAQDs and the QWs to tune the tunnel coupling, which is necessary to achieve high fidelity coherent spin transfer in the hybrid device under development.

HL 64.12 Thu 10:00 P1A

Simulation of Mode Competition Phenomena in Nitride Laser Diodes — •Eduard Kuhn, Lukas Uhlig, Matthias Wachs, Ulrich T. Schwarz, and Angela Thränhardt — Institut für Physik, Technische Universität Chemnitz

Due to their small separation of longitudinal modes, Fabry-Pérot type laser diodes show rich mode competition effects. For example streak camera measurements show cyclic mode hopping, where the currently active longitudinal mode changes from lower to higher wavelengths. This effect can be explained by beating vibrations of the carrier densities in the quantum wells. In this work we simulate the mode dynamics using a model based on the semiconductor Bloch equations and compare the results with streak camera measurements. We also discuss the influence of the cavity length on the mode dynamics and how different scattering terms affect the interaction between longitudinal modes.

HL 64.13 Thu 10:00 P1A

Passively mode-locked p-doped quantum dot lasers for stable optical pulse trains — •Dominik Auth[1], Vladimir V. Korenev[2,3], Artem V. Savelyev[2], Mikhail V. Maximov[2,3], Alexey E. Zhukov[2,3], and Stefan Breuer[1] — [1]Institute of Applied Physics, Technische Universität Darmstadt, 64289 Darmstadt, Germany — [2]St. Petersburg Academic University RAS, ul. Khlopina 8/3, 194021 St. Petersburg, Russia — [3]Peter the Great St. Petersburg Polytechnic University, St. Petersburg 195251, Russia

Monolithic mode-locked edge-emitting semiconductor quantum dot lasers emitting at 1.25 micrometer are ideal sources for the generation of short optical pulses for short-reach inter and intra data-center links. In this contribution, the emission dynamics of InAs/InGaAs quantum dot lasers with different gain-to-absorber section lengths and different p-doping concentrations in the GaAs barrier sections are investigated. The focus is on spectral, radio-frequency and time-domain analysis highlighting the influence of the absorber section length and the doping concentration on the pulse train stability and obtained mode-locking area in dependence on the gain injection current and absorber reverse bias voltage for these devices. This work is supported by the Russian Foundation for Basic Research (project #18-502-12081).

HL 64.14 Thu 10:00 P1A

Electric field dependence of the biexciton decay in a single quantum dot — •Björn Jonas, Sebastian Krehs, Alex Widhalm, Kai Spychala, Timo Langer, Dirk Reuter, and Artur Zrenner — Physics Department, Paderborn University, Warburger Straße 100, 33098 Paderborn, Germany

The decay of biexcitons in single quantum dots is commonly used to generate polarization entangled photon paires. In order to gain control over the emission energy, the QDs are often embedded in diode structures. This allows for tuning via the quantum confined stark effect. Aside from the beneficial effect of energy tuning, the applied electric fields can also induce single particle tunneling and hence charging of the QD. Both effects can decrease the efficiency of quantum light sources. In this work we studied the decay of biexcitons in a single QD embedded in a symmetric PIN-diode. We resonantly excited the biexciton-state via 2-photon absorbtion with a cw-laser and observed its optical decay depending on the applied electric field. This data was then compared with electric field dependend photocurrent measurements.
We find that under forward bias the intensities of the XX- and X-emission are equaly affected by negative charging of the QD. Under reverse bias the X-emission is selectively decreased by tunneling. Furthermore the faster tunneling rate of the electrons leads to the generation of positivly charged excitons, which is clearly detected by an emerging trion line. Based on these results we propose a tailored sample structure, that symmetrises the tunneling times of electrons and holes and therefore increases the efficiency of the light source.

HL 64.15 Thu 10:00 P1A

Resonance fluorescence on plasmon-quantum dot hybrids — •Gerhard Johannes Schäfer[1], Armando Rastelli[2,3], and Markus Lippitz[1] — [1]Experimentalphysik III, Universität Bayreuth, Bayreuth, Germany — [2]Institute for Integrative Nanosciences, IWF Dresden, Dresden, Germany — [3]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, Linz, Austria

Resonance fluorescence spectroscopy is a well-established tool to investigate single quantum dots in bulk experiments. I present experiments on single GaAs quantum dots using a high NA microscope objective in a closed cycle cryostat. In a next step these structures are coupled to plasmonic structures.

HL 64.16 Thu 10:00 P1A

Self-assembled low-density InAs quantum dots/quantum dot molecules — •Akshay Kumar Verma, Timo Langer, and Dirk Reuter — Paderborn University, Department Physik, Warburger Str. 100, 33098 Paderborn

In recent years, low-density InAs Quantum dots (QDs)/Quantum dot molecules (QDMs) have been fabricated and studied by single dot spectroscopy for their unique optical and electrical properties. For single dot based experiments, the density requirement is around 10^8 QDs/cm^2 ($\sim$1QD/μm^2) or below for which a dot does not interact with neighbouring dots and can optically be addressed individually. Self-assembled InAs quantum dot layer(s) were grown on GaAs (100) substrates by molecular beam epitaxy (MBE) using two growth approaches, In-gradient approach, and annealing approach, resulting in densities from 10^8-10^{10} QDs/cm^2. The size, shape, and density of QDs were controlled by a variation of the growth parameters. In the annealing approach, we deposit a subcritical InAs amount with continuous substrate rotation, with subsequent annealing. The transition energies can be tuned by using the In-flush technique. We have grown two vertically InAs QDs layers separated by GaAs barrier, so called QDMs. The QDs have been analyzed by atomic force microscopy and photoluminescence (PL). By carefully adjusting the substrate temperature and In amount, we were able to obtain QD densities of $\sim 10^7$-10^8 QDs/cm^2 homogenously over an entire 3" wafer. We suggest that the low-density InAs QDs/QDMs grown by annealing approach provide us a large fraction of the wafer for further experiments.

HL 64.17 Thu 10:00 P1A

Gain, dispersion and alpha measurements of p-doped quantum dot lasers — •Felix Wilke[1], Matteo Angelozzi[2], Paolo Bardella[2], Christoph Weber[1], Dominik Auth[1], Vladimir V. Korenv[3,4], Artem V. Saveleyev[3], Mikhail V. Maximov[3,4], Alexey E. Zhukov[3,4], and Stefan Breuer[1] — [1]Institute of Applied Physics, Technische Universität Darmstadt, 64289 Darmstadt, Germany — [2]Department of Electronics and Telecommunications, Politecnico di Torino, 10129 Torino, Italy — [3]St. Petersburg Academic University RAS, ul. Khlopina 8/3, 194021 St. Petersburg, Russia — [4]Peter the Great St. Petersburg Polytechnic University, St. Petersburg 195251, Russia

We report on the experimental investigations on the role of p-doping on the spectrally resolved modal gain and absorption, group delay dispersion and linewidth enhancement factor in two-section InAs/InGaAs semiconductor quantum dot lasers emitting at around 1250 nm. The net modal gain curves are obtained during post-processing and three methodologies are employed: namely Fourier-transform infrared spectroscopy [Hofstetter et al. PTL 11,1372 (1999)], Hakki-Paoli [Hakki et al. JAP 46,1299 (1975)] and mode sum [Cassidy JAP 56, 3096 (1984)]. This work is supported by the Russian Foundation for Basic Research (project #18-502-12081).

HL 64.18 Thu 10:00 P1A

Ultrashort dynamics of an InP/AlGaInP QD SESAM — •Marius Grossmann[1], Julian Obermeier[2], Roman Bek[3], Thorsten Schumacher[2], Markus Lippitz[2], Michael Jetter[1], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQST) and Research Center SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]Department of Physics, University of Bayreuth, 95440 Bayreuth, Germany — [3]Twenty-One Semiconductors, Kiefernweg 4, 72654 Neckartenzlingen, Germany

Mode-locked vertical external-cavity surface-emitting lasers (VECSELs) provide ultrashort pulses across a wide wavelength range. Furthermore, semiconductor bandgap engineering allows the additional flexibility to custom-tailor the pulse train properties.

To this end quantum dots (QDs) are a key component because their 0D-nature contributes beneficial properties when employed in a semiconductor saturable absorber mirror (SESAM). These include independently adjustable saturation fluence and modulation depth as well as a fast relaxation, all advantageous for mode locking of VECSELs.

In this contribution we present the ultrafast properties of an

InP/AlGaInP QD SESAM investigated via degenerate pump-probe spectroscopy in the red spectral range.

HL 64.19 Thu 10:00 P1A

Comparison of optical excitation schemes for InAs/In(Ga)As/ GaAs quantum dots emitting in the telecom C-band — •Richard Schaber, Cornelius Nawrath, Fabian Olbrich, Michael Jetter, Simone Luca Portalupi, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart

Semiconductor quantum dots (QDs) exhibit excellent non-classical emission properties, most notably high single photon purity and photon indistinguishability values as well as a high fidelity of entangled photon pairs. With these, the essential prerequisites as light sources for applications in quantum communication are fullfilled.

We present InAs/In(Ga)As/GaAs QDs emitting at 1550nm (telecom C-band) wavelengths which matches the absolute absorption minimum of standard silica fibers. Coherence properties of the emitted photons are compared under different optical excitation schemes. Non-resonant (above band) excitation is investigated as well as (quasi-)resonant schemes, highlighting the superior suitability of the latter for possible appplications regarding coherence.

HL 64.20 Thu 10:00 P1A

1550 nm quantum dots grown in an InGaAs well — •Marcel Schmidt[1], Aimeric Courville[2], Andreas D. Wieck[1], and Arne Ludwig[1] — [1]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Germany — [2]CNRS, Université Côte d'Azur, CRHEA, France

Self-assembled quantum dots (QDs) emitting at 1.55 μm are very promising for future optical fiber transmitted quantum information exchange as the attenuation in the optical fiber has an absolute minimum at this wavelength. The QDs are nearly ideal sources for single indistinguishable photons or entangled photon pairs which can be used for quantum information purposes like quantum key distribution or quantum repeaters. We present first results of QDs grown in an asymmetric InGaAs quantum well[1]. The QDs are grown on a pseudomorphic InGaAs layer. By stopping the rotation during QD growth, both the InAs quantity and the deposition rate are modified. As a result, the QD density and morphology varies along the growth gradient. A further layer of InGaAs, with a higher In content than the subsequent layer, is applied on top of the QDs. Photoluminescence maps preformed on the so embedded QDs indicate regions with lower intensity along the gradient. AFM measurements taken from these spots show a higher density of ripened islands and thus potentially more dislocations serving as non-radiative recombination channels.

1.) Zhang et al., 1.55 μm InAs/GaAs quantum dots and high repetition rate quantum dot SESAM mode-locked laser. Scientific reports **2**, 477 (2012).

HL 64.21 Thu 10:00 P1A

Grating Couplers on a III-V Semiconductor Platform for Quantum Photonic Applications — •Stephanie Bauer, Simone Luca Portalupi, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQ^{ST}) and SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart

Quantum photonic integrated circuits are a compact and promising platform for quantum information technologies. In contrast to silicon-based systems, photonic circuits on a III-V semiconductor platform bear the advantage of the direct implementation of quantum dots with their outstanding properties as non-classical light sources. However, some applications require the coupling of light into single mode fibers e.g. for the connection of distinct quantum nodes. For this task, grating couplers are very promising due to the outstanding coupling efficiencies(<85%) and good fiber alignment tolerances.

Here, we present the fabrication and characterisation of waveguide integrated grating couplers on a GaAs/AlGaAs platform. Their coupling efficiency is optimized for a wavelength in the near infrared regime, matching the emission wavelength of InAs quantum dots.

HL 64.22 Thu 10:00 P1A

Time-resolved high-frequency Lock-In transport measurements on self-assembled quantum dots — •Felix Schaumburg[1], Jens Kerski[1], Jakob Penner[1], Arne Ludwig[2], Andreas D. Wieck[2], Martin Geller[1], and Axel Lorke[1] — [1]Faculty of Physics and CENIDE, University Duisburg-Essen, Germany — [2]Chair of Applied Solid State Physics, Ruhr-University Bochum, Germany

Time-resolved transconductance measurements on self-assembled quantum dots (QDs) can be used to access excited spin- and charge states in an all-electrical measurement [1], an important step towards quantum state manipulation and detection for future quantum information technologies. For fast and high-fidelity measurements, the signal-to-noise ratio (SNR) of the read-out signal is of great importance. We present transconductance measurements with an significantly increased SNR up to single-shot measurements. For this, we combined transconductance with a Lock-In measurement scheme using the resonance frequency of an LC circuit. We use a high-mobility electron transistor (HEMT) with a layer of QDs, which are coupled to a two-dimensional electron gas (2DEG). This allows us to observe the tunnelling dynamics between the 2DEG and the QDs. A sinusoidal MHz-ac-voltage in resonance with the LC circuit is applied to the 2DEG in the Lock-In measurement. The transmitted signal is analysed with a Lock-In-Amplifier, exhibiting the regular transients of transconductance with an enhanced SNR.

[1] K. Eltrudis et al., Appl. Phys. Lett. **111**, 092103 (2017).

HL 64.23 Thu 10:00 P1A

Self mode-locked single section quantum dot optical frequency comb laser subject to short optical self-injection — •Matthias Hagen[1], Dominik Auth[1], Christoph Weber[1], Benedikt Schwarz[2,3], Luke F. Lester[4], and Stefan Breuer[1] — [1]Institute of Applied Physics, Technische Universität Darmstadt, 64289 Darmstadt, Germany — [2]Institute of Solid State Electronics, TU Wien, 1040 Vienna, Austria — [3]John A. Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts 02138, USA — [4]Bradley Department of Electrical and Computer Engineering, Virginia Polytechnic Institute and State University, Blacksburg, Virginia, 24061, USA

Frequency modulated optical frequency comb generation in self-mode locked single section quantum dot lasers with short fabry-perot cavity lengths of 1 mm have been studied experimentally and by simulation [Weber et al., Optics Letters 44(14), pp. 3478-3481 (2019)]. Ultra short optical self-injection of optical frequency comb quantum cascade lasers has been reported to change and control the group delay dispersion of the optical frequency comb [Hillbrand et al., Optics Letters 43(8), pp. 1746-1749 (2018)]. In this contribution we study the impact of ultrashort optical self-injection onto frequency-modulated optical frequency combs in self-mode locked quantum dot lasers with respect to change in group delay dispersion and intermode-beat-frequency tuning.

HL 64.24 Thu 10:00 P1A

Examination of self-assembled quantum dots in a density-modulated pattern with capacitance-voltage spectroscopy — •Nikolai Spitzer, Nikolai Bart, Andreas Wieck, and Arne Ludwig — Ruhr-Universität Bochum, Lehrstuhl für Angewandte Festkörperphysik - Universitätsstraße 150, 44801 Bochum

Self-assembled InAs quantum dots (QDs) on GaAs with a QD density modulation were grown by molecular beam epitaxy. The QDs can be arranged in stripe patterns whose properties can be changed by a gradient in the GaAs sublayer beneath the QDs. We suspect that the formation of QDs is favoured by atomic rough areas as opposed to flat areas during molecular epitaxial growth. The differences in the sublayer are due to the profile of the molecular beam. Capacitance-voltage spectroscopy is used to investigate the properties of the quantum dots arranged in this way at different densities.

HL 64.25 Thu 10:00 P1A

Manipulating quantum dot luminescence via strong THz fields — •Moritz Heindl and Georg Herink — Experimental Physics VIII, University of Bayreuth, Germany

The investigation and manipulation of ultrafast electron dynamics at the nanoscale requires precise characterization of local electric field transients. For this purpose, the field-dependent change of the luminescence of semiconductors due to the quantum confined Stark effect can be employed. Here, we present an experimental scheme to locally modify quantum dot luminescence by field enhancement at planar nanostructures, e.g. micro-antennas and micro-slits. For ultrafast probing and control, we employ high-field single-cycle THz pulses

based on the tilted-pulse front scheme.

HL 64.26 Thu 10:00 P1A

Spin noise spectroscopy in single InGaAs quantum dots — •Kai Hühn, Julia Wiegand, Jens Huebner, and Michael Oestreich — Inst. for Solid State Physics, Leibniz University Hannover, Appelstraße 2, 30167 Hannover, Germany

In this work we present Spin noise spectroscopy measurements of single Quantum Dots in high magnetic fields reaching from 300mT to 1.4 T. Some theory for the magnetic field dependence of the heavy-hole spin lifetime has been formulated. Additionally the Zeeman splitting and the diamagnetic shift has been investigated to determine Trion g-factor of 1.25. A new fit model has been established, which connects the spin noise power with the spin noise width. This enabled a new way of extrapolating the intrinsic lifetime of an Lorentzian shaped inhomogenius broadened quantum dot.

HL 64.27 Thu 10:00 P1A

Fast switching of quantum dot photons in a Mach-Zehnder interferometer — •Fabio Rimek[1], Pia Lochner[1], Hendrik Mannel[1], Arne Ludwig[2], Andreas D. Wieck[2], Martin Geller[1], and Axel Lorke[1] — [1]Faculty of Physics and CENIDE, University Duisburg-Essen, Germany — [2]Chair of Applied Solid State Physics, Ruhr-University Bochum, Germany

A Mach-Zehnder interferometer can be used to measure the coherence of a photon stream by a two-path experiment. In the ultimate limit of a single photon in the interferometer, it is also a realization for the so-called which-path experiment, where a single photon occupies both paths of the interferometer.
In this contribution, we will use single photons from a single self-assembled quantum dot in the Heitler regime with coherence lengths exceeding the dimensions of the interferometer to realize a time-resolved which-path experiment. A major challenge is an electro-optical polarization switch in the wavelength range of the photons from the self assembled InAs/GaAs quantum dots (∼950 nm). The polarisation switch should switch the photon polarisation faster than the photon residence time in the Mach-Zehnder interferometer. Depending on the polarization, the path can be determined in the interferometer. The switching of the polarization is caused by a superposition of two perpendicularly polarized waves, exhibiting a phase difference that can be varied by an electro-optic modulator (EOM). The polarization is stabilized by an PID controlled feedback loop, which eliminates fluctuations of the phase due to other influences.

HL 64.28 Thu 10:00 P1A

Semiclassical modelling of coupled quantum dot-cavity systems: From polariton-like dynamics to Rabi oscillations — •Kevin Jürgens, Frank Lengers, Tilmann Kuhn, and Doris E. Reiter — Institut für Festkörpertheorie, Universität Münster, Münster

Semiconductor quantum dots (QDs) in a photonic cavity are strongly coupled light-matter systems with numerous applications in quantum information technology. Due to the photonic confinement, the interaction of the QDs with the cavity mode is increased. Here we present a semiclassical model to describe the dynamics of the coupled QD-light system: The QDs are modelled as a planar ensemble of quantum mechanical two-level systems coupled to the electric field and the light field is described by Maxwell's equations in one dimension. We explicitly take into account the coupling between the QD polarization and the electric field, i.e. we solve the coupled Maxwell-Bloch equations. We show that, depending on the initial value of the light field amplitude, a sharp transition between two regimes with fundamentally different dynamics and spectra emerges. For low amplitudes we find exciton polariton-like dynamics and for high amplitudes Rabi oscillations. The spectrum of the exciton polariton shows the typical anticrossing behavior when tuning the transition frequency of the QD through resonance, and for high amplitudes we see the energy splitting of the dressed states. We confirm our findings in an analytical model.

HL 64.29 Thu 10:00 P1A

Frequency Shift of Electronic Resonances in Self Assembled InAs Quantum Dots — •Ibrahim A. Engin, Ismail Bölükbaşı, Sven Scholz, Andreas D. Wieck, and Arne Ludwig — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-UniversitätBochum, D-44780 Bochum, Germany

Self-assembled InAs quantum dots (SAQD) proved promising semiconductor structures as single-photon sources and provide possibilities for quantum memories. Therefore understanding the physical properties is important and in progress. We investigate electronic resonances in InAs SAQDs by using C(V)-spectroscopy.

The thermal shift of the s-states has been reported and described with a master equation [1], which has been improved further to model excitonic and non-equilibrium states in such SAQD [2]. The model shows contrarily shifting in dependence of frequency and temperature.

Here we investigate both s- and p-states in dependence of temperature and frequency to measure the shifting characteristics of p-peaks and observe the dominancy of the frequency shift for s-states. The superposition of thermal and frequency shift are being analyzed. Adjustments to the master equation model are needed.

[1] Brinks, F. et al., "Thermal shift of the resonance between an electron gas and quantum dots: what is the origin?" New J. Phys. 18, 123019 (2016).

[2] Valentin, S. et al., "Illumination-induced nonequilibrium charge states in self-assembled quantum dots", Phys. Rev. B 97, 045416 (2018).

HL 64.30 Thu 10:00 P1A

Ridge-width dependent beam profile analysis of InAs/InGaAs quantum dot lasers — •Adrian Hamel[1], Christoph Weber[1], Dominik Auth[1], Vladimir V. Korenev[2,3], Artem V. Savelyev[2], Mikhail V. Maximov[2,3], Alexey E. Zhukov[2,3], and Stefan Breuer[1] — [1]Institute of Applied Physics, Technische Universität Darmstadt, 64289 Darmstadt, Germany — [2]St. Petersburg Academic University RAS, ul. Khlopina 8/3, 194021 St. Petersburg, Russia — [3]Peter the Great St. Petersburg Polytechnic University, St. Petersburg 195251, Russia

Monolithic mode-locked edge-emitting semiconductor quantum dot lasers with narrow ridge widths to broad ridge widths emitting at 1.25 micrometer are ideal sources for the generation of broad optical frequency combs for short-reach inter and intra data-center links. In this contribution, the beam profile of InAs/InGaAs quantum dot lasers with 5 micrometer, 10 micrometer and 50 micrometer broad ridge waveguides and different doping concentration in the GaAs barriers are studied experimentally. The work focuses on the comparison of near and far field beam profile. This work is supported by the Russian Foundation for Basic Research (project #18-502-12081).

HL 64.31 Thu 10:00 P1A

Telecom wavelength InP-based quantum dots for quantum communication — Andrei Kors, Johann Peter Reithmaier, and •Mohamed Benyoucef — Institute of Nanostructure Technologies and Analytics (INA), CINSaT, University of Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

Self-assembled semiconductor quantum dots (QDs) emitting at optical fiber communication wavelengths, particularly in the telecom C-band, which offers the lowest attenuation losses in silica fibers is highly interesting for quantum communication applications.

Here, we report our effort on the growth of low density InAs/InP QDs using molecular beam epitaxy, fabrication of InP-based microcavities emitting at telecom wavelengths, and their optical properties. Fabrication of symmetric QDs with low density is obtained by careful control of various growth parameters. Low-temperature single-dot spectroscopy exhibits high-intensity sharp excitonic emission lines with vanishing fine-structure.

HL 64.32 Thu 10:00 P1A

Photoluminescene Spectroscopy of Self-Assembled InAs/GaAs Quantum Dots grown in a Density-Modulated Pattern by Molecular Beam Epitaxy — •Peter F. Zajac, Nikolai Bart, Andreas D. Wieck, and Arne Ludwig — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Universitätsstraße 150, 44801 Bochum

Self-assembled InAs/GaAs Quantum Dots (QDs) with a modulation of QD density perpendicular to the growth direction were grown by molecular beam epitaxy (MBE). The modulation corresponds to a striped pattern, whose properties can be modified by varying the growth parameters of the buffer layers underneath the QDs. It is proposed that the pattern is caused by the deposition profile of the molecular beam causing the formation of atomically rough and smooth surface areas which lead to an earlier nucleation of QDs at rougher regions in comparison to flat surfaces. With Photoluminescence Spectroscopy (PL) measurements at room temperature and 100 K the properties of such grown QDs in the different regimes of QDs density are studied in

order to understand the growth process and to tune the QD emission.

HL 64.33 Thu 10:00 P1A

Sensing electrical fields in nanostructures via quantum dot luminescence — •Sofie Krietenstein and Georg Herink — Experimental Physics VIII, University of Bayreuth, Germany

Quantum dot luminescence can be modified in the presence of external electrical fields, particularly due to the Quantum-Confined-Stark-Effect.

In this contribution, we present a detection scheme for sensing local electrical fields in nanostructures via changes of luminescence spectra and lifetimes. Specifically, we employ the Dispersive Fourier Transform based on the group velocity dispersion of optical fibers to map spectral information to the temporal domain. We present measurements on colloidal quantum dots embedded in voltage-biased gold nanostructures using different detection schemes.

HL 64.34 Thu 10:00 P1A

Probing the time dynamics of a continuously driven quantum dot under the influence of phonons — •Doris E. Reiter — Institut für Festkörpertheorie, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Semiconductor quantum dots are ideal object to study light-matter interaction in a quantum system. When a quantum mechanical two-level system is driven by a continuous wave excitation after an instantaneous switch on, the dynamics shows Rabi oscillations. These Rabi oscillations could be probed by an ultrashort laser pulse resulting in a Mollow triplet-like spectrum for resonant driving. The Mollow triplet consists of a single peak at the driving frequency and two peaks at the Rabi frequency with half the amplitude. In contrast to an atomic system, the quantum dot is embedded in the solid state matrix and therefore is subject to the interaction with phonons. The electron-phonon interaction results in a damping of the Rabi oscillations and accordingly the optical spectrum after the damping exhibits only the two side peaks. We derive analytical equations to describe both the dynamics and the probe signals of the system within a simple rate equation model. We validate our model by comparison with solution using a standard correlation expansion. The analytical results allow to scrutinize the influence of phonons on optically excited quantum dots.

HL 64.35 Thu 10:00 P1A

Chirped single photons from a semiconductor quantum-dot — •David Bauch[1], Dirk Heinze[1], Artur Zrenner[1], and Stefan Schumacher[2] — [1]Department of Physics and CeOPP, Paderborn University, Paderborn, Germany — [2]College of Optical Sciences, University of Arizona, Tucson, AZ 85721, USA

On demand sources for controlled single photon emission are essential for quantum information theory. Exciton emission or cascaded biexciton-exciton emission in semiconductor quantum dots offer the potential for optically controlled generation of a single photon [1] and polarization-entangled twin photons [2]. In contrast to pure optical control, externally applied time-dependent electrical fields enable control of the (bi-)exciton resonance (electronic chirp), resulting in changes of the excitation dynamics and the resulting photon emission. Combining both optical and electronic control of the photon emission might be significant for future integration into optoelectronic devices. Here we investigate the influence of electronic chirps on the generation of single photons via (bi-)exciton (two-)photon emission and biexciton-exciton emission cascades and determine quantum properties and spectral characteristics of the emitted photons in a high- and low-quality resonator. For exciton emission we show suppression of Rabi-splitting in high-quality cavities and on-demand triggering of photon emission while retaining spectral properties.

[1]: Heinze, D., Breddermann, D., Zrenner, A., Schumacher, S. Nat. Commun. 6, 8473 (2015). [2]: Heinze, D., Zrenner, A., Schumacher, S. Phys. Rev. B 95, 245306 (2017).

HL 64.36 Thu 10:00 P1A

Multi-particle theory of magneto-optical properties of GaAs/AlGaAs quantum dots — •Diana Csontosová[1,2], Armando Rastelli[3], and Petr Klenovský[1,2,4] — [1]Department of Condensed Matter Physics, Faculty of Science, Masaryk University, Kotlářská 267/2, 61137 Brno, Czech Republic — [2]Czech Metrology Institute, Okružní 31, 63800 Brno, Czech Republic — [3]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, Altenbergerstr. 69, 4040 Linz, Austria — [4]Central European Institute of Technology, Masaryk University, Kamenice 753/5, 62500 Brno, Czech Republic

We have theoretically studied the size effect of GaAs/AlGaAs quantum dots on magneto-optical properties of neutral excitonic states. We employed a combination of the envelope function approximation based on 8-band $\mathbf{k}\cdot\mathbf{p}$ theory and the method of configuration interaction similar to Ref [1]. The magnetic field was applied in the growth direction. The results of our calculations are in very good agreement with available experimental data. [2] By comparing the results of single- and multi-particle calculations, we find that correlations play crucial role on the magneto-optical properties of our dots.

[1] Huber, D., *et al.*, arXiv:1909.04906 (2019).
[2] Löbl, M. C., *et al.*, Phys. Rev. B **100**, 155402 (2019).

HL 64.37 Thu 10:00 P1A

Interal photo-emission of electrons from a quantum dot — •Pia Lochner[1], Jens Kerski[1], Annika Kurzmann[1], Andreas D. Wieck[2], Arne Ludwig[2], Martin Geller[1], and Axel Lorke[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [2]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Germany

Resonance fluorescence (RF) on excitonic transitions in confined quantum systems (like self-assembled quantum dots) is ideally free of any charge generation in the environment. The light field from the laser should only couple to the optical transitions. However, it as been shown recently that even under resonant excitation, free electrons can be generated in the environment by intra-band electron excitation from a nearby charge reservoir. These electrons can be *captured* by the dot and quench the exciton transition of the RF signal [1].

In this contribution, we demonstrate by time-resolved RF measurements on a single self-assembled quantum dot an internal photo-effect that *emits* electrons from the QD by an intraband excitation. The dot is in our sample only weakly-coupled to an electron reservoir with tunneling rates below 1/ms. We show a linear dependence of the optically-generated emission rate on the excitation intensity and use a rate equation model to deduce the involved rates. Our results demonstrate that also under resonant excitation, free electrons can be generated by an internal photo-effect that can influence the optical properties of a dot.

[1] A. Kurzmann, et al., APL **108**, 263108 (2016).

HL 64.38 Thu 10:00 P1A

Carrier and energy transfer in colloidal quantum dot semiconductor hybrids — •Mikko Wilhelm, Shyam Kommadath, Salwa Khokhar, and Wolfram Heimbrodt — Philipps-Universität Marburg

Colloidal quantum dots are attractive for functionalization of semiconductors in electronic and opto-electronic devices like solar cells, field effect transistors or spintronic devices. CdS/ZnS and CdSe/ZnS core/shell quantum dots of different sizes synthesized in solution are deposited via knife coating on different semiconductor substrates. Depending on the band alignment between the quantum dots and the semiconductor substrate, energy and charge transfer is observed. The interaction between the quantum dots and semiconductor substrate is studied with optical spectroscopy. The results of continuous wave and time resolved photoluminescence measurements at different temperatures from 10K to room temperature are presented and discussed.

HL 64.39 Thu 10:00 P1A

Magneto-optical studies of manganese doped collodial core shell CdS/ZnS quantum dots — •Johannes Röder[1], Mikko Wilhelm[1], Nadeem Sabir[1], Wolfgang Parak[2], and Wolfram Heimbrodt[1] — [1]Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Universität Hamburg, 22761 Hamburg, Germany

The magnetic field dependency of the photoluminescence of colloidal core shell CdS/ZnS quantum dots doped with manganese in the ZnS shell are investigated. The focus of this investigations was on the influence of the Mn position in the core shell dots on the magneto-optical properties. There are 2 different samples and 2 reference samples investigated: One were Mn is directly grown on the CdS core together with a ZnS shell and another were Mn is introduced after the CdS core is already covered with a ZnS shell. Samples were Mn is directly grown on the CdS core without a ZnS shell and a CdS core with 2 shell layers of ZnS without any Mn are used as reference samples. To investigate the temperature dependency the quantum dots were transferred from solution via drop casting on a quartz substrate. The results of these measurements will be discussed in detail.

HL 64.40 Thu 10:00 P1A

Tracking the mixing of single-particle states in correlated multi-particle complexes of quantum dots — •Diana Csontosová[1,2] and Petr Klenovský[1,2,3] — [1]Department of Condensed Matter Physics, Faculty of Science, Masaryk University, Kotlářská 267/2, 61137 Brno, Czech Republic — [2]Czech Metrology Institute, Okružní 31, 63800 Brno, Czech Republic — [3]Central European Institute of Technology, Masaryk University, Kamenice 753/5, 62500 Brno, Czech Republic

By deconvolution of the Configuration interaction (CI) calculation of the electronic states in the quantum dots (QDs), we investigate (i) the content of single-particle states in multi-particle eigenstates of excitonic complexes, (ii) the heavy-light hole mixing in those, and (iii) their probability densities. Our approach enables us to track the aforementioned parameters for arbitrary size of the CI basis, i.e., including the effects of correlation. This provides us a way to find the most probable final states of excited trions or more precise determination of heavy-light hole mixing in the CI states. Our method enables a more precise study of the effects of tuning of emission properties of QDs using externally applied fields (electric, magnetic, strain).

HL 64.41 Thu 10:00 P1A

Conductance spectroscopy on quantum dot molecules — •Carsten Ebler, Giang N. Nguyen, Alexander R. Korsch, Andreas D. Wieck, and Arne Ludwig — Ruhr-Universität Bochum, 44801 Bochum, Germany

Quantum dot molecules (QDM) have shown to be a good approach increasing the T2 time in quantum bits [1]. For a controlled charging of QD charge states and a better understanding of the interaction and crosstalk inside the QDM, we use two epitaxially grown self-assembled InAs quantum dot layers (SAQD) in close tunnel contact to each other. We establish the QDM in tunnel contact with an inverted GaAs/Al0.3Ga0.7As HEMT structure containing a 2-dimensional electron gas (2DEG), manipulate the system with electronical and optical pulses and perform time resolved conductance measurements [2] of the 2DEG to readout the charge occupation of the QDMs. The charge state is read out over conductivity changes in the channel of the HEMT and the resulting transient contains multi-exponential components. We make use of the inverse Laplace transformation to distinguish between the different time constants representing tunnel contributions into the different quantum dot layers.

[1] Weiss et. al, PRL 109 (2012) [2] Marquardt et. al, APL 95 (2009)

HL 64.42 Thu 10:00 P1A

Influence of electric and magnetic fields on the line broadening of semiconductor quantum dots — •Tim Strobel, Jonas H. Weber, Hüseyin Vural, Julian Maisch, Simone L. Portalupi, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

Photonic quantum technologies, such as quantum networks and quantum computing are based on two-photon interference (TPI). Implementations of actual TPI experiments inevitably require single photons with high indistinguishability. Semiconductor quantum dots (QDs) are an excellent choice with respect to such quantum applications. They can be used for on-demand emission of indistinguishable photons, a property, which is inevitable to successfully implement two-photon inteference experiments with up-scaled complexity using multiple sources. QD emission spectra with a linewidth reaching the transform limit are desired to yield maximum indistinguishability of photons from remote sources. Charge and spin noise, inherent to the semiconductor device, can drastically increase the linewidth to a multiple of the transform limit. Those two sources of noise are subject of current research and scientific discussion. Optimizing the perfomance demands an understanding of the noise sources. Here, we present an investigation on the influence of electric and magnetic fields on the QD emission linewidth. In this talk, measurement techniques to uncover the behaviour of those effects will be presented.

HL 64.43 Thu 10:00 P1A

Capacitance-voltage spectroscopy on no-wetting layer quantum dots — •Ismail Bölükbasi, Sven Scholz, Andreas D. Wieck, and Arne Ludwig — Ruhr-Universität Bochum, D-44780 Bochum, Germany

Quantum dots have interesting physical properties and allow research in zero dimensional systems. They are used in modern displays and may become important for the progress of semiconductor and information technology in the form of qubits in quantum computers and quantum memories or quantum communication applications.

Quantum dots are created by molecular-beam-epitaxy (MBE) in Stranski-Krastanov growth. InAs is deposited epitaxially onto GaAs and grows without relaxation to up to 1.5 monolayers of InAs. This layer is called the wetting layer, on top of which the self-organized quantum dots form.

We find, that a monolayer of AlAs after the growth of the quantum dots can suppress certain states in this wetting layer[1], allowing to purify their photoluminescence spectra from electronic contributions such as for example a two-dimensional-electron gas would induce. Capacitance-voltage and photoluminescence measurements are carried out to investigate the effects of this monolayer of AlAs on the physical properties of the quantum dots and the modified charging behaviour around flat band conditions.

[1] Löbl, M. C. et al. Excitons in InGaAs quantum dots without electron wetting layer states. Commun. Phys. 2, 93 (2019)

HL 64.44 Thu 10:00 P1A

Spin Noise Spectroscopy Setup for single GaAs Quantum Dots resonant at the Rb D-line — •Tianjiao Sun, An Zhao, Xin Cao, Fei Ding, Jens Hübner, and Michael Oestreich — Institute for Solid State Physics,Appelstraße 2, D-30167 Hannover, Germany

Electrons and holes confined in single quantum dots (QDs) have attracted much attention since they are potential candidates for semiconductor quantum information qubits. We use spin noise spectroscopy, to access the spin dynamics of confined carriers in single quantum dots, as well as the interaction of single confined carriers with the nuclear environment[1]. In addition, a recent report shows for (InGa)As QDs an occupation noise contribution in resonant spin noise measurements which reveals the dynamics of charge exchange between the QD and its environment due to Auger recombination[2]. Here, we aim for the investigation of the intrinsic spin and charge dynamics in a new type of symmetric GaAs QDs[3]. The low strain in these QDs can enable a prolonged spin coherence time compared to (InGa)As QDs. Furthermore, the optical transition at the Rb D-line is promising for a potential realization of coherent coupling of solid-state and atomic qubit implementations.

[1] J. Hübner, F. Berski, R. Dahbashi, and M. Oestreich, physica status solidi (b) 251, 1824 (2014).

[2] J. Wiegand, D. S. Smirnov, J. Osberghaus, L. Abaspour, J. Hübner, and M. Oestreich, Phys. Rev. B 98, 125426(2018).

[3] R. Keil, M. Zopf, Y. Chen, B. Höfer, J. Zhang, F. Ding, and O. G. Schmidt, Nat. Commun. 8, 15501 (2017).

HL 64.45 Thu 10:00 P1A

Carbon nanodots: Luminescence properties tuned by microcavity devices — •Lukas Trefflich[1], Nicole Weizenmann[2], Frank Dissinger[3], Gabriele Benndorf[1], Chris Sturm[1], Rüdiger Schmidt-Grund[1,4], Siegfried R. Waldvogel[3], Ralf Seidel[2], and Marius Grundmann[1] — [1]Felix Bloch Institute for Solid State Physics, Universität Leipzig — [2]Peter Debye Institute for Soft Matter Physics, Universität Leipzig — [3]Institute for Organic Chemistry, Johannes Gutenberg Universität Mainz — [4]now at: Institute of Physics, Technische Universität Ilmenau

The carbon nanodots (cdots) made from citric acid and a stabilizing amine component emit bright light in the spectral range between 390 nm and 600 nm. To investigate their size-dependent luminescence properties, we separate them with gel-electrophoresis and perform time- and energy-resolved photoluminescence (PL). We propose a streched exponential law [1] for the emission decay. The mean luminescence lifetime depends on the emission wavelength (cf. [2]) and the particle size. We obtain lifetimes in the range of 0.6 ns to 2 ns. The emission of the cdots can be enhanced by incorporating them in a planar microcavity. That allows to tune the emission wavelength of the device by varying the optical thickness of the cavity layer. We produce such a device with pulsed laser deposition and characterize it with power dependent PL. The power-dependence fits to a multimode laser-model [3], indicating lasing, with a threshold intensity of 32 MW cm^{-2}. [1] Milovanov et al., Phys. Rev. B, 2007, **76** [2] Kahn and Kim, Sci. Rep., 2019, **9** [3] Casperson, J. Appl. Phys., 1975, **46**

HL 64.46 Thu 10:00 P1A

Excited States in Bilayer Graphene Double Quantum Dots — •Alexander Rothstein[1], Luca Banszerus[1,2], Samuel Möller[1],

Eike Icking[1,2], Kenji Watanabe[3], Takashi Taniguchi[3], Christian Volk[1], and Christoph Stampfer[1,2] — [1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany, EU — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany, EU — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan

Due to its small spin orbit interaction and negligible hyperfine coupling as well as the possibility to open up a band gap, bilayer graphene (BLG) offers a promising platform for future spin-based quantum computation devices. Recent progress in the fabrication techniques and the possibility to fully pinch off current in BLG allow to electrostatically confine single- and double quantum dots by a smooth potential, which can be studied with regard to their electronic configuration.* Here, we present a remarkable degree of control of finger-gate based double quantum dots structure enabling to modify controllably the electron number in each of the quantum dots from zero up to a few electrons. We show an increasing inter dot tunnel coupling, as well as an increasing capacitive interdot coupling with a growing dot occupation. At a finite bias voltage, we can resolve the excited state spectrum of the first electrons in the double quantum dot and extract their energies as function of an applied out-of-plane magnetic field.

HL 64.47 Thu 10:00 P1A

Homodyne Spin Noise Spectroscopy of Single Quantum Dots — •Pavel Sterin, Kai Hühn, Julia Wiegand, Jens Hübner, and Michael Oestreich — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany

Spin noise spectroscopy (SNS) is a technique that can be used to investigate the spin dynamics of sensitive semiconductor systems in a quasi-non-perturbative way. However, for the most delicate systems like, e.g., single InGaAs quantum dots it seemed that SNS had reached its limits: classic setups exhibit an electrical noise that dominates the measurements at intensities low enough to keep the residual absorption acceptable [1]. Further reduction of the intensity is limited by prohibitively long integration times [3].

We propose a setup that employs homodyne SNS as first demonstrated by [2],[3] and [4]. An all optical amplification is realized by coupling the experiment to a homodyne interferometer. This modification enables efficient integration times and a quantum-limited, i.e., optimal, signal-to-noise ratio. Finally, the new setup will allow us to gain insight into unperturbed spin dynamics of single quantum dots.

[1] Dahbashi, et al. Phys. Rev. Lett. 112, 156601, (2014).
[2] Cronenberger, et al. Rev. Sci. Instrum. 87, 093111 (2016).
[3] Sterin, et al. Phys. Rev. Applied 9, 034003 (2018).
[4] Petrov, et al. Phys. Rev. B 97, 125202 (2018).

HL 64.48 Thu 10:00 P1A

Negatively charged silicon vacancies V_{Si}^- in 4H-silicon carbide for quantum applications — •Julius Röwe and Martin S. Brandt — Walter Schottky Institut and Physik-Department, Technische Universität München, Garching, Germany

Since many, in particular bipolar electronic devices can be fabricated from silicon carbide, color centers such as the negatively charged silicon vacancy V_{Si}^- are intensively studied in this material for possible applications in quantum-based information and sensing. However, to make full use of the technological advantage, an efficient spin-to-current conversion is crucial for the coherent electrical read-out of these color centers. We study the fundamental properties of V_{Si}^- in 4H-SiC by photoconductivity measurements under near-resonant illumination and observe two-photon excitation of the ground state into the conduction band. Raster scanning of the detection volume allows spatial and lateral resolution of the photoconductivity in the micrometer range and an understanding of the properties of the electrical contacts to the SiC photoconductor. In addition, we will discuss the possibility to locally generate V_{Si}^- e.g. by helium ions.

HL 64.49 Thu 10:00 P1A

Nuclear spin dynamics in n-GaAs — •Lida Abaspour, Pavel Sterin, Jan Gerrit Lonnemann, Eddy Rugeramigabo, Jens Hübner, and Michael Oestreich — Institute for Solid States Physics, Leibniz University of Hannover, Appelstraße 2, D-30167 Hannover

Interaction of electron and nuclear spins in semiconductors became more important over the last few years for applications in spin based quantum information [1, 2]. However, the knowledge to understand the exact spin dynamics of such a complex system is not complete.

In this work, we measure the nuclear spin relaxation rate in a set of n-GaAs samples in a magnetic field much larger than the local fields. In this way the dipolar and quadrupolar effects can be ignored. The interaction of the nuclei with localized impurities (insulating samples) is different from conduction band electrons (metallic samples). In order to unravel the complex processes involved in the spin dynamics of this system, we use the results from magnetotransport measurements of the same samples [3] which yield access to the fraction of the localized doping in each sample. This helps us to explain the behavior of the nuclear spin relaxation rate in dependence of doping. The temperature dependence in insulating sample gives us more information about the spin dynamics of the system in terms of phonon interaction.

[1] F. Berski et al.,Phys. Rev. Lett, 115, 176601 (2015).
[2] M. Vladimirova, et al. Phys. Rev. B, 95, 125312 (2017).
[3] J. G. Lonnemann, et al. Phys. Rev. B, 96, 045201 (2017).

HL 64.50 Thu 10:00 P1A

Optically detected magnetic resonance spectroscopy of excitons in porous silicon and partially hydroxylated silicane — •Jonathan Zerhoch and Martin S. Brandt — Walter Schottky Institut and Physik-Department, Technische Universität München

Porous silicon and partially hydroxylated silicane, also known as siloxene, exhibit the strongest luminescence of any silicon-based material. We employ both continuous wave and pulsed optically detected magnetic resonance spectroscopy (ODMR) to study the recombination processes in these materials. In both, we observe a luminescence enhancing signature of the allowed $\Delta m_s = \pm 1$ and the forbidden $\Delta m_s = \pm 2$ transitions of triplet excitons and use the former to estimate their diameter. In addition, the resonance of dangling bond defects overlapping the triplet exciton signature and quenching the luminescence is observed. The technique of pulsed ODMR enables coherent control of the spin systems and, as expected, we find that the $\Delta m_s = \pm 1$ transition of the triplet exhibits a Rabi frequency which is a factor of $\sqrt{2}$ higher than the Rabi frequency of the spin-1/2 dangling bond defect. The observed dipolar broadened Pake-doublet gives rise to a wide distribution of electron-hole distances that appears to suppress the observation of Rabi oscillations at the $\Delta m_s = \pm 2$ resonance. Furthermore, we investigated the dynamical properties of the spin-1 and spin-1/2 systems providing T_2 times and the timescales of the different recombination processes.

HL 64.51 Thu 10:00 P1A

Manipulation of exceptional points in planar anisotropic photonic structures — •E. Krüger[1], C. Sturm[1], S. Richter[1,2], J. Zúñiga-Pérez[3], H.-G. Zirnstein[4], L. Trefflich[1], C. Deparis[3], B. Rosenow[4], R. Schmidt-Grund[1,5], and M. Grundmann[1] — [1]Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Germany — [2]ELI Beamlines/Fyzikální Ústav AV ČR, Czech Republic — [3]Université Côte d'Azur, CRHEA-CNRS, France — [4]Universität Leipzig, Institut für Theoretische Physik, Germany — [5]TU Illmenau, Leipzig, Institut für Physik, Germany

We present different approaches for establishing exceptional points (EP) in planar dielectric microcavities with broken cylindrical symmetry, realized by using anisotropic cavity layer materials.

Such EPs represent non-Hermitian degeneracies in momentum space, related to a local complex-square-root topology of the resonator eigenenergies. The eigenmodes coalesce along these directions, yielding degeneracy in energy, broadening and polarization.

We prove the exceptional-point nature experimentally and theoretically for ZnO-based microcavities by monitoring the square-root topology around such an EP. Furthermore, we show how the crystal symmetry and the crystal orientation of the cavity layer material as well as the geometrical cavity design influence the occurence and the position of the EPs in momentum space. We discuss also different approaches for breaking the system reciprocity in the cavity plane, thereby paving the way for topological non-trivial photonic systems.

[1] S. Richter et al., Phys. Rev. Lett. **123** (2019)

HL 65: 2D Materials and their Heterostructures III (joint session DS/HL)

Time: Thursday 11:00–12:30 Location: CHE 89

HL 65.1 Thu 11:00 CHE 89

Controllable growth of few-layer graphene — •Victor Aristov[1,2], Alexander Chaika[2,3], Olga Molodtsova[1,4], Sergey Babenkov[1,5], Dmitrii Potorochin[1,4,6], Andrea Locatelli[7], Tevfik Mentes[7], Alessandro Sala[7], and Dmitry Marchenko[8] — [1]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [2]Institute of Solid State Physics of the Russian Academy of Sciences, Chernogolovka, Moscow District 142432, Russian Federation — [3]CRANN, School of Physics, Trinity College Dublin, Dublin 2, Ireland — [4]ITMO University, 197101 Saint Petersburg, Russian Federation — [5]Institut fuer Physik, Johannes Gutenberg-Universita*t, D-55099 Mainz, Germany — [6]Institute of Experimental Physics, TU Bergakademie Freiberg, D-09599 Freiberg, Germany — [7]Elettra Sincrotrone Trieste, I-34149 Basovizza, Trieste, Italy — [8]Helmholtz-Zentrum Berlin fuer Materialien und Energie, D-12489 Berlin, Germany

Utilizing vicinal SiC/Si(001) wafers one can synthesize self-aligned graphene nanoribbons that exhibit energy transport gap on the order of 1 eV, large positive in-plane magnetoresistance, and the potential to work as a spin filter, opening opportunities for electronic and spintronic applications. This work demonstrates the capabilities to control the lattice and boundary orientations and the layer thickness in-situ, during the few-layer graphene synthesis in an ultra-high vacuum [1]. Supported by the RFBR (Grant Nos. 17-02-01139, 17-02-01291). [1] V.Yu.Aristov et al., ACS Nano 13, 526 (2019)

HL 65.2 Thu 11:15 CHE 89

Proximity-induced spin Hall effect in graphene/WSe_2 van der Waals heterostructures with tunable, highly efficient spin-to-charge conversion — •Franz Herling[1,2], C.K. Safeer[1], Josep Ingla-Aynés[1], Nerea Ontoso[1], Luis E. Hueso[1,3], and Fèlix Casanova[1,3] — [1]CIC nanoGUNE, 20018 Donostia-San Sebastian, Basque Country, Spain — [2]QuESTech, Horizon 2020 ITN, Marie Sklodowska-Curie Action (No 766025) — [3]IKERBASQUE, Basque Foundation for Science, 48013 Bilbao, Basque Country, Spain

The proximity effect in two-dimensional materials opens ways to achieve important functions for future spintronic devices. In van der Waals heterostructures, transition metal dichalcogenides (TMD) can be used to enhance the spin-orbit coupling of graphene leading to highly efficient spin-to-charge conversion (SCC) by spin Hall effect (SHE) that is predicted to be controllable by a gate voltage. Here, we report for the first time the observation of the SHE in graphene proximitized with WSe_2. By Hanle precession measurements, we quantify the spin transport and SCC parameters from 10 K up to room temperature. Exceptional for graphene/TMD devices, the sole mechanism is the SHE for all measurements and no Rashba-Edelstein effect is observable. Importantly, we are able to amplify and turn off the SCC by applying a back-gate voltage, demonstrating the long-awaited milestone of an electrically-tunable SHE. The amplified SCC shows a high efficiency, measured with an unprecedented SCC length of up to 41 nm (with a lower limit of 20 nm).

HL 65.3 Thu 11:30 CHE 89

Thermal conductivity and thermal diffusivity of suspended few-layer h-BN using modified 3ω method — •Sofia Blanter[1], Nicola Paradiso[1], Denis Kochan[2], Kenji Watanabe[3], Takashi Taniguchi[3], and Christoph Strunk[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

We present measurements of thermal conductivity and thermal diffusivity for few-layer suspended hexagonal boron nitride between 25 and 300 K. The measurements are performed on 5-13 nm thick and suspended over a length of 2-10 μm h-BN flakes using a modified version of the 3 omega method.

We generate a temperature gradient by an AC current through a metal heater. Then we measure the temperature difference and the phase shift of the AC temperature response between the heater and a thermometer a small distance away. This allows us to assess the thermal diffusivity of the flake separately from that of the substrate.

Varying the distance between the heater and thermometer, we observe that the phase shift becomes temperature independent for short distances.

HL 65.4 Thu 11:45 CHE 89

Dimensional crossover due to broken symmetry and enhanced thermoelectric performance in graphene antidot lattices — •Mustafa Neşet Çinar and Hâldun Sevinçli — Deparment of Materials Science and Engineering, Izmir Institute of Technology, 35430 Urla Izmir Turkey

Graphene antidot lattices (GALs) are monolayers with periodically placed holes in otherwise pristine graphene. We investigate the electronic properties of symmetric and symmetric GAL structures having hexagonal holes, and show that anisotropic GALs can display a dimensional crossover such that quasi-one-dimensional (Q1D) electronic structures can be realized in two-dimensional systems around the charge neutrality point. We investigate the transport and thermoelectric properties of these Q1D GALs by using non-equilibrium Green function (NEGF) method. Dimensional crossover manifests itself as transmission plateaus, a characteristic feature of Q1D systems, and enhancement of thermoelectric efficiency, where thermoelectric figure of merit, zT, can be as high as 0.9 at room temperature. We further study the transport properties in the presence of Anderson disorder and and that mean-free-paths of Q1D electrons of anisotropic configuration are much longer than those of isotropic one at the same energies.

HL 65.5 Thu 12:00 CHE 89

Electronic structure of thin topological insulator films — •Thomas Naimer, Klaus Zollner, and Jaroslav Fabian — Universität Regensburg, Deutschland

We investigate the electronic structure of thin slabs of the 3D topological insulators Bi2Se3 and Bi2Te3 by means of density functional theory. We present an extensive study of the effects of perpendicular electric fields on the topological surface states. Additionally we examine exchange proximity effects in Cr2Ge2Te6-Bi2Te3 heterostructures. We acknowledge the support of the EU Graphene Flagship program.

HL 65.6 Thu 12:15 CHE 89

Interacting two-electron states in electrostatically confined bilayer graphene quantum dots — •Angelika Knothe and Vladimir Fal'ko — National Graphene Institute, University of Manchester, Manchester M13 9PL, United Kingdom

Successfully utilizing the properties of two-dimensional materials in quantum nanostructure devices could lead to unprecedented electronics applications. We study the possible states of two interacting electrons in a quantum dot electrostatically confined in gapped bilayer graphene. The properties of the material's electronic structure, such as the three minivalleys around each valley, and the corresponding orbital magnetic moment, translate into the features of the dot states. In the weakly gapped case, the single-particle level scheme is that of an almost quadratic band, featuring a singly-degenerate ground state and angular momentum duplet degeneracies. For a sufficiently strong gap, threefold degenerate "minivalley triplets" emerge. For two electrons in the dot, the long-range part of the screened Coulomb interaction defines the orbital configuration of the interacting two-particle state. Short-range contributions breaking the symmetries on the lattice scale determine the ordering in spin and valley space. We identify the set of orbital, spin, and valley levels of the interacting two-particle states.

HL 66: Thin Oxides and Oxide Layers II (joint session DS/HL)

Time: Thursday 11:00–12:15 Location: CHE 91

HL 66.1 Thu 11:00 CHE 91

Structural, Optical and Electrical Properties of Indium Tungsten Oxide upon High Temperature Annealing — •Dorothee Menzel and Lars Korte — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium Photovoltaik, Kekulestrasse 5, 12489 Berlin, Germany

High work function metal oxides, such as tungsten oxide (WOx) have recently been investigated as charge selective p-contacts for silicon heterojunction solar cells: They provide a higher optical transparency, and due to their high work function (WF) it is expected that they can improve the cell's fill factor due to a more efficient carrier separation. However, WOx suffers from a rather poor conductivity. Indium oxide (InOx), on the other hand, has a moderate WF but a much higher conductivity. We vary the ratio of In-to-W oxide by thermal co-evaporation, spanning the full range from pure WOx to pure InOx and search for a tradeoff of high WF and high conductivity. Using in-situ (X-ray and UV) PES and surface photovoltage measurements, we found a pronounced decrease of the WF from 6.3eV for pure WOx down to 4.5eV for 40% of InOx-content in the InWOx mixture. This was accompanied by a decrease of the band bending in the c-Si substrate by 200meV [1]. Further studies focused on the material properties, such as optical, electrical and structural properties of indium tungsten oxide thin films on glass. We will discuss the changes in these properties with changing In-to-W ratio and upon high temperature annealing up to 700°C.

[1] D. Menzel et al., Appl. Phys. Lett., 112, 1-13, 2018.

HL 66.2 Thu 11:15 CHE 91

In-situ observation of sub-unit-cell nonlinear polarization in superlattices of layered oxides — •Johanna Nordlander[1], Marco Campanini[2], Marta D. Rossell[2], Manfred Fiebig[1], and Morgan Trassin[1] — [1]ETH, Zurich, Switzerland — [2]EMPA, Dübendorf, Switzerland

When approaching the 2D-limit of a material, finite size, edge or confinement effects often lead to phenomena that differ from the bulk behavior and promote novel functionalities. In materials with a layered structure, the individual sub-unit-cell layers that form their fundamental building blocks may exhibit a different symmetry, and hence different properties, than those of the parent material. For example, strong nonlinear optical properties may arise from broken inversion symmetry in fractional unit-cells of an otherwise centrosymmetric layered oxide. Here we use in-situ optical second harmonic generation (ISHG) during thin-film deposition to access these unique symmetry properties of sub-unit-cell layers in ultrathin, naturally layered hexagonal manganites. A strong nonlinear polarization directly originating from the inversion-symmetry breaking of individual half-unit-cell layers leads to a striking modulation of ISHG intensity connected to the periodic cancellation and reappearance of a non-centrosymmetric thin-film structure as each half-unit-cell layer is added during thin-film synthesis. We thus reveal the unexpectedly strong optical response of these sub-unit-cell blocks that perfectly cancel in the bulk limit. We furthermore make use of this characteristic dynamic ISHG signature to create oxide superlattices through sub-unit-cell symmetry control.

HL 66.3 Thu 11:30 CHE 91

Ellipsometric study of defect induced magnetism in spinel ferrite thin films — •Vitaly Zviagin[1], Chris Sturm[1], Pablo Esquinazi[1], Marius Grundmann[1], and Rüdiger Schmidt-Grund[1,2] — [1]Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik — [2]Now at: Technische Universität Ilmenau, Institut für Physik

We present the magnetic properties of normal spinel $ZnFe_2O_4$ (ZFO) thin films in dependence on fabrication and annealing temperature as well as atmosphere. The increase in the net magnetic response with decreasing substrate temperature correlates with the increase in cation disorder, evident by an increase in $O^{2-}2p$-$Fe^{3+}_{Td}3d$ electronic transition amplitude in the dielectric function (DF) spectra.[1] Absorption in the low energy range (∼0.9 eV) is related to an electronic transition between d orbitals of Fe^{2+} and Fe^{3+} cations and shows a strong dependence on fabrication and annealing atmosphere. Comparing the cation distribution in film bulk (optical transitions in the DF) to near-surface region (X-ray absorption), it is found that an inhomogeneous cation distribution leads to a weaker magnetic response in films of inverse configuration, whereas defects in normal spinel are likely to be found at the film surface. The presented results show that it is possible to engineer and to probe the defect distribution in the magnetic spinel ferrite film structure and to tailor their magnetic properties on demand.

[1] V. Zviagin *et al.*, Appl. Phys. Lett. **108**, 13 (2016)

HL 66.4 Thu 11:45 CHE 91

Fast sweep and voltage pulse studies on HfO_2/TiO_2- bilayer resistive switching memories — •Nils Quiring[1], Felix Cüppers[1], Alexander Hardtdegen[1], Susanne Hoffmann-Eifert[1], and Rainer Waser[1,2] — [1]PGI-7, Forschungszentrum Jülich GmbH, Germany — [2]IWE-2, RWTH Aachen University, Germany

Redox-based resistive random access memories (ReRAM) are promising contenders for future information technology applications. Compared to the respective monolayers, bilayer oxide stacks of HfO_2/TiO_2 revealed enhanced switching stability [1]. Yet, the origin of this stability is not fully understood. The inherent variability of properties such as the resistance states, switching voltages and times need further investigation.

In this study, bilayer oxide stacks of HfO_2/TiO_2 sandwiched between a Pt and a Ti electrode are electrically characterized by voltage sweep and pulse measurements. The switching behavior at different voltages, durations and signal waveform geometries with a current limitation is examined. Cells during switching are characterized with respect to cycle to cycle and device to device variability.

[1] A. Hardtdegen et al., " Improved Switching Stability and the Effect of an Internal Series Resistor in HfO_2/TiO_2 Bilayer ReRAM Cells " *IEEE TED*, vol. 65, 8, 2018, pp. 3229-3236.

HL 66.5 Thu 12:00 CHE 91

TiO_x formation during ALD metal oxide growth on Ti for resistive switches — •Ivonne Bente, Stephan Aussen, and Susanne Hoffmann-Eifert — Peter Grünberg Institut, Forschungszentrum Jülich GmbH

We studied the formation of TiO_x at the interface of Ti metal and a metal oxide film, which is grown onto the Ti layer by atomic layer deposition (ALD). For the metal oxide we investigated stoichiometric oxide films (MO) including Al_2O_3, TiO_2 and HfO_2 layers. The 25 nm thick dense Ti films are deposited on thermal oxidized Si wafers in an off-axis sputter tool with a base pressure $< 10^{-10}$ mbar. The Ti films with hexagonal crystal structure exhibit a low surface roughness. The films were transferred under ultra-high vacuum into an ALD plasma system. 2 to 3 nm thick oxide layers are deposited at 250°C using O_2-plasma as the oxygen source and standard metalo-organic precursors for the metal sources. The resulting stacks are investigated by x-ray photoelectron spectroscopy showing different Ti oxidation states (0 to 4^+) and a clear TiO_x thickness dependence on the ALD process. The switching behavior of the resulting stacks is investigated. In addition, complementary resistive switching experiments are performed on equivalent stacks, i.e. Pt/MO/TiO_x/Ti. The correlation between the XPS results and the resistive switching characteristics (pristine leakage current, electroforming voltage, etc.) is discussed.

HL 67: Frontiers in Electronic-Structure Theory - Focus on Electron-Phonon Interactions V (joint session O/HL/DS/CPP)

Time: Thursday 15:00–17:30 Location: GER 38

Invited Talk HL 67.1 Thu 15:00 GER 38

Huge quantum effects on the 250 K superconducting lanthanum hydride — •Ion Errea — University of the Basque Country, Donostia/San Sebastián, Spain

The discovery of superconductivity at 200 K in the hydrogen sulfide system at large pressures was a clear demonstration that hydrogen-rich materials can be high-temperature superconductors. The recent synthesis of LaH10 with a superconducting critical temperature (Tc) of 250 K place these materials at the verge of reaching the long-dreamed room-temperature superconductivity. Here we show that quantum atomic fluctuations stabilize in the superconducting pressure range a high-symmetry Fm-3m crystal structure consistent with experiments, which has a colossal electron-phonon coupling of 3.5. Even if ab initio classical calculations predict this structure to distort below 230 GPa yielding a complex energy landscape, the inclusion of quantum effects evidences the Fm-3m as the true ground state. The agreement between the calculated and experimental Tc values further supports this phase as responsible for the 250 K superconductivity. The relevance of quantum fluctuations questions many of the crystal structure predictions made for hydrides within a classical approach that at the moment guide the experimental quest for room-temperature superconductivity. Furthermore, quantum effects are revealed to be crucial to stabilize solids with extraordinary electron-phonon coupling, which may otherwise be destabilized by the large electron-phonon interaction, reducing the pressures needed for their synthesis.

HL 67.2 Thu 15:30 GER 38

Self-Interaction Corrected SCAN for Solids: All-Electron Implementation with Numeric Atom-Centered Basis Functions — •Sheng Bi[1], Igor Ying Zhang[2], Christian Carbogno[1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Fudan University, Shanghai, China

For all semi-local density-functional approximations (DFAs), electronic self-interaction errors lead to an erroneous description of charge-transfer processes, a systematic underestimation of band gaps in semiconductors, and incorrect total energies [1]. These errors can be alleviated via localized-orbital scaling corrections [2] or via self-interaction corrections (SIC) [3]. In this work, we have implemented a reciprocal-space formulation of self-consistent SIC in the all-electron, numeric atomic-orbitals code *FHI-aims*, which is applicable for all semi-local DFAs, including the promising meta-GGA "strongly constrained and appropriately normed" (SCAN) functional [4]. We validate our implementation by inspecting charge transfer, cohesive energies, and band gaps for a test set of molecules and solids, showing that SIC considerably improves SCAN calculations and yields results on par with standard *GW* calculations at a fraction of the computational cost. This allows us to use SCAN-SIC for studying the adsorption of organic molecules on the H-Si(111) surface.

[1] A. J. Cohen *et al.*, *Chem. Rev.* **112**, 289 (2011).
[2] N. Q. Su *et al.*, *Proc. Natl. Acad. Sci.* **115**, 9678 (2018).
[3] Z. Yan *et al.*, *Phys. Rev. A* **95**, 052505 (2017).
[4] J. Sun *et al.*, *Phys. Rev. Lett.* **115**, 036402 (2015).

HL 67.3 Thu 15:45 GER 38

Understanding the lattice dynamics of 3D hexagonal boron nitride (h-BN): beyond the LDA approach — •Luigi Cigarini, Michal Novotný, and František Karlický — Department of Physics, Faculty of Science, University of Ostrava, Czech Republic

It is fundamental to achieve a clear depiction of the lattice dynamics of 3D h-BN in order to understand the experimental outcomes. Five different stacking conformations are possible for 3D h-BN and at least two or three of them are systematically present in samples in variable amounts [1-2], resulting as a source of irreproducibility for experiments, such as the infrared optical response [3-4].

The lattice dynamics of h-BN is particularly tough to describe, stated the different nature of the forces participating in it: covalent bonds and Van der Waals interactions. The LDA approach seemed to be the most effective compromise, at the DFT level [1,5-6].

In this work we explain the surprisingly good performance of LDA. We also show that it is possible to achieve better results, in comparison with experimental IR spectra, by using, instead, the GGA approach to DFT and treating separately the two parts of the dynamical matrix. Besides, we found that IR spectroscopy is able to give some information about stacking composition. [1]. Liu, L. et al., Phys. Rev. B, 68(10), 104102 (2003). [2]. Constantinescu, G. et al., Phys. Rev. Lett., 111(3), 036104 (2013). [3]. Çamurlu, H.E. et al., Ceram. Int., 42(5), 6312-6318 (2016). [4]. Mukheem, A. et al., Nanomaterials, 9(4), 645 (2019). [5]. Cuscó, R. et al., Phys. Rev. B, 97(15), 155435 (2018). [6]. Serrano, J. et al., Phys. rev. lett., 98(9), 095503 (2007).

HL 67.4 Thu 16:00 GER 38

Error Estimation of Energy-per-Atom of Semiconductor Compounds Using Statistical Learning — •Daniel T. Speckhard[1,2], Sven Lubeck[2], Christian Carbogno[1], Luca Ghiringhelli[1], Claudia Draxl[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Humboldt-Universität zu Berlin, Institut für Physik and IRIS Adlershof, Berlin, Germany

Material databases such as NOMAD give researchers the ability to work with millions of material simulation results [1]. However, it is typically unclear to which extent calculations performed with different numerical settings and computer codes can be trusted and related to each other. This project presents statistical learning strategies to model errors in energies for two all-electron DFT codes, *FHI-aims* and **exciting**, for different basis-set sizes and **k**-point densities. Specifically, we use mutual information scores to select features that are able to capture the energy-per-atom errors. With respect to several metrics, random forest regression on the selected features shows the most promising results. This work lays the foundation for estimating errors in DFT data in NOMAD and helps to save computing resources by *a priori* predicting the DFT simulation settings required to achieve a desired level of precision. This also enables us to estimate the basis-set and **k**-point converged results of not fully converged calculations.

[1] C. Draxl and M. Scheffler, *J. Phys. Mat.*, **2** 036001 (2019). https://nomad-coe.eu

HL 67.5 Thu 16:15 GER 38

Force balance approach for advanced approximations in density functional theories — •Mary Leena Tchenkoue[1], Markus Penz[1], Iris Theophilou[1], Michael Ruggenthaler[1], and Angel Rubio[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, New York NY 10010, USA

We propose a systematic and constructive way to determine the exchange-correlation potentials of density-functional theories including vector potentials. The approach does not rely on energy or action functionals. Instead it is based on equations of motion of current quantities (force balance equations) and is feasible both in the ground-state and the time-dependent setting. This avoids, besides differentiability and causality issues, the optimized-effective-potential procedure of orbital-dependent functionals. We provide straightforward exchange-type approximations for different density functional theories that for a homogeneous system and no external vector potential reduce to the exchange-only local-density and Slater Xα approximations.

HL 67.6 Thu 16:30 GER 38

Combining embedded mean field theory with linear-scaling density functional theory — •Joseph Prentice[1,2], Robert Charlton[2], Arash Mostofi[2], and Peter Haynes[2] — [1]St Edmund Hall and Department of Materials, University of Oxford, Oxford, UK — [2]Department of Materials, Department of Physics and the Thomas Young Centre, Imperial College London, London, UK

We demonstrate the capability of embedded mean field theory (EMFT) within the linear-scaling density-functional theory code ONETEP, which enables DFT-in-DFT quantum embedding calculations on systems containing thousands of atoms at a fraction of the cost of a full calculation. We perform simulations on a wide range of systems from molecules to complex nanostructures to demonstrate the performance of our implementation with respect to accuracy and efficiency. This work paves the way for the application of this class of quantum embedding method to large-scale systems that are beyond the reach of existing implementations.

HL 67.7 Thu 16:45 GER 38

Topological semimetallic phase in PbO_2 promoted by temperature — •Bo Peng[1], Ivona Bravić[1], Judith L. MacManus-Driscoll[2], and Bartomeu Monserrat[1] — [1]Cavendish Laboratory, University of Cambridge, United Kingdom — [2]Department of Materials Science and Metallurgy, University of Cambridge, United Kingdom

Materials exhibiting topological order host exotic phenomena that could form the basis for novel developments in areas ranging from low-power electronics to quantum computers. The past decade has witnessed multiple experimental realization and thousands of predictions of topological materials. However, it has been determined that increasing temperature destroys topological order, restricting many topological materials to very low temperatures and thus hampering practical applications. Here, we propose the first material realization of temperature promoted topological order. We show that a semiconducting oxide that has been widely used in lead-acid batteries, β-PbO_2, hosts a topological semimetallic phase driven by both thermal expansion and electron-phonon coupling upon increasing temperature. We identify the interplay between the quasi-two-dimensional nature of the charge distribution of the valence band with the three-dimensional nature of the charge distribution of the conduction band as the microscopic mechanism driving this unconventional temperature dependence. Thus, we propose a general principle to search for and design novel topological materials whose topological order is stabilized by increasing temperature. This provides a clear roadmap for taking topological materials from the laboratory to technological devices.

HL 67.8 Thu 17:00 GER 38

How Electric Fields Affect Intermolecular van der Waals Interactions — •Mohammad Reza Karimpour, Dmitry Fedorov, and Alexandre Tkatchenko — University of Luxembourg, 1511 Luxembourg, Luxembourg

van der Waals (vdW) dispersion interactions between atoms or molecules originate from electromagnetic forces caused by the zero-point quantum-mechanical fluctuations of electronic charge densities. They are ubiquitous in nature and present in many areas of physics, chemistry, biology, and nanotechnology. Recently, it has been shown that the strength of vdW interactions can be controlled and tailored by external electric charges [1]. In addition, an external field strongly modifies the dispersion interaction between two hydrogen atoms and can change both its spatial dependence and its attractive or repulsive character [2]. To describe such important phenomena in large molecular systems, we employ the Many-Body Dispersion (MBD) method [3] based on the quantum Drude oscillator model. Since the conventional MBD method includes only dipole-dipole coupling, it does not capture the effects of external fields on vdW interactions. Therefore, we first extend the approach to dipole-quadrupole and quadrupole-quadrupole couplings. Then, the developed formalism is applied to calculate the MBD energy in the presence of an external electric field for low-dimensional systems including bilayer graphene.

[1] Kleshchonok and Tkatchenko, Nat. Commun. **9**, 3017 (2018)
[2] Fiscelli *et al.* arXiv:1909.03517 (2019)
[3] Tkatchenko *et al.* Phys. Rev. Lett. **108**, 236402 (2012)

HL 67.9 Thu 17:15 GER 38

Electronic structure of β-SiAlON: effect of Al/O doping and of finite temperature — •Saleem Ayaz Khan[1], Ondrej Šipr[2], Jiří Vackář[2], Robin Niklaus[3], Wolfgang Schnick[3], and Jan Minár[1] — [1]University of West Bohemia, Plzen, Czech Republic — [2]Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic — [3]LMU Munich, Germany

Electronic structure of a series of ordered and disordered β-Si_{6-z}Al_{z}O_{z}N_{8-z} systems is investigated by means of ab initio calculations, using the FLAPW method as implemented in the wien2k code and Green function KKR method as implemented in the SPR-KKR code. Finite temperature effects are included within the alloy analogy model. We found that the trends with the Al/O doping are similar for ordered and disordered structures. The electronic band gap decreases with increasing z by about 1 eV when going from z=0 to z=2. The optical gap decreases analogously as the electronic band gap. The changes in the density of states (DOS) at Si and N atoms introduced by doping β-Si_{3}N_{4} with Al and O are comparable to the DOS at Al and O atoms themselves. The bottom of the conduction band in β-Si_{6-z}Al_{z}O_{z}N_{8-z} is formed by extended states residing on all atomic types. Increasing the temperature leads to a shift of the bottom of the conduction band to lower energies. The amount of this shift increases with increasing doping z.

HL 68: Nitrides: Preparation and characterization II

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

HL 68.1 Thu 15:00 POT 112

Impact of high free-carrier concentrations on optical properties of cubic GaN — •Elias Baron[1], Rüdiger Goldhahn[1], Michael Deppe[2], Donat J. As[2], and Martin Feneberg[1] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Germany — [2]Department Physik, Universität Paderborn, Germany

The zincblende III-nitrides are possible candidates for replacing the wurtzite phase nitrides in certain applications such as quantum-dot-based devices. Despite their metastable nature, several improvements concerning control and quality have been reported. Free-electron concentrations n above $10^{20}\mathrm{cm}^{-3}$ are achievable by using Ge as a donor in zincblende GaN and AlGaN. We present a characterization of thin film zincblende GaN, deposited by plasma-assisted molecular beam epitaxy on 3C-SiC/Si substrates in (001) orientation. The complex dielectric functions (DF) in the mid-infrared are obtained by spectroscopic ellipsometry, from which the transverse-optical phonon and plasma frequencies are determined. These results are corroborated by Raman experiments. Utilizing Kane's model for the band structure in the vicinity of the Γ-point of the Brillouin zone, taking into account many-body effects like band-gap renormalization and Burstein-Moss shift, and the optical effectice electron mass determined by the plasma frequency, an all-optical determination of the free-carrier concentration of zincblende GaN is achieved.

HL 68.2 Thu 15:15 POT 112

Absolute internal quantum efficiency of GaInN/GaN quantum wells under steady state conditions — •Savutjan Sidik[1], Philipp Henning[1,2], Philipp Horenburg[1], Heiko Bremers[1,2], Uwe Rossow[1], and Andreas Hangleiter[1,2] — [1]Institut für Angewandte Physik, Technische Universität Braunschweig — [2]Laboratory for Emerging Nanometrology, Technische Universität Braunschweig

An accurate determination of the internal quantum efficiency (IQE) is essential in optimizing the efficiency of GaInN/GaN quantum wells (QWs). A common approach to determine the IQE from temperature-dependent photoluminescence (PL) measurements is based on the assumption that the IQE is 100 % at low temperature. The temperature-dependent integrated PL intensity is normalized to the different incident laser power levels, then normalizing the normalized PL intensity to the maximum value for each temperature and power density gives the IQE. Recently, we have been able to verify this assumption for selected samples using time-resolved PL measurements. In this contribution, we compare samples with known and unknown low-temperature IQE based on their absolute low-temerature PL intensity under otherwise identical conditions. On the one hand, this allows a verification of the 100 % cases. On the other hand, the absolute low-temperature IQE can be assessed by such a comparison for arbitrary samples.

HL 68.3 Thu 15:30 POT 112

Size-effect of donors on the lattice parameters of wurtzite GaN — •Elias Kluth, Karsten Lange, Matthias Wienecke, Jürgen Bläsing, Hartmut Witte, Armin Dadgar, Rüdiger Goldhahn, and Martin Feneberg — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Germany

We present experimental results on the size effect of the donors Si and Ge in wurtzite GaN. Thin film samples grown by metal-organic vapour phase epitaxy on sapphire with $(11\bar{2}0)$ surfaces were investigated by Hall-effect, high resolution x-ray diffraction, high resolution Raman spectroscopy, and infrared spectroscopic ellipsometry experiments. Phonons and lattice parameters were determined and systematic shifts as a function of carrier and donor concentrations were found. Several contributions are considered: i) epitaxial strain due to epitaxy on foreign substrates, ii) influence of electrons on the lattice parame-

ters, iii) the effect of donor ions on the surrounding GaN matrix which is the so called "size-effect". By comparing GaN:Si with GaN:Ge but similar carrier concentrations, we are able to distangle the different contributions. We report quantitative results of the size-effect of Ge and Si in GaN and phonon deformation potentials for several phonon modes.

HL 68.4 Thu 15:45 POT 112

Electronic properties of $ZnSi_{1-x-y}Ge_xSn_yN_2$ semiconductors — •Masako Ogura, Dan Han, Monika Pointner, Laura Junkers, and Hubert Ebert — Ludwig-Maximilians-University Munich, Munich, Germany

Heterovalent ternary nitrides $Zn(Si,Ge,Sn)N_2$ have a great potential for application in optoelectronics and photovoltaics. We have investigated the mixed crystal system $ZnSi_{1-x-y}Ge_xSn_yN_2$ by means of first-principles electronic structure calculations using the Korringa-Kohn-Rostoker (KKR) Green's function method in combination with the coherent potential approximation (CPA) alloy theory.

Concerning the band gap, good agreement with available experimental data could be achieved by means of the modified Becke-Johnson exchange functional. Calculating the Bloch spectral functions as a function of energy and k-vector allowed to determine the finite lifetime of electron and hole states as well as the corresponding effective masses for the conduction and valence bands, respectively. In addition, representative results for X-ray absorption and emission spectra for the 1s-state of N will be presented.

HL 68.5 Thu 16:00 POT 112

Thermally activated spreading resistance of Si- and Ge-doped lattice matched GaN/InAlN periodic stacks — •Hartmut Witte[1], Cleophace Seneza[1], Prabha Sana[2], Christoph Berger[1], Armin Dadgar[1], and André Strittmatter[1] — [1]Institute of Physics, Otto-von-Guericke-University Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany — [2]Fraunhofer Institute for Microstructure of Materials and Systems IMWS, Walter-Huelse-Strasse 1, 06120 Halle, Germany

Si- or Ge-doped lattice-matched GaN/InAlN periodic stack structures were grown by MOVPE for applications as photonic band gap layers in the n-type region of GaN blue laser structures. For electrical transport measurements, mesa structures were realized with ohmic contacts on the bottom and the top of the stack. Besides the sheet resistance, a spreading resistance is observed depending on the contact geometry. Both IV- and CV-characteristics show rectifying behavior at low free electron concentrations and strong ohmic behavior at high electron concentrations. Temperature-dependent Hall- effect measurements verify metallic conduction associated with degenerately doped semiconductors. Contact arrangements for which a higher spreading resistance is found show an opposite temperature dependence of the resistance in IV- measurements. A defect assisted current mechanism via extended defects or the GaN/InAlN interfaces could be presented and will be investigated using CV- and thermal admittance spectroscopy. Kelvin probe microscopy and conductive atomic force microscopy will be employed to analyze surface-related electrical conduction.

HL 68.6 Thu 16:15 POT 112

100% quantum efficiency in III-nitride quantum wells at low temperatures: experimental verification by time-resolved photoluminescence — •Philipp Henning, Savutjan Sidik, Philipp Horenburg, Heiko Bremers, Uwe Rossow, and Andreas Hangleiter — Institut für Angewandte Physik & Laboratory for Emerging Nanometrology, Technische Universität Braunschweig, 38106 Braunschweig, Germany

Using time-resolved photoluminescence (PL) measurements, we present an experimental verification for 100% internal quantum efficiency (IQE) of III-N quantum wells at low temperatures. Conventional IQE measurements, such as temperature- and power-dependent PL, require a low-temperature normalization, where usually an IQE of 100% is assumed. This assumption neglects remaining nonradiative recombination processes, such as tunneling to nonradiative centers, that may be present even at low temperatures. From time-resolved PL measurements, charge carrier lifetimes for radiative and nonradiative recombination can be evaluated separately. We state that the low-temperature IQE corresponds to 100%, whenever the effective charge carrier decay is dominated only by radiative recombination. In this case, the temperature-dependent measurements show a synchronous rise of the effective lifetimes together with the radiative lifetimes, since only the radiative lifetime increases with temperature in a 2D system, while nonradiative processes are thermally activated. Thereby, absolute IQE measurements become possible, since we provide a robust indicator for nonradiative recombination at low temperatures.

HL 68.7 Thu 16:30 POT 112

V-groove patterning of 3C-SiC/Si(001) substrates for cubic GaN epitaxy — •Mario Littmann, Dirk Reuter, and Donat J. As — Universität Paderborn, Department Physik, Warburger Straße 100, 33098 Paderborn

Meta-stable cubic GaN (c-GaN) can be grown by molecular beam epitaxy on 3C-SiC/Si(001) substrates. However, the high lattice mismatch results in many crystal defects. A possible solution to reduce the amount of defects is the pre-pattering of the substrate. In previous works, it was reported that it is possible to create defect-free c-GaN inside a V-shaped groove with an opening angle of 70°. In this case, the walls of the groove match the {111}-facets of the cubic crystal.
In this work, we developed a lithography and etching procedure to create V-shaped grooves inside a 3C-SiC substrate. Electron-beam lithography is applied to create a structure with a width of 100 nm. Reactive-ion etching (RIE) is used to etch a V-shaped groove into the substrate. The RIE process is based on Sulfur hexafluoride to ensure a high lateral etch rate. Scanning electron microscopy (SEM) reveals that the walls are formed by {111}-facets of the cubic crystal. In addition, the first attempts to grow c-GaN on the pre-patterned substrates are discussed. The crystal quality is investigated by high-resolution X-ray diffraction and photoluminescence spectroscopy. The structures are further analyzed by SEM and atomic force microscopy.

HL 69: Quantum dots and wires III

Time: Thursday 15:00–18:00 Location: POT 151

Invited Talk HL 69.1 Thu 15:00 POT 151

Scaling networks of compound semiconductor nanowires — •Anna Fontcuberta i Morral — Ecole Polytechnique Fédérale de Lausanne, EPFL

Nanowires are filamentary crystals with a tailored diameter between few and 100 nm [1,2]. Their shape anisotropy and size confer them with advantageous properties in a variety of areas ranging from photonics to quantum computing [3-6]. In all applications, deterministic site selective growth of nanowires is absolutely necessary. In this talk we will explain how nanowires can be obtained in arrays both free standing and lying on a substrate, in a scalable manner. We will also show how the properties such as enhanced light absorption and mobility can be engineered, opening the path to advanced functionality.

[1] P. McIntyre, A. Fontcuberta i Morral, Materials Today Nano https://doi.org/10.1016/j.mtnano.2019.100058 [2] L. Güniat et al, Chemical reviews 119, 8958-8971 (2019) [3] P. Krogstrup et al, Nature Photon. 7, 306 (2013) [4] R. Frederiksen et al, ACS Photon. 4, 2235-2241 (2017) [5] M. Friedl et al, Nano Lett. 18, 2666 (2018) [6] J. Vukajlovic-Plestina, Nature Comm. 10, 869 (2019)

HL 69.2 Thu 15:30 POT 151

Ultra-doped Germanium nanowires using ion implantation and flash-lamp anneling — •Ahmad Echresh, Mao Wang, Yufang Xie, Slawomir Prucnal, Yordan M. Georgiev, and Lars Rebohle — Helmholtz Zentrum Dresden Rossendorf, Dresden, Germany

Germanium (Ge) is a promising high mobility channel material for future nanoelectronics. Materials with high carrier mobility can enable increased integrated circuit functionality or reduced power consumption. Hence, Ge based nanoelectronic devices could offer improved performance at reduced power consumption compared to Si electronics. In this work, Germanium-on-insulator (GeOI) substrates were doped with phosphorous (P) using ion beam implantation followed by flash lamp annealing (FLA). During FLA, the implanted layer recrystallized and P was electrically activated. Then, Ge nanowires were fabricated

using electron beam lithography and inductively coupled plasma etching. Raman spectra showed amorphisation of the Ge structure after implantation and good recovery after FLA. Rutherford backscattering spectrometry measurements were used to verify the crystal quality of Ge layer before and after FLA. Moreover, Hall effect measurement configuration is designed for single Ge nanowires to determine the carrier mobility and carrier concentration. The results of these measurements will be shown at the conference. The goal is to fabricate a p-n junction along the Ge nanowires and use them as infrared sensors.

HL 69.3 Thu 15:45 POT 151

Electrical Characterisation of Te-doped InAs Nanowires — •Anton Faustmann[1], Pujitha Perla[1,3], Detlev Grützmacher[1,2,3], Mihail Lepsa[2,3], and Thomas Schäpers[1,3] — [1]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Peter Grünberg Institute (PGI-10), Forschungszentrum Jülich, 52425 Jülich, Germany — [3]JARA-Fundamentals of Future Information Technology (JARA-FIT), Jülich-Aachen Research Alliance, Germany

InAs features high electron mobility and absence of a Schottky barrier at metal interfaces enabling ohmic contacts. In combination with large g-factor and high Rashba spin-orbit coupling this makes InAs nanowires a promising candidate for research of quantum effects.

InAs nanowires with Te doping grown by molecular beam epitaxy were investigated in terms of their electrical transport properties at both room and cryogenic temperatures. The nanowires were grown in a catalyst-free vapour-solid process without using Au droplets. In contrast to Si, which shows amphoteric behaviour, Te acts as n-type dopant. It furthermore offers the possibility of an increased overall doping level. The Te doping concentration was found to affect both the morphology of the nanowires as well as electrical properties. The shape of the nanowires depends on Te uptake. Their intrinsic as well as contact resistances decrease considerably at increased doping level. Field-effect measurements using a global back gate show great effect on the conductance, however no complete pinch-off was observable with conductance saturating at high negative gate voltages. Resistances were found to be only slightly increased at cryogenic temperatures.

HL 69.4 Thu 16:00 POT 151

Polar optical phonons' splitting in nanowires — •Norma Rivano[1], Thibault Sohier[1,2], and Nicola Marzari[1] — [1]Theory and Simulation of Materials (THEOS) and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — [2]nanomat/QMAT/CESAM and European Theoretical Spectroscopy Facility, Université de Liège, Belgium

The need for an accurate description of the vibrational properties of 1D materials is strongly motivated by the growing interest in low-dimensionality in general and semiconductor nanowires in particular. Dimensionality has been shown to have an important impact on materials' properties, thus being crucial for both fundamental understanding and technological applications. At small momenta, longitudinal and transverse polar-optical modes are known to undergo a frequency splitting which depends upon the phonon wave-vector, the effective charges, the dielectric properties and the dimensionality of the system. Indeed, in the long-wavelength limit, the amount of electrostatic energy built up by the longitudinal polar-optical phonons is finite in 3D, but it vanishes in 2D. Here, we show that it also vanishes in 1D, but with a different asymptotic behavior. We also discuss the role of the nanowire's radius, which is particularly relevant for characterization through Raman spectroscopy. To this aim, we develop an analytical model and compare it with ab-initio simulations. We provide insights into the vibrational physics of nanowires as well as a ready-to-use tool for the experimental community to encourage further studies.

30 min. break.

HL 69.5 Thu 16:45 POT 151

Fluorescence spectral diffusion of single type-II semiconductor ZnSe/CdS dot-in-rod nanostructures at room and cryogenic temperatures — •Hans Werners, Sven-Hendrik Lohmann, Christian Strelow, Alf Mews, and Tobias Kipp — Institut für Physikalische Chemie, Universität Hamburg, Grindelallee 117, 20146 Hamburg, Germany

In this work, we investigate type-II dot-in-rods, where the intrinsic band offset leads to a spatial separation of the electron and hole wavefunctions. Fluorescence measurements at room temperatures of our ZnSe/CdS DRs show a monoexponential decay and an emission energy that can be assigned to an interface recombination between an electron in the shell and a hole in the core. The ensemble fluorescence lifetimes exceeds 100 ns at room temperature. We use confocal fluorescence spectroscopy at cryogenic temperatures and observe abrupt spectral shiftings of the emission line over time, superimposed on smoother spectral diffusion processes. The spectral diffusion covers a larger range in energy than for type-I CdSe/CdS DRs [1], indicating the larger susceptibility of type-II structures to external stimuli, like surface charges. At cryogenic temperatures, we measure shorter fluorescence lifetimes compared to room temperature measurements. We observe a biexponential decay and the fluorescence lifetime-intensity distribution (FLID) suggest stable trion emission at low temperatures. To further analyze the temperature dependency of the charge carrier dynamics, we use time resolved transient absorption measurements.

[1] Lohmann et al., ACS Nano 11, 12185-12192 (2017)

HL 69.6 Thu 17:00 POT 151

Monolithic co-integration of III-V compound semiconductors on silicon using a multiple step relaxation technique — •Ramasubramanian Balasbramanian[1], Vitalii Sichkovskyi[1], Johann Peter Reithmaier[1], Larisa Popilevsky[2], Gadi Eisenstein[2], Galit Atiya[3], and Yaron Kauffmann[3] — [1]University of Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germnany — [2]Russel Berrie nanotechnology Institute, Technion, Haifa 32000, Israel — [3]Material Science and Engineering Dep., Technion, Haifa 32000, Israel

Monolithic co-integration of III-V compound semiconductors on Si intends to combine advantages of both materials in a single chip. Si possesses excellent electronic, thermal and mechanical properties, whereas III-V materials exhibit excellent photonic properties due to their direct band gap. Development of defects, due to the differences in thermal expansion coefficient and lattice constants between III-V materials and Si, are filtered using Dislocation Filtering Layers (DFLs) which are either strained layer super lattices or highly strained QDs. Here, we report on the integration of InP and GaAs on 5° off-cut Si wafers by MBE using DFLs. The grown structures are characterized using high resolution transmission electron microscopy (HRTEM), atomic force microscopy and photo luminescence (PL) spectroscopy. HRTEM studies showed an efficient dislocation reduction by DFLs. The InP based laser structure grown on top of such DFL buffer showed PL properties comparable to the reference one grown directly on InP . RWG lasers are being processed and results will be discussed during the conference.

HL 69.7 Thu 17:15 POT 151

Fabrication and Characterization of Reconfigurable Field Effect Transistors — •Muhammad Bilal Khan, Sayantan Ghosh, Slawomir Prucnal, René Hübner, Artur Erbe, and Yordan M. Georgiev — Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

To complement scaling down of CMOS, new device concepts have been introduced. These concepts include undoped silicon nanowire (SiNW) based reconfigurable field effect transistors (RFETs). In an RFET, SiNWs are nickel silicided at both ends. This results in silicide-Si-silicide Schottky junctions. Two distinct gate electrodes are placed on these junctions. By controlling the electrostatic potential on the gate electrodes, the RFET is programmed to p- or n-polarity. We report on fabrication and electrical characterization of top-down fabricated SiNW based RFETs. Flash lamp annealing is used for silicidation instead of rapid thermal annealing for better control over the silicidation process. Different gate dielectrics are used to improve the device performance.

HL 69.8 Thu 17:30 POT 151

Influence of UiO-66 Metal-Organic Framework Synthesis on contacted Carbon Nanotubes — •Marvin J. Dzinnik[1], Benedikt B. Brechtken[1], Hendrik A. Schulze[2], Peter Behrens[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstraße 2, 30167 Hannover, Germany — [2]Institut für Anorganische Chemie, Leibniz Universität Hannover, Callinstrasse 9, 30167 Hannover, Germany

Carbon Nanotubes (CNT) and metal-organic framework (MOF) hybrid materials are candidates for novel sensors [1]. While in previous experiments MOFs were synthesized on carbon nanotube networks [1] we are presenting measurements on individual multi-walled CNTs with UiO-66 MOFs.

We show the electronic properties of CNT samples before and after the MOF synthesis. DC-transport measurements were used in order to investigate the change in conductivity due to the MOF synthesis. The measured conductance decreased by a factor of 30. The electrical properties of the CNTs after the synthesis show Tomonaga-Luttinger liquid behavior indicating that the carbon nanotube still behaves as a one-dimensional system. In a further experiment a MOF between a contact and the CNT was used as a dielectric medium in a transistor setup. A positive gate voltage leads to a lower conductance of the CNT showing the gate action.

[1] H. A. Schulze et al., ChemNanoMat, 5, 1159-1169, (2019).

HL 69.9 Thu 17:45 POT 151

Shell-filling and spin-valley coupling in gate-defined BLG quantum dots — Luca Banszerus[1,2], •Samuel Möller[1], Eike Icking[1], Christian Volk[1], Kenji Watanabe[3], Takashi Taniguchi[3], and Christoph Stampfer[1,2] — [1]2.Physikalisches Institut A, RWTH Aachen University, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, Germany — [3]National Institute for Materials Science,1-1 Namiki, Tsukuba, 305-0044, Japan

We present a gate-defined single quantum dot in electrostatically gapped bilayer graphene with full occupational control up to the first electron. Quantum dot states are examined by applying perpendicular and in-plane magnetic fields to the sample at low and high bias, allowing to extract addition energies and g-factors. We obtain the electron g-factor of 2 and valley g-factors in the order of 30, depending on the orbital state. Each orbital state (shell) is occupied four times due to the spin and valley degrees of freedom in graphene. Single particle states are found sufficient to describe the ground state (excited states) of the quantum dot up to occupations of 12(8) electrons. The order of states in which electrons enter the quantum dot is extracted and found to be constant across shells. Remarkably, we find the fourfold degeneracy at zero magnetic field is lifted. Instead, two pairs each with two states of opposite spin and valley form. We denote this phenomenon to an effective spin-valley coupling of 0.5 meV.

HL 70: Spin phenomena in semiconductors

Time: Thursday 15:00–16:45 Location: POT 251

HL 70.1 Thu 15:00 POT 251

Spin noise spectroscopy for nuclear relaxation dynamics in InGaAs epilayer — •Clara Rittmann, Aleksandr Kamenskii, Alex Greilich, and Manfred Bayer — Experimentelle Physik II, Technische Universität Dortmund, 44221 Dortmund, Germany

We study the dynamic nuclear spin polarization in Indium Gallium Arsenide (InGaAs) epilayer under the circular excitation using a spin noise spectroscopy. The sample consists of a 10μm thick epitaxial layer of n-doped InGaAs with 3% of Indium, grown on a GaAs substrate. First, we characterize the unperturbed spin dynamics of resident electrons using the spin noise technique. It allows us to determine the spin relaxation time and the g-factor of the electron system. Further, we discover that an additional off-resonant circular excitation has a strong effect on the Larmor precession of the electron spins, without affecting the spin noise amplitude. This is related to the dynamic nuclear polarization by the optically oriented spins, which in their turn are affected by the induced Overhauser field, produced by the nuclear system. Finally, we study the common time evolution of the electron-nuclear system detecting the spin noise of the residual electrons.

HL 70.2 Thu 15:15 POT 251

High-throughput computational discovery of $In_2Mn_2O_7$ as a high Curie temperature ferromagnetic semiconductor for spintronics — •Wei Chen[1], Janine George[1], Joel B. Varley[2], Gian-Marco Rignanese[1], and Geoffroy Hautier[1] — [1]Institute of Condensed Matter and Nanoscicence (IMCN), Université catholique de Louvain, Louvain-la-Neuve 1348, Belgium — [2]Lawrence Livermore National Laboratory, Livermore, California 94550, USA

Robust ferromagnetism and attractive semiconducting properties are critical for achieving highly spin-polarized transport in spintronic devices, yet combining the two requirements in one material remains an open problem. Here we conduct a search for concentrated ferromagnetic semiconductors through high-throughput computational screening of over 40000 known compounds. Among the very few identified ferromagnetic semiconductors, we show that the manganese pyrochlore oxide $In_2Mn_2O_7$, hitherto unknown to spintronic applications, is particularly promising for spin transport as it combines a low electron effective mass (0.29 m_0), a large exchange splitting of the conduction band (1.1 eV), good stability in air, and a Curie temperature (130 K) among the highest of concentrated ferromagnetic semiconductors. We rationalize the high performance of $In_2Mn_2O_7$ by the unique hybridization among O-2p, Mn-3d, and In-5s states. We further find that Sn and Mo can be effectively incorporated on the In site while acting as shallow donors, indicative of n-type dopability.

HL 70.3 Thu 15:30 POT 251

Spatial and temporal evolution of electron spins in [110] **grown GaAs quantum wells** — •Karl Schiller, Sergiu Anghel, and Markus Betz — Experimentelle Physik 2, Technische Universität Dortmund, Otto-Hahn-Straße 4a, 44227 Dortmund, Germany

Spin-orbit interaction (SOI) is a key mechanism in manipulating electron spins in non-centrosymmetric semiconductor heterostructures and can be understood in terms of an effective magnetic field B_{eff} acting on the moving electrons. At the same time, the SOI can serve as a source of dephasing (D'yakonov-Perel mechanism), as the precession frequency becomes dependent on the electron trajectory. However, this mechanism is suppressed in [110] quantum wells (QWs) for spins aligned along the same direction as the B_{eff} and, consequently, long spin lifetimes can be achieved [1].

We have investigated spatial and temporal evolution of optically injected spin distributions for QWs with different thicknesses. For that, we have used non-degenerate and time-resolved magneto-optic Kerr rotation microscopy. The output of a mode-locked Ti:Sapphire oscillator is split into circularly polarized pump pulse at 1.57 eV, which excites a spin distribution, and linear polarized probe pulse to detect it, with its energy depending on the QW thickness. We have observed pronounced anisotropic spin diffusion between the [001] and [1$\bar{1}$0] directions for QW thicknesses of 20 nm, 14 nm and 9.6 nm.

[1] Y. Ohno et al., Phys. Rev. Lett. **83**, 4196 (1999)

HL 70.4 Thu 15:45 POT 251

Extended electron spin dephasing in isotopically purified ZnSe — •Phillip A. Greve[1], Evgeny A. Zhukov[1], Erik Kirstein[1], Nataliia Kopteva[2], Irina A. Yugova[1,3], Alexander Pawlis[4], Dimitri R. Yakovlev[1,5], Alexander Greilich[1], and Manfred Bayer[1] — [1]Experimentelle Physik Technische Universität Dortmund 44221 Dortmund Germany — [2]Spin Optics Laboratory, St. Petersburg State University, Ul'anovskaya 1, Peterhof, St. Petersburg 198504, Russia — [3]Physical Faculty of St. Petersburg State University, 198504 St. Petersburg, Russia — [4]Department Physik, Universität Paderborn, 33098 Paderborn, Germany — [5]Ioffe Physical-Technical Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia

We demonstrate a very long spin dephasing time of electrons bound to defect centers in fluorine-doped isotopically purified ZnSe epilayer. The sample was implanted with fluorine after the MBE growth, which led to a broad defect band of high PL intensity about 0.5 eV under the free exciton transition of ZnSe. Using a time-resolved pump-probe Kerr rotation technique, we were able to measure a dephasing time over 300 ns at cryogenic temperatures. The g factor of 2 indicates a strong localization of electrons. The state characteristics and dependencies on temperature, magnetic field, and sample structure are discussed.

HL 70.5 Thu 16:00 POT 251

Absence of giant Rashba effect in the valence band of CsPbBr3 — •Maryam Sajedi[1,2], Maxim Krivenkov[1,2], Dmitry Marchenko[1], Andrei Varykhalov[1], Jaime Sánchez-Barriga[1], and Oliver Rader[1] — [1]Helmholtz Zentrum Berlin für Materialien und Energie, Albert Einstein Str 15, D-12489, Berlin, Germany — [2]Department of physics, Potsdam University, Am Neuen Palais 10, D-14415, Potsdam Germany

We have employed spin- and angle-resolved photoemission spectroscopy of CsPbBr3 single crystal to verify the presence of Rashba

spin-orbit coupling effect in the highest lying occupied state. We uncover the entire three-dimensional Brillouin zone (BZ) momentum-space, and the dispersion of the topmost bulk valence band (VB) at high symmetry R-point. We use density functional theory (DFT) calculations to compare the ground state electronic structure of the particular perovskite compound with corresponding dispersive bands from photoemission (PES) experiments. By direct experimental evidence from the results of spin-resolved band structure experiments, we exclude a large Rashba effect in the global valence band maximum (VBM) at R-point of bulk BZ.

HL 70.6 Thu 16:15 POT 251

Single-shot spin readout of a spin qubit in silicon measured using a neural network — •Tom Struck[1], Javed Lindner[1], Arne Hollman[1], Floyd Schauer[2], Dominique Bougeard[2], and Lars Schreiber[1] — [1]JARA-FIT Institute Quantum Information, RWTH Aachen University, Germany — [2]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Regensburg, Germany

Spin qubits have proven to be a promising candidate for quantum computing, with the field advancing quickly in recent years. One challenge is the fast and reliable qubit state detection. A popular method used for single-shot read-out of an electron spin qubit is spin-selective tunnelling [1,2] combined with charge readout by a single electron transistor (SET). Depending on the qubit's spin state, the SET senses an approx. 60 pA current rise with a statistically distributed timing. Reliable and fast interpretation of the current trace is particularly challenging. Here we compare the traditional current threshold analysis with current trace classification by a neural network. This spin-state classifier is highly noise resilient, allowing a decrease in measurement time by a factor of five. The calculation time per trace is only 30 μs, rendering the implementation of fast-feedback loops possible. [1] J. M. Elzerman et al., Nature 430, 431 (2004) [2] Arne Hollman et al. arXiv:1907.04146v1

HL 70.7 Thu 16:30 POT 251

Spin relaxation induced by valley-orbit coupling in a single Si quantum dot — •Amin Hosseinkhani and Guido Burkard — Department of Physics, University of Konstanz, Germany

The spin of isolated electrons in Silicon quantum dot heterostructures is a promising candidate for quantum information processing. While silicon offers weak spin-orbit coupling and nuclear-spin free isotopes, the valley degree of freedom in silicon couples to spin and can degrade the qubit performance by opening a relaxation channel. We build on the effective mass theory and find exact solutions for the envelope function of a single quantum dot along the applied electric field. We take into account a few miscuts at the Si/barrier interface and study how the wavefunction evolves in the magnetic field. We then obtain the valley phase and splitting for a single quantum dot spin qubit as a function of the applied magnetic and electric field. These enable us to develop the theory of spin-relaxation induced by valley-orbit coupling. We show that it is important to consider all four physical spin-valley states into the qubit logical states in order to describe the qubit relaxation.

HL 71: Focus Session: Tailored Nonlinear Photonics II

The research field of nonlinear photonics is driven by the tailoring and control of nonlinear light-matter interactions and by the application of nonlinear concepts for advanced light management. Current research activities are driven by concepts from quantum optics, coherent optics, and solid-state physics. The progress in the field strongly benefits from advanced solid-state materials, nanostructures, and photonic structures, as well as from extremely intense and efficient ps and fs laser sources. The application of new concepts paves technically viable routes towards advanced nonlinear photonic devices, which are indispensable for the implementation of efficient frequency conversion, conditional photonic functionalities, and photonic quantum technologies.

Organizers: Artur Zrenner (Universität Paderborn), Thomas Zentgraf (Universität Paderborn) and Manfred Bayer (TU Dortmund)

Time: Thursday 15:00–17:15 Location: POT 51

Invited Talk HL 71.1 Thu 15:00 POT 51

Quadratic nanomaterials for nonlinear integrated photonic devices — •Rachel Grange — ETH Zurich, Department of Physics, Institute for Quantum Electronics, Zurich, Switzerland

Nonlinear optics is present in our daily life with many applications, e.g. light sources for microsurgery or green laser pointer. All of them use bulk materials such as glass fibres or crystals. Generating nonlinear effects from materials at the nanoscale can expand the applications to integrated devices. However, nonlinear signals scale with the volume of a material. Therefore, finding nanostructured materials with high nonlinearities to avoid using high power and large interaction length is challenging. Here I will show several strategies to maximize nonlinear optical signals in nano-oxides with noncentrosymmetric crystalline structure and semiconductors. I will demonstrate how we enhance second-harmonic generation by using the scattering properties of individual barium titanate nanoparticles, and III-V standing nanodisks. Our results suggest that a strong increase of the nonlinear signal can be obtained without using plasmonics or hybrid nanostructures.

Then, I will present innovative fabrication approaches of metal-oxides materials that are very different from standard semiconductors or metals. First, solution-processing of nano-oxides may solve, at the same time, the low nonlinear signal and the low throughput of photonic crystal cavity fabrication to obtain cost-effective disposable devices. Second, we also developed lithography processes to obtain lithium niobate nanowaveguides or metasurfaces.

Invited Talk HL 71.2 Thu 15:30 POT 51

Resonant nanostructured surfaces for parametric frequency conversion — •Frank Setzpfandt — Institute of Applied Physics, Abbe Center of Photonics, Friedrich-Schiller-Universität Jena

Metasurfaces composed of high-refractive-index nanoparticles supporting electric and magnetic Mie-type resonances offer unique opportunities for controlling the properties of transmitted or reflected light. Recent technological advances furthermore enabled the fabrication of Mie-resonant nanoparticles from materials with strong second-order nonlinearity, like gallium arsenide and lithium niobate. Metasurfaces based on these materials are a versatile platform for efficient nonlinear frequency conversion using parametric three-wave mixing, e.g. by second-harmonic or sum-frequency generation. They enable control of emission direction and polarization of the nonlinearly generated light through the geometry of the nanoparticles. I will discuss our recent advances in understanding and controlling nonlinear frequency conversion in dielectric metasurfaces made from gallium arsenide and lithium niobate, which feature very different nonlinear properties. Alternatively, efficient frequency conversion is also possible using strong material resonances e.g. in 2D transition metal dichalcogenides, where the nonlinear susceptibility can be notably increased in the vicinity of the resonance. I will demonstrate that nanostructuring transition metal dichalcogenides also enables spatial control of second-harmonic light generated in the 2D material, without using Mie resonances.

HL 71.3 Thu 16:00 POT 51

Optimizing the single-photon emission from a quantum-dot biexciton based on a direct two-photon transition — Tom Praschan[1], •Dirk Heinze[1], Artur Zrenner[1], Andrea Walther[2], and Stefan Schumacher[1,3] — [1]Department of Physics and Center for Optoelectronics and Photonics Paderborn (CeOPP), Paderborn University, Warburger Strasse 100, 33098 Paderborn, Ger-

many — [2]Department of Mathematics, Humboldt-Universität zu Berlin, Unter den Linden 6, 10099 Berlin, Germany — [3]College of Optical Sciences, University of Arizona, Tucson, Arizona 85721, USA

Semiconductor quantum dots are excellent candidates for on-demand single photon sources. A partly stimulated party spontaneous two-photon process from the biexciton state to the ground state of the quantum dot makes it possible to tailor the properties of the emitted single photon all-optically with a laser pulse [1,2]. An optimized and complex control pulse can steer the emission process into the desired emission path [3]. Here, we optimize the pulse parameters numerically to trigger the direct two-photon process with its maximum emission probability. We include phonon assisted processes [4] near the quantum dot resonances into our theoretical analysis and calculate single photon properties. Considering an emission into a high-Q cavity we find that on-demand single photon emission is possible for realistic parameters. [1] D. Heinze et al. Nat. Commun. 6, 8473 (2015). [2] D. Breddermann et al. Phys. Rev. B 94, 165310 (2016). [3] D. Breddermann et al. Phys. Rev. B, 97,125303 (2018). [4] D. Heinze et al. Phys. Rev. B, 95, 245306 (2017).

HL 71.4 Thu 16:15 POT 51

ZnO-based dielectric nanoantennas for nonlinear applications — •Christian Golla, Nils Weber, Sophia Thies, Thomas Zentgraf, and Cedrik Meier — Department Physik, Universität Paderborn, 33098 Paderborn, Germany

Boosting nonlinear optical effects like second and third harmonic generation on the nanoscale is a subject of many theoretical and experimental studies. Here, plasmonic nanoantennas play an important role due to their capability of enhancing local electric fields and thus increasing the efficiency of nonlinear processes. However, intrinsic losses caused by metals limit the efficiency of such devices especially in the visible regime. In this context, nanostructures made of dielectric materials emerged as complementary candidates to plasmonic systems in recent years. These structures allow the confinement and magnification of electric and magnetic fields to subwavelength volumes based on Mie resonances. Due to the low absorption compared to metals they are considered as an alternative to overcome the limitations of plasmonic structures. In our work, zinc oxide based nanoantennas on sapphire substrates are investigated. Not only enhancement of the generation of second and third harmonic light but also the realization of a metasurface in the linear regime are demonstrated. Furthermore, preliminary results for combining the nonlinear character and the metasurface are shown.

HL 71.5 Thu 16:30 POT 51

Indirect optical transitions induced by a refractive index front — Mahmoud Gaafar[1,2], Hagen Renner[1], Manfred Eich[1,3], and •Alexander Petrov[1,4] — [1]Institute of Optical and Electronic Materials, Hamburg University of Technology, Hamburg, Germany — [2]Department of Physics, Menoufia University, Menoufia, Egypt — [3]Institute of Materials Research, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — [4]ITMO University, St. Petersburg, Russia

Refractive index fronts in dispersive waveguides can lead to indirect transition of light where frequency and wavenumber is changed. At the new position on the dispersion relation light might have strong change of the group velocity. Adjusting the front velocity and dispersion relation, reflection, transmission and trapping by the front are possible. We experimentally implement the free carrier front in silicon waveguides by the two photon absorption of the pump pulse and show all three effects. In case of trapping, also known as optical push broom effect, the light is trapped in the front and strongly compressed in time and space. Also transitions to zero group velocity are possible to stop and store optical pulses. We will make an overview of the possible front induced transitions and provide the outlook for the further research.

HL 71.6 Thu 16:45 POT 51

Acoustically induced bistability switching and memory effect in confined exciton-polariton condensates — •Alexander Kuznetsov, Klaus Biermann, and Paulo Santos — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

Bistability is a remarkable and useful property of nonlinear exciton-polariton (EP) quasiparticles. In this work, we demonstrate the switching of trapped EPs between bistable states by 0.4 GHz acoustic strain pulses. A microsecond-long strain pulse, piezoelectrically generated on-demand, triggers the bosonic stimulation (Bose-Einstein-like condensation) from an initial state below the condensation threshold to the final state above the threshold, i.e., the bistability switching. The system remains in this final state for as long as the optical pump is supplied (recorded time up to 15 minutes). Thus, the reported effect is a novel concept for an on-chip optical memory with electro-acoustic triggering based on confined EP condensates.

HL 71.7 Thu 17:00 POT 51

Second Harmonic Generation on excitons and magnon-sideband in the antiferromagnet Cr_2O_3 — •Johannes Mund[1], Victor V. Pavlov[2], Roman V. Pisarev[2], Dmitri R. Yakovlev[1,2], and Manfred Bayer[1,2] — [1]Experimentelle Physik 2, Technische Universität Dortmund, Germany — [2]Ioffe Institute, Russian Academy of Sciences, St. Petersburg, Russia

We present results of optical second harmonic generation (SHG) in Cr_2O_3 on Frenkel excitons formed by $^4A_1$-^2E states of Cr^{3+} ions in the near infrared range $1.7 - 1.78$ eV. As was shown in previous work [1], the electric-dipole SHG is allowed in Cr_2O_3 due to its particular antiferromagnetic ordering below $T_N = 307.5$ K. In addition, it was possible to image the antiferromagnetic domains in a Cr_2O_3 sample by SHG [2]. We investigated detailed SHG polarization dependencies for linearly and circularly polarized light of the exciton states using femtosecond laser pulses. In magnetic field B, applied parallel and perpendicular to the sample optical c-axis, further information on exciton symmetries and optical selection rules were obtained. Moreover, in our spectra, we succeed for the first time to observe SHG signals on the exciton-magnon-sideband.

[1] M. Fiebig et al. PRL 73, 2127 (1994)
[2] M. Fiebig et al. Appl. Phys. Lett 66, 2906 (1995)

HL 72: Focus Session: Functional Metal Oxides for Novel Applications and Devices III (joint session HL/DS)

electronics, power electronics, high-electron-mobility transisitors, memristors, topological quantum computation and so on. These functionalities typically require homo- or heteroepitaxial layers of high crystallinity with bendable amorphous semiconducting oxides as an exception. This session sets a focus on growth of bulk and thin films, experimental and theoretical investigation of their physical properties as well as fabrication and characterization of demonstrator devices.

Organizers: Oliver Bierwagen (Paul-Drude-Institut für Festkörperelektronik, Berlin), Holger Eisele (TU Berlin), Jutta Schwarzkopf (Leibniz-Institut für Kristallzüchtung, Berlin) and Holger von Wenckstern (Universität Leipzig).

Time: Thursday 15:00–16:30 Location: POT 81

HL 72.1 Thu 15:00 POT 81

Ab-initio investigation of first-order Raman scattering in gallium oxide — •Rouven Koch, Pasquale Pavone, Dmitrii Nabok, and Claudia Draxl — Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, Germany

In this work, we investigate the Raman tensors and first-order spectra of the β and α phase of Ga_2O_3 by means of first-principles calculations using the *ab-initio* methodology implemented in the software package

`exciting` [1]. We start from the determination of the equilibrium crystal structure of both polymorphs. Then, we explore the lattice dynamics of the two phases, paying special attention to the characterization of the phonons at the Γ point. The peculiar properties of the polar phonon modes of the β phase are addressed, including the LO-TO splitting and reflectivity spectra. Then, we compute the frequency-dependent dielectric tensors within the random-phase approximation. The lattice-dynamical properties and the dielectric tensors are used for the calculation of the Raman spectra in different polarizations. The obtained polarized Raman spectra for α- and β-Ga_2O_3 are compared to available data in the literature [2]. Our results highlight the fact that excitonic effects do not play a significant role on off-resonance Raman spectra. The overall good agreement with the experiments indicates the accuracy of the approximations used in this calculation.

[1] A. Gulans *et al.*, J. Phys.: Condens. Matter **26** (2014) 363202;
[2] C. Kranert *et al.*, Scientific Reports **6** (2016) 35964.

HL 72.2 Thu 15:15 POT 81

Raman-Spectroscopy of corundum-like α-Ga_2O_3 grown by HVPE — •Jona Grümbel[1], Pingfan Ning[1,3], Jürgen Bläsing[1], Dae-Woo Jeon[2], Martin Feneberg[1], and Rüdiger Goldhahn[1] — [1]Otto-von-Guericke-Universität Magdeburg — [2]Korean Institute of ceramic Engineering and Technology, Seoul, South Korea — [3]School of Electronics and Information Engineering, Tiangong University, China

Ga_2O_3 is a high-bandgap semiconductor, whose stable β-phase is already applicable to semiconductor power devices like FETs and Schottky-Diodes. The metastable, corundum-like α-phase is less discussed, but allows bandgap-engineering by alloying with α-Al_2O_3 (sapphire) or α-In_2O_3.

Here, we investigate the lattice vibrations in the context of crystal quality. Therefore, three different samples grown by three different variations of HVPE (halide vapor phase epitaxy) are investigated. For the characterization of phonon modes, Raman Spectroscopy is employed.

All seven Raman-active phonon modes are identified in different Raman setup configurations. We investigate the correlation of phonon energies and lattice parameters as determined by x-ray diffraction. A small but detectable influence of phonon deformation potentials is found. Moreover, we find a very pronounced influence of crystal quality - as witnessed by ω-scan relative amplitudes - on certain Raman-active phonon modes which might be used as marker for ample quality.

HL 72.3 Thu 15:30 POT 81

Raman spectroscopy as a tool to determine the Néel temperature of NiO thin films in correlation with their structural characteristics — •Johannes Feldl, Melanie Budde, Carsten Tschammer, Oliver Bierwagen, and Manfred Ramsteiner — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e. V., Hausvogteiplatz 5–7, 10117 Berlin, Germany

NiO is one of the most common natural antiferromagnetic (AF) oxides and a transparent p-type semiconductor making this material interesting for both, applications in the fields of spintronics and transparent-oxide electronics. One of the crucial magnetic parameters of AF materials is the Néel temperature (T_N). For thin epitaxial films of NiO, T_N will depend on the growth conditions and their resulting structural properties and is therefore expected to deviate from the value of 523 K for bulk NiO. Here, we utilize Raman spectroscopy to study the magnetic and structural properties of NiO thin films. The films are grown on MgO(100) substrates by plasma-assisted molecular beam epitaxy at different substrate temperatures. For the assessment of the structural properties, Raman scattering by optical phonons is analysed. Regarding the experimental determination of T_N, we demonstrate a reliable approach by analyzing the temperature dependence of the two-magnon (2M) peak in the Raman spectra. The obtained T_N values are below 480 K and are found to be correlated with the in-plane strain and the degree of lattice disorder in the NiO films.

HL 72.4 Thu 15:45 POT 81

Phonons and free-carrier contributions of spinel $ZnGa_2O_4$ by spectroscopic ellipsometry — •Alwin Wüthrich[1], Martin Feneberg[1], Zbigniew Galazka[2], and Rüdiger Goldhahn[1] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Germany — [2]Leibniz Institute for Crystal Growth, Berlin, Germany

Ga based spinels with the general formula of $MeGa_2O_4$, where Me is a divalent metal, such as $MgGa_2O_4$ or $ZnGa_2O_4$ offer an ultra wide band gap and good electrical conductivity. These transparent semiconducting oxides (TSOs) have been receiving greater interest in the last years due to an outstanding importance in a wide range of scientific disciplines, such as photoelectronics, sensing systems or optical applications. Here, bulk $ZnGa_2O_4$ single crystals were grown directly from the melt by the vertical gradient freeze (VGF) method. This study presents a characterisation of these bulk crystals by spectroscopic ellipsometry, from which the complex dielectric function (DF) was deduced. Free-carrier concentrations (n) up to 10^{19} cm^{-3} were investigated in the infrared spectral range, where the phonons and plasmons were determined. The former agrees well to prior theoretical and experimental studies while from the latter the dependence of the effective electron mass on n is achieved, indicating a non-parabolicity of the conductive band.

HL 72.5 Thu 16:00 POT 81

Electric and Thermoelectric Properties of $ZnGa_2O_4$ Bulk Crystals — •Johannes Boy[1], Martin Handwerg[1], Rüdiger Mitdank[1], Zbigniew Galazka[2], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin, Germany — [2]Leibniz Institute for Crystal Growth, Max-Born-Strasse 2, 12489 Berlin, Germany

In the past years, intense research has been done in the field of oxide semiconductor materials, which are promising candidates for the design of novel high power devices, optoelectronics and sensing systems due to their wide bandgap. $ZnGa_2O_4$ is a transparent material of blue coloration, with a high bandgap E_g=4.6 eV at room temperature [1]. The majority charge carrier type is n-type. Electron mobilities up to 100 cm^2/Vs with charge carrier concentrations in the order of 10^{18} - 10^{19} cm^{-3} have been reported [1]. In this work, we manufactured microlabs on the chip [2] to investigate the temperature dependence of the Seebeck coefficient S, Hall charge carrier density n and mobility μ between T = 10 K and T = 320 K. At high bath temperatures $T > 230K$, the scattering is determined by electron-phonon-interaction. At low bath temperatures (between 10 and 150 K) we observe a temperature-independent maximum, which can be explained by electrons interacting with ionized impurities. The room temperature Seebeck coefficient is $S_{(300K)} = (-120 \pm 3)$ μV/K and decreases with decreasing bath temperature.[1] Z. Galazka, *et al.*; APL Materials **7**, 022512 (2019).
[2] J. Boy, *et al.*; APL Materials **7**, 022526 (2019).

HL 72.6 Thu 16:15 POT 81

Low-frequency noise characterization of MOCVD-grown β-Gallium Oxide — •Christian Golz[1], Günter Wagner[2], Saud Bin Anooz[2], Zbigniew Galazka[2], Andreas Popp[2], Fariba Hatami[1], and W. Ted Masselink[1] — [1]Department of Physics, Humboldt-Universität zu Berlin, Newton-Str. 15, D-12489 Berlin, Germany — [2]Leibniz Institute for Crystal Growth, Max-Born-Str. 2, 12489 Berlin, Germany

Low-frequency noise spectroscopy was used to characterize defects and trap states in β-Ga_2O_3 epilayers. These high-quality Si-doped layers were homoepitaxially grown by metal-organic chemical vapour deposition (MOCVD)[1] on insulating Mg-doped β-Ga_2O_3 substrates prepared from bulk crystals obtained by the Czochralski method [2].

For noise measurements, lithographically defined Greek cross mesa structures were etched using hot H_3PO_4. Ohmic Ti/Au contacts were processed by e-beam evaporation. Generation-recombination noise, thermal noise, and 1/f noise are well resolved. Measured Hooge parameter values between 10^{-5} and 10^{-3} indicate a high structural quality of the epilayer. Generation-recombination noise was analyzed between 80 K and 400 K, finding up to three deep trap levels. Each of these deep traps is characterized in terms of their density, thermal activation energy, capture cross section prefactor, and binding energy.

[1] R. Schewski et al., APL Mater. 7, 022515 (2019); [2] Z. Galazka et al., ECS J. Solid State Sci. Technol. 6, Q3007 (2017)

HL 73: Semiconductor Surfaces (joint session O/HL)

Time: Thursday 15:00–17:30 Location: REC C 213

HL 73.1 Thu 15:00 REC C 213

Time-resolved reflection anisotropy spectroscopy reveals the impact of surface non-idealities for water adsorption on GaP — •Matthias M. May[1], Helena Stange[1], Jonas Weinrich[2], Thomas Hannappel[3], and Oliver Supplie[3,4] — [1]Helmholtz-Zentrum Berlin, Germany — [2]Ferdinand-Braun-Institut, Berlin, Germany — [3]Technische Universität Ilmenau, Germany — [4]Humboldt-Universität zu Berlin, Germany

The initial interaction of water with semiconductor surfaces typically leads to surface chemical reactions, which determine the electronic structure of the solid–liquid interface as well as stability against corrosion. Access to this interface to reveal the nature of the interaction is, however, challenging. Here, we study gallium phosphide-based (100) surfaces exposed to H_2O by means of time-resolved reflection anisotropy spectroscopy during water adsorption in vacuum [1]. We show that the introduction of imperfections in the form of surface steps via substrate off-cut variation or trace contaminants not only changes the dynamics of the interaction, but also its qualitative nature. While the clean surface without steps does not show any presence of oxygen after several 10 kL of exposure at room temperature, this changes with the introduction of trace carbon or a substrate off-cut. The decay rate of the surface optical anisotropy allows us to estimate activation energies of the surface reactions. Our findings emphasise the challenges for the comparability of experiments with idealised electronic structure models.

[1] May et al., *SciPost Physics* **6**, 058 (2019).

HL 73.2 Thu 15:15 REC C 213

Ion-Induced Surface Nanostructures of Germanium(001) — •Ricardo de Schultz, Denise Erb, and Stefan Facsko — Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstraße 400, 01328 Dresden, Germany

Ion beam irradiation can lead to various self-organized surface nanopatterns depending on the irradiation conditions and the sample material. In this case, the surface patterns of Ge(001), which evolve during high-fluence 1 keV ion irradiation with Ar^+ ions at elevated temperatures, have been studied. Whereas at room temperature the semiconductor surface would become amorphous during ion irradiation, high temperatures enhance the diffusion so that bulk vacancies and interstitials can recombine before the next ion hits the same surface region. Thus the surface stays crystalline. This results in a biased surface diffusion because of the Ehrlich-Schwoebel barrier at step edges and kinks.

The periodic surface patterns that emerge on Ge(001) reflect the four-fold symmetry of the crystalline surface. These patterns consist of a checkerboard of inward and outward oriented pyramids. For normal ion incidence their bases are square and oriented along the <100> crystal direction. For two different azimuthal ion incidence angles - along <110> and <100> - the emerging patterns have been examined for different polar incidence angles and compared to simulations. These indicate that the height gradient dependent sputter erosion plays an important role during pattern formation.

HL 73.3 Thu 15:30 REC C 213

Structural and Electronic Properties of the FeSi(110) Surface — •Biao Yang[1], Martin Uphoff[1], Yi-Qi Zhang[1], Joachim Reichert[1], Ari P. Seitsonen[2], Andreas Bauer[3], Christian Pfleiderer[3], and Johannes V. Barth[1] — [1]Physics Department E20, Technical University of Munich, D-85748 Garching, Germany — [2]Département de Chimie, École Normale Supréieure, 24 rue Lhomond, F-75005 Paris, France — [3]Physics Department E51, Technical University of Munich, D-85748 Garching, Germany

Iron silicide (FeSi) is a fascinating material which has attracted numerous research efforts for decades.[1] It has B20 crystal structure featuring cubic unit cell without an inversion center. To gain insight into the unusual surface properties of this system, we successfully prepare the atomically flat FeSi(110) surface with the Ar ion sputtering and annealing treatment. By scanning tunneling microscopy (STM), we clearly resolve a step-terrace topography and the details of the atomic lattice. The atomically resolved STM images and DFT calculations give strong indications for the surface termination, where the topmost comprises of one Fe and one Si atom. Furthermore, a small energy gap of 80 meV close to the Fermi level is derived by scanning tunneling spectroscopy (STS). Intriguingly, two in-gap states are identified for the first time. References 1. V. Jaccarino, G. K. Wertheim, J. H. Wernick, L. R. Walker, S. Arajs. Phys. Rev. 1967, 160, 476.

HL 73.4 Thu 15:45 REC C 213

Detection of stress hormone cortisol in saliva using silicon nanowire field effect transistors with a portable measurement system — •Stephanie Klinghammer[1], Nadia Licciardello[1], Tetiana Voitsekhivska[2], Clemens Kirschbaum[3], Larysa Baraban[1], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf e.V., Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany — [3]3Department of Psychology, TU Dresden, 01062 Dresden Germany

The accurate and rapid detection of various targets from patients on portable point-of-care devices is attracting great attention in bio- and nanotechnology for more than a decade [1]. Here, we demonstrate a portable, label-free and real-time sensing platform based on silicon nanowire field effect transistors which is capable for detection of several small molecules [2]. We particularly focus on the sensitive recognition of the stress hormone cortisol by using aptamers as receptors in order to allow high sensitive screenings in physiological conditions. We show the working principle by determination of cortisol levels in saliva of volunteers and compared to levels obtained with conventional ELISA method.

References: [1] Patolsky F, Zheng G, Lieber CM. 2006. Nanomed. 1(1):51*65 [2] Voitsekhivska T, Suthau E, Wolter K-J. 2014. in IEEE. 173-178

Invited Talk HL 73.5 Thu 16:00 REC C 213

Coupling of electronic and atomic degrees of freedom in surface-stabilized quasi-1D systems — •Wolf Gero Schmidt — Lehrstuhl für Theoretische Physik, Universität Paderborn

Minute structural changes may lead to drastic modifications of the electronic properties of quasi-1D systems, while, on the other hand, an electronic charge redistribution, induced, e.g., by optical excitations or surface vibrations may induce pronounced structural modifications in such systems. This is illustrated in my talk using two prominent examples: (i) Localized photoholes at the Brillouin zone boundary of the In/Si(111)(8x2) nanowire system are shown to drive an ultrafast (8x2) $\longrightarrow$ (4x1) phase transitions that is accompanied by the formation of metallic In-In bonds along the wire direction [1,2]. (ii) A Si $sp^3 \longrightarrow sp^2+p$ rehybridization accompanied by a lateral surface charge transfer is demonstrated to destabilize the Si(553)-Au spin chains [3] with respect to a diamagnetic surface ground state that complies with electron counting heuristics [4]. Thermal excitation leads to soft Au chain vibrations that alter transiently the Au electron affinity and eventually the hybridization of the Si step edge atoms.

[1] T Frigge et al., Nature 544, 207 (2017).
[2] CW Nicholson et al., Science 362, 821 (2018).
[3] SC Erwin, FJ Himpsel, Nat. Commun. 1, 58 (2010).
[4] C Braun et al., PRB 98, 121402(R) (2018).

HL 73.6 Thu 16:30 REC C 213

Determining surface phase diagrams including anharmonic effects — •Yuanyuan Zhou, Matthias Scheffler, and Luca M. Ghringhelli — Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin-Dahlem, Germany

A prerequisite for analyzing and understanding the electronic properties and the function of surfaces is the detailed knowledge of their structure under realistic conditions. We have developed a replica-exchange grand-canonical (REGC) algorithm that enables the unbiased calculation of pressure-temperature phase diagrams of surfaces or clusters in reactive atmospheres including anharmonic effects. [1] Moreover, the multi-canonical sampling yields the temperature-pressure dependence (map) of all equilibrium observables that can be measured within the given model Hamiltonian. For instance, structural parameters such as the radial distribution function, or the HOMO-LUMO gap. This allows for rational design, where *operando* condition are taking fully

into account. Our approach is demonstrated by studying Si clusters and the Si(100) surface in a hydrogen atmosphere, by coupling REGC with *ab initio* molecular dynamics. All interactions are described at the density-functional-theory level, with the Perdew-Burke-Ernzerhof gradient-corrected exchange-correlation functional. In particular, we show how to determine *observable structures* at finite temperature and pressure, i.e., obtained by ensemble averaging the sampled structures. [1] Y. Zhou, M. Scheffler, and L. M. Ghringhelli, Phys. Rev. B. 100, 174106 (2019).

HL 73.7 Thu 16:45 REC C 213

Doping-induced metal-insulator transition in Au atomic wires — •Zamin Mamiyev[1], Simone Sanna[2], Christoph Tegenkamp[1], and Herbert Pfnür[1] — [1]Appelstrasse 2 Institut für Festkörperphysik, Leibniz Universität Hannover, Hannover, Germany — [2]Institut für Theoretische Physik, Justus-Liebig- Universität Gießen

Close coupling between structural and electronic parameters has been demonstrated in the past for arrays of quasi one-dimensional Au chains on Si surfaces. Here we employ plasmon spectroscopy and LEED to study electronic and structural modifications as a result of surplus Au concentrations, x, starting at 0.48 ML on Si(553) and at 0.65 ML on Si(111). For the Si(111)-Au surface an abrupt metal-insulator transition (MIT) was observed by adding more than 0.05 ML Au. In contrast, the Si(553)-Au surface shows a rather gradual decrease of plasmon frequency up to x= 0.1 ML. Moreover, self-doping with Au on Si(553)-Au improves the chain quality up to x=0.03 ML, resulting also in an increase of plasmon intensity. Further addition of Au at room temperature leads to a vanishing plasmon frequency, coupled with the disappearance of the ×2 periodicity. By annealing the doped samples at 630°C the Au atoms form small clusters with $(\sqrt{3}\times\sqrt{3})$R30° symmetry, while the metallicity of the Au chains is fully recovered, but the structural imperfections in the chains as well. The appearance of $\sqrt{3}$-order indicates local restructuring into larger terraces and their spatial separation from the Au-chains. This proves that not only the amount of dopant but also its distribution is important for reversible MIT on such surfaces. These findings were corroborated by DFT calculations.

HL 73.8 Thu 17:00 REC C 213

Selective Excitation of Amplitude Modes Driving the In/Si(111) Peierls Transition — •Hannes Böckmann-Clemens, Jan Gerrit Horstmann, and Claus Ropers — 4th Physical Institute, Solids and Nanostructures, University of Göttingen, Göttingen 37077,Germany

The use of laser pulses to actively steer a system along the transition pathway from a reactant towards a desired product state is a fundamental scheme in the field of femtochemistry. Transferring this concept to solid-state surface systems requires the ultrafast manipulation of coherent phonons, associated with the reaction coordinate. Here, we demonstrate the mode-selective vibrational control over the Peierls metal-to-insulator phase transition of In/Si(111) by means of tailored pulse sequences. We explore the potential energy surface spanned by the amplitude modes of the system via selection of specific pathways along the transition path. We identify two essential modes, identify their separate roles in controlling the transition, and carry out experiments with mode-selective excitation.

HL 73.9 Thu 17:15 REC C 213

Novel electronic junctions in an atomic wire array: metallic states, charge density waves and solitonic excitations — •Abdus Samad Razzaq[1], Sun Kyu Song[2], Han Woong Yeom[2], and Stefan Wippermann[1] — [1]Max-Planck-Institut für Eisenforschung, Germany — [2]Pohang University, South Korea

The Si(111)-(4x1)In atomic wire array is an extremely popular model for one-dimensional (1D) electronic systems. It features a reversible, temperature-induced metal insulator transition into a charge density wave (CDW) ordered ground state with (8x2) translational symmetry. Close to the phase transition temperature, both phases can coexist and form novel types of electronic junctions between the metallic (4x1) phase and the insulating CDW-ordered (8x2) phase. Furthermore, the CDW phase is 4-fold degenerate, giving rise to solitonic excitations of the CDW, that take the form of phase boundaries between different CDW ground states. Combining scanning tunnelling microscopy (STM) and ab initio molecular dynamics (AIMD) calculations, we explore the microscopic structures of interfaces between distinct electronic phases at the atomic scale. These models enable insights into soliton propagation and soliton-mediated charge transport. Financial support from the German Research Foundation (DFG), grant no. FOR1700, and BMBF NanoMatFutur, grant no. 13N12972, is gratefully acknowledged.

HL 74: Poster IIIA

This poster session includes contributions from the following topic:

- 2D semiconductors and van der Waals heterostructures

Please put up your poster at the beginning of the session and remove the poster immediately after the session. The person peresenting the poster should attend it for at least half of the session duration and indicate the time when to find him/her at the poster.

Time: Thursday 15:00–17:30 Location: P2/2OG

HL 74.1 Thu 15:00 P2/2OG

Radiation-modulation of mono-layer MoSe2 nano emitters by LSPs — •Yuhao Zhang and Stefan Linden — Physikalisches Institut, Universität Bonn

Nano emitters based on transition metal dichalcogenide (TMDC) monolayers is considered as a potential resource for nano-photonic technologies. It is necessary to develop methods to optimize the radiation of this kind of nano emitters. Localized surface plasmons (LSPs) is considered as one of the best choice due to it is a no- propagation method and it is convenient to be controlled. Here, we produced MoSe2 monolayers by mechanical exfoliation, and then the monolayers are transferred to plasmonic nanoantennas by PDMS stamps. In order to change the resonance of LSPs that they produced, the sizes of the nanoantennas are changed from 100 nm to 400 nm. Then the radiation of the nano emitters coupled to different resonance LSPs are measured by a PL microscope. The result shows that the radiation of mono-layer MoSe2 nano emitters is modulated by the resonance of LSPs. When the LSP is resonance with radiation of the nano emitters, the radiation is enhanced 1.5 times compared to the monolayers on the glass substrate. With the resonance of LSPs is off, the radiation of nano emitters descend continuously until they are near-resonance with high-order LSPs. Our results agree well with the FEM simulations. This effect provides an efficient tool to optimize the radiation of TMDC nano emitters.

HL 74.2 Thu 15:00 P2/2OG

Theory of near-field optics in transition metal dichalcogenides — •Robert Salzwedel, Andreas Knorr, and Malte Selig — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

In recent years transition metal dichalcogenides (TMDCs) attracted much attention due to their strong Coulomb and light matter interaction leading to tightly bound excitons with large optical oscillator strength. Due to their finite thickness, those excitons have been shown to be very sensitive to their environment, for instance to a change in their dielectric surrounding [1] or the deposition of a self assembled layer of molecules [2].

Here we present a microscopic theory which is based on a self consistent solution of Maxwell and Bloch equations to study phenomena which are associated with the nearby environment of the TMDC layer, for instance the trapping of excitons by external molecules placed on top of the layer. As an outlook, our approach also allows the description of the launch of in-plane exciton-polaritons and their propagation

through the layer.

[1] P. Steinleitner et al., Nano Lett.18, 1402 (2018)
[2] M. Feierabend et al., Nat. Commun. 8, 14776 (2017)

HL 74.3 Thu 15:00 P2/2OG

Direct Measurement of the Radiative Pattern of Exciton Complexes in a Tungsten Diselenide Monolayer — •Lorenz Maximilian Schneider[1], Shanece S. Esdaille[2], Daniel A. Rhodes[2], Katayun Barmak[3], James C. Hone[2], and Arash Rahimi-Iman[1] — [1]Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, Marburg, 35032, Germany — [2]Department of Mechanical Engineering, Columbia University, New York, NY 10027, USA — [3]Department of Applied Physics and Applied Math, Columbia University, New York, NY 10027, USA

Due to the extraordinary high Coulomb interaction found in monolayers of transition-metal dichalcogenides, not only the binding energies of higher-order excitonic complexes are in the tens of meV's but also their fine structure is considerable, arising from the short- and long-range part of the Coulomb exchange integral. Such strong electronic interaction also leads to the hybridization of dark excitonic states into one dipole-allowed for z-polarization but spin-forbidden exciton branch, referred to as "grey" exciton, and another one that is both spin and dipole forbidden. While there have been some indirect measurement reports revealing the presence of the grey z-polarized exciton mode, no direct measurement of the radiation pattern has been performed. Here, we present an investigation of a high-quality h-BN encapsulated monolayer, where angle resolved spectroscopy has been used to directly reveal and extract the radiation pattern of bright and grey excitons. The in-plane and out-of-plane dipole modes can indeed be directly identified by their emission under low and high emission angles.

HL 74.4 Thu 15:00 P2/2OG

Microwave Studies of Graphene/hBN Heterostructures — •Vincent Strenzke[1], Udai Singh[1], Marta Prada[2], Lars Tiemann[1], and Robert Blick[1] — [1]Center for Hybrid Nanostructures, Universität Hamburg, Hamburg, Germany — [2]I. Institute for Theoretical Physics, Universität Hamburg, Hamburg, Germany

Recently, it has been revealed that the band structure of monolayer graphene exhibits a small band gap in the range of tenth of μeV that results from intrinsic spin orbit interaction. Such low energies can be probed in magnetotransport experiments at cryogenic temperatures, by employing a resistively detected microwave resonance method. In this work, graphene was combined with hexagonal boron nitride (hBN), i.e., a two-dimensional material which is a superior substrate for high-quality electronics as compared to silicon substrates. In these graphene/hBN heterostructures, we observed additional features in the microwave resonance spectrum, signalling additional interactions and phenomena. For further fundamental studies on the properties of two-dimensional van der Waals materials, it will be interesting to employ this method on e.g. bilayer graphene or transition metal dichalcogenide heterostructures with a controlled stacking order.

HL 74.5 Thu 15:00 P2/2OG

Magnetic resonance studies of spin defects in a Van der Waals crystal — •Matthias Diez[1], Andreas Gottscholl[1], Christian Kasper[1], Victor Soltamov[1], Andreas Sperlich[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Spin defects in wide-bandgap semiconductors have shown to be promising systems in terms of realising quantum information processing, quantum sensing and quantum computing. While spin centers in 3D materials especially the NV-center in diamond or silicon vacancy in silicon carbide have been extensively studied, similar defects in 2D materials are yet to be discovered. In this work, we use optically detected magnetic resonance (ODMR) and electron paramagnetic resonance (EPR) to study a recently found spin defect in irradiated hexagonal boron nitride (hBN) in more details [1]. In particular, we identified the defect to be a negatively charged boron vacancy (V_B^-) and determined the parameters of its spin Hamiltonian by analyzing the temperature, illumination and angular dependencies. The defect has a triplet ground state (S=1) with a zero field splitting of $\approx$ 3.5 GHz. These results stimulate the search also for other types of spin defects in 2D materials and heterostructures.

[1] Gottscholl et al., arXiv:1906.03774 (2019)

HL 74.6 Thu 15:00 P2/2OG

Probing spin-valley polarization dynamics in $MoSe_2$/WSe_2 heterostructures — •Michael Kempf[1], Florian Raab[2], Markus Schwemmer[2], Andreas Hanninger[2], Philipp Nagler[2], Christian Schüller[2], and Tobias Korn[1] — [1]Institute of Physics, University of Rostock, Rostock, Germany — [2]Institute of Physics, University of Regensburg, Germany

Transition metal dichalcogenides (TMDC) have revealed many intriguing properties in recent years. For valleytronics especially, the coupling of spin and valley degree of freedom shows great promise. Combined with valley-selective optical selection rules, a chosen spin polarization can easily be introduced into these systems. Keeping possible future applications in mind, a long spin polarization lifetime is of great importance, yet in pristine monolayer TMDC this is strongly limited due to ultrafast exciton recombination and electron-hole exchange. Through two-color time-resolved Kerr rotation and ellipticity measurements we are able to study the spin-valley dynamics in n-doped $MoSe_2$ and compare it to the undoped case. Here we observe a drastic lifetime increase from the order of pico to nanoseconds, significantly exceeding the lifetimes of excitons and trions. This can be attributed to a transfer of spin polarization to resident carriers [1]. Following a similar reasoning we investigate two-dimensional $MoSe_2$/WSe_2 heterostructures, electrons and holes are spatially separated. This in turn suppresses their radiative recombination as well as exchange interaction thus leading to an increase of spin polarization lifetime.

[1] M. Schwemmer et al. Appl. Phys. Lett. 111, 082404 (2017).

HL 74.7 Thu 15:00 P2/2OG

Diffusion of dark excitons in monolayer WSe_2 at cryogenic temperatures — •Koloman Wagner[1], Jonas Zipfel[1], Jonas D. Ziegler[1], Edith Wietek[1], Barbara Meisinger[1], Takashi Taniguchi[2], Kenji Watanabe[2], and Alexey Chernikov[1] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]National Institute for Materials Science, Tsukuba, Ibaraki, Japan

Exciton propagation is studied in hBN-encapsulated WSe_2 at liquid helium temperature through spatially- and time-resolved photoluminescence microscopy. To monitor diffusion we detect signatures from phonon-assisted recombination of low-energy, inter-valley dark exciton states. At low excitation densities we find efficient diffusion that appears to be intrinsically limited by exciton scattering with linear acoustic phonons in WSe_2. These observations highlight the negligible role of localization through residual disorder and support the assignment of the studied spectral features to originate from free exciton states. At higher densities we detect an effective increase of the diffusion coefficient with distinct signatures of bimolecular recombination, qualitatively similar to the observations at room temperature.

HL 74.8 Thu 15:00 P2/2OG

Time-resolved Faraday Rotation on single-layer MoSe2 — •Simon Raiber[1], Gabriela Hirschinger[1], Matthias Dietl[1], Tobias Korn[2], and Christian Schüller[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg — [2]Institut für Physik, Universität Rostock

For an atomically thin layer of MoSe2, a direct band gap emerges at the K points of the hexagonal Brillouin zone. The broken inversion symmetry of the crystal structure gives rise to chiral selection rules, allowing to create a valley polarization. Faraday rotation is sensitive to spin and hence can give direct access to the valley polarization.

We have performed time-resolved Faraday rotation experiments with a femtosecond time resolution on an exfoliated MoSe2 single-layer sample at low temperatures. Measuring the total carrier life time and taking into account direct radiative recombination, dephasing via intervalley exchange interaction and exciton-phonon relaxation processes, we can give a detailed view on the evolution of the valley polarization and determine the corresponding decay times. In the presence of out-of-plane magnetic fields of up to 8 Tesla, it was possible to generate a valley polarization that is independent of the helicity of the incident light. We find that the valley life times exhibit a pronounced magnetic field dependence.

HL 74.9 Thu 15:00 P2/2OG

Photoluminescence monitoring during laser-thinning of transition metal dichalcogenides — •Christian Tessarek, Oleg Gridenco, Kathrin Sebald, Stephan Figge, Jürgen Gutowski, and Martin Eickhoff — Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, D-28359 Bremen, Germany

Laser-thinning is a promising tool for processing of two-dimensional materials such as transition metal dichalcogenides (TMDCs) [1]. By laser exposure it is possible to reduce the number of layers locally from multi- down to a monolayer. For a precise layer-by-layer etching process, thinning and simultaneous monitoring is required which can be performed by Raman or photoluminescence (PL) spectroscopy.

This study focusses on PL monitoring during laser-thinning of different trilayer TMDCs such as MoS_2, WS_2 and ReS_2. It will be shown that MoS_2 and WS_2, which are direct bandgap semiconductors for monolayers, can be thinned down layer-by-layer. The spectral position of the indirect bandgap transition clearly indicates the number of layers, changes abruptly from tri- to bilayer and vanishes for a monolayer. Moreover, a strong increase of the direct bandgap emission indicates thinning from a bi- to a monolayer. Limitations of PL monitoring will also be discussed using the example of ReS_2, which remains an indirect bandgap semiconductor even for a monolayer.

[1] A. Castellanos-Gomez et al., Nano Letters 12, 3187 (2012).

HL 74.10 Thu 15:00 P2/2OG

Looking for interlayer excitons in hybrid WSe_2/MoS_2 heterostructures — •Rico Schwartz[1], Alina Christine Schubert[1], Antony George[2], Andrey Turchanin[2], and Tobias Korn[1] — [1]Institut für Physik, Universität Rostock, D-18059 Rostock, Germany — [2]Institut für Physikalische Chemie, Friedrich-Schiller-Universität Jena, D-07743 Jena, Germany

Fabrication and optical spectroscopy of transition metal dichalcogenide (TMDC) monolayers and their heterostructures have been intensely studied by a lot of work groups in recent years. One interesting aspect is the excitation of interlayer excitons, that means excitons whose electrons and holes are placed in different monolayers and thus in different materials.

TMDC heterostructures are mostly fabricated by deterministic stacking of exfoliated flakes, which limits their size to a few tens of microns. CVD growth, in contrast, allows large-scale TMDC films which might be interesting for future industrial applications.

We study a hybrid heterostructure consisting of a CVD-grown WSe_2 monolayer on a Si/SiO_2 substrate [1] combined with an exfoliated MoS_2 flake. In photoluminescence studies, we observe a pronounced quenching of intralayer exciton emission in our heterostructure, indicating interlayer charge transfer. Additionally, we find emission from interlayer excitons comparable to those in samples fabricated using only exfoliated layers [2].

[1] A. George et al., J. Phys.: Mater. **2**, 016001 (2019)
[2] J. Kunstmann et al., Nature Physics **14**, 801-805 (2018)

HL 74.11 Thu 15:00 P2/2OG

Control of proximity-induced spin-orbit coupling in graphene/TMDC heterostructures — •Tobias Rockinger, Tobias Völkl, Dieter Weiss, and Jonathan Eroms — Institute of Experimental and Applied Physics, Universität Regensburg, Universitätsstraße 31, 93053 Regensburg

Graphene is known as an ideal candidate for spintronic devices because of its long spin relaxation times. However, for spintronic applications we have to create spin currents as well. Spin currents cannot be created in graphene directly because of graphene's low intrinsic spin-orbit coupling (SOC). Z. Wang et al. [1] showed that one can induce SOC into graphene by proximity-coupling with TMDCs. Because the proximity-induced SOC varies from sample to sample, we strive for a better control over the induced SOC. Theoretical predictions by Y. Li et al. [2] and A. David et al. [3] show that proximity-induced SOC depends on the twist angle between graphene and the TMDC. We therefore fabricated graphene/TMDC heterostructures where the twist angle is controlled during a van der Waals stacking process. To get comparable samples we only use single layer TMDCs on graphene. Four-terminal magnetotransport measurements at low temperatures revealed weak localization and weak anti-localization, showing weak or strong SOC, respectively. The measurements of our first samples agree with theory and show signs of the expected dependence of SOC on the twist angle.
[1] Z. Wang et al., Phys. Rev. X 6, 041020 (2016) [2] Y. Li et al., Phys. Rev. B 99, 075438 (2019) [3] A. David et al., Phys. Rev. B 100, 085412 (2019)

HL 74.12 Thu 15:00 P2/2OG

Dry-transfer process of graphene / hBN heterostructures — •Khairi Fahad Elyas, Asem Ben Kalefa, Lina Bockhorn, Gunnar Schneider, Christopher Belke, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, 30167 Hannover

Graphene is the first in a large family of two-dimensional (2D) van der Waals (vdW) materials to attract a lot of attention due to its remarkable properties. One of these properties is a zero band gap. The second most popular vdW material after graphene is hexagonal boron nitride (h-BN). The h-BN is a ideal insulator with wide band gap (4.5 eV).
Here, we demonstrate the dry-release transfer of monolayer and bilayer graphene of the size up to 20 μm by using poly (propylene) carbonate (PPC) films. We also transfer a few layers h-BN with size up to 45 μm. Due to the strong adhesion between PPC and 2D materials at room temperature, we show that single-layer to low-layer graphene as well as less-layered h-BN can be produced on a spin coated PPC films /SiO_2 / Si substrate by the mechanical peeling method. This method is useful for sample preparations for different applications like TEM measurements. Based on the dry-release transfer samples with high purities are achieved.
We also demonstrate electronic and magnetotransport measurements on graphene/hBN heterostructures.

HL 74.13 Thu 15:00 P2/2OG

Benchmarking calculated excited state properties of 2D materials on substrates and in van de Waals heterostructures against experiments — •Anders Christian Riis-Jensen and Kristian Sommer Thygesen — Technical University of Denmark, Institute of Physics

2D materials and van der Waals heterostructures exhibit extraordinary optical properties because of the reduced screening in two dimensional materials. Due to the possible lattice mismatch and relative twist angle between the layers constituting a van der Waals heterostructure, accurate many-body ab-initio calculations for such many layers heterostructures are not possible.

By combining many-body ab-initio calculations with electrostatic and perturbative models, we calculate quasi-particle band gaps and intra- and interlayer exciton energies in many layers van der Waals heterostructures, and benchmark to what accuracy these properties can be calculated compared to experimental measurements. Furthermore, we show what discrepancy can be expected between ab-initio calculations and experiments for optical properties due to the effect of substrate screening and show how the screening of 2D materials on bulk substrates can be accurately modelled by a generalized analytical 2D hydrogen model. At the end of the talk I will discuss a new screening regime for 2D materials on strongly screening substrates, where the exciton behavior is very different from the well-known picture in 2D materials and van der Waals heterostructures.

HL 74.14 Thu 15:00 P2/2OG

Manipulating transition-metal dichalcogenide monolayers with proximity effects — •Lanqing Zhou[1,2], Sven Borghardt[1,2], Detlev Grützmacher[1,2], and Beata Kardynal[1,2] — [1]PGI-9, Forschungszentrum Jülich, Julich, Germany — [2]Department of Physics, RWTH Aachen University, 52074 Aachen, Germany

Transition-Metal Dichalcogenides (TMDs) monolayers have been shown to exhibit many interesting physical properties related to their crystal structure and strong spin-orbit interactions. In addition,their properties can be manipulated using proximity fields generated when they are placed in contact with functional molecules or films.Here we interface molybdenum diselenide and tungsten diselenide monolayers with thin films of chromium triiodide and chromium trichloride. Both chromium trihalides (CrX3, X =Cl,I) are layered materials which are electronic insulators that are also ferromagnetic at low temperatures. In this contribution, we examine the effects of proximity magnetic field and the band alignment between W(Mo)Se2 and CrX3 on the excitonic states in the heterostructure. The excitonic states are probed via temperature dependent and polarization resolved photoluminescence. We show that both type-I and type-II heterostructures can be fabricated using different combination of monolayers of TDMs and CrX3. We will also show that in the type-II heterostructure the dominant effects originate from the charge transfer between the two component materials. Finally, we explore the use electric field to manipulate the charge separated complexes.

HL 74.15 Thu 15:00 P2/2OG

Computational Design of Quantum Defects in Low-Dimensional Semiconductors — •Fabian Bertoldo and Kristian Thygesen — Technical University of Denmark, Kgs. Lyngby,

Denmark

2D materials are known to host intriguing electronic properties and thus offer a fascinating platform for quantum photonics. In particular, 2D materials have been shown to host single-photon emitters (SPE). It is therefore vital to investigate the influence of defects within different host materials which are much easier to create and control in monolayers compared to bulk systems. Based on the computational 2D materials database (C2DB) [1] we first perform a computational screening for intrinsic point defects of stable theoretically predicted and experimentally known low-dimensional semiconductors. We will present a tool within the atomic simulation environment (ASE) [2] to automatically identify intrinsic point defects for given structures and calculate their respective formation energies as well as their charge transition energies.

[1] The Computational 2D Materials Database: High-throughput modeling and discovery of atomically thin crystals, S. Haastrup et al. 2D Materials 5, 042002 (2018)

[2] The atomic simulation environment - a Python library for working with atoms, A. Larsen et al. Journal of Physics: Condensed Matter, 29(27): 273002, 2017

HL 74.16 Thu 15:00 P2/2OG

Manufacturing and magnetotransport properties of weakly coupled double trilayer graphene — •Xiao Xiao, Sung Ju Hong, Christopher Belke, and Rolf Haug — Festkörperphysik-Institut, Hannover, Germany

We have investigated magnetotransport of double trilayer graphene (DTLG). The DTLG was fabricated by stacking two trilayer graphene (TLG) flakes with polypropylene carbonate in a dry transfer method. Analysing the edges of the two flakes in the optical microscope, we identified a large twist angle around 24°. This is consistent with the electrical measurement which show the superposition of two independent magnetotransport properties. As in twisted bilayer graphene, the large twist angle seems to result in a weak coupling between the two layers. In the observed Landau fan diagram, one of the DTLG turns out to be ABA-stacked TLG. Furthermore, we found an additional high carrier density which comes from the other TLG.

HL 74.17 Thu 15:00 P2/2OG

STM-induced excitonic luminescence of a 2D semiconductor — Delphine Pommier[1], •Rémi Bretel[1], Luis Parra López[2], Florentin Fabre[2], Andrew Mayne[1], Elizabeth Boer-Duchemin[1], Gérald Dujardin[1], Guillaume Schull[2], Stéphane Berciaud[2], and Eric Le Moal[1] — [1]Institut des Sciences Moléculaires d'Orsay, CNRS, Université Paris Sud, Université Paris-Saclay, F-91405 Orsay, France — [2]Institut de Physique et Chimie des Matériaux de Strasbourg, Université de Strasbourg, CNRS, IPCMS, UMR 7504, F-67000 Strasbourg, France

Transition metal dichalcogenides (TMDs) are 2D layered materials that have gained a lot of interest as their unique and tunable excitonic properties are very promising for new compact optoelectronic devices. To fully understand processes involving excitons requires studies at the nanometer scale. Scanning tunneling microscopy (STM) may be used to carry out such studies, as a local electrical source for the excitation of excitons in TMDs. In this work, we report the STM-induced light emission (STM-LE) of the semiconducting, direct bandgap monolayer (1ML) molybdenum diselenide (MoSe2) at room temperature in air. The emitted light is collected in transmission through an oil-immersion objective. STM-LE is compared with laser-induced photoluminescence. The emission is identified as the radiative decay of bright A exciton and the excitation mechanism here is found to be a resonant energy transfer, which contrasts with previous results from other electroluminescence studies on TMDs [1].

[1] Pommier et al, Physical Review Letters 123.2 (2019): 027402.

HL 74.18 Thu 15:00 P2/2OG

Phase transition measurements of atomically thin 1T-TaS2 probed with ultrafast electron diffraction — •Mashood Tariq Mir, Arne Ungeheuer, Ahmed Hassanien, Arne Senftleben, and Thomas Baumert — Institute of Physics and CINSaT, University of Kassel, Heinrich-Plett-Strasse 40, D-34132 Kassel, Germany

The layered transition metal dichalcogenides (TMDs) host a rich collection of physical properties which may open many different applications with atomically thin films such as sensors, electronic switching or energy storage. Among those materials, 1T-TaS2 exhibits a complex phase diagram depending on temperature encompassing charge density waves (CDW) with diverse commensurabilities. We aim to use femtosecond laser pulses to induce rapid structural changes and probe the following with ultrafast electron diffraction (UED). In this work, free-standing single-crystalline sample were prepared down to a few nanometer thicknesses to allow electron diffraction in transmission mode. The samples were mechanically exfoliated from different adhesive surfaces. The preparation method was optimized using atomic force microscopy and optical microscopy to isolate atomically thin flakes.

In addition, we present an initial UED study of CDW phases of 1T-TaS2. Upon lattice heating, the material undergoes several phase transitions. We are focusing on the reversible phase transition from the nearly commensurate to incommensurate phase in which the commensurate phase disappears, while the incommensurate phase emerges without causing irreversible damage to the underlying crystal.

HL 74.19 Thu 15:00 P2/2OG

Effect of ion irradiation on electrical and optical properties of molybdenum disulfide — •Zahra Fekri[1], Phanish Chava[2], Tommaso Venanzi[3], Gregor Hlawacek[4], Antony George[5], Andrey Turchanin[6], and Artur Erbe[7] — [1]HZDR — [2]HZDR — [3]HZDR — [4]HZDR — [5]University Jena — [6]University Jena — [7]HZDR

Since silicon transistors are reaching their physical limit to shrink, there is a need for the discovery of new materials to keep on with Moore's law. Two-dimensional (2D) materials, which have gained enormous attention since the discovery of graphene, could enable transistors to keep scaling. MoS2 is among the most well-known 2D materials due to its unique properties. Tunable bandgap, high mobility, and flexibility make MoS2 a promising material in future electronics, sensing and photo-detection applications. The ability to modify materials at the atomic scale is crucial for the fabrication of novel nanodevices. The electrical and optical properties of MoS2 strongly depend on defects. Deficiencies in the structure can be detected by spectroscopic techniques which provide the understanding of new functionalities of MoS2 based devices. Helium ion microscope promises to be a suitable tool to create controllable defects on 2D materials. A nice aspect of this method is that the electrical measurement can occur in situ in the microscope so that the effect of irradiation can be assessed immediately. This research focuses on modifying the electrical and optical properties of MoS2 based field effect transistor using helium ion microscope.

HL 74.20 Thu 15:00 P2/2OG

Optical characterization of ion implanted monolayer molybdenum dichalcogenides — •Minh Bui[1], Stefan Rost[2], Manuel Auge[3], Jhih-Sian Tu[1], Sven Borghardt[1], Hans Hofsäss[3], and Beata Kardynał[1] — [1]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Peter Grünberg Institut (PGI-1 / IAS-1), Forschungszentrum Jülich, 52425 Jülich, Germany — [3]II. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Monolayers (MLs) of semiconducting transition metal dichalcogenides (TMDCs) possess unique band structure leading to exotic optical properties, suitable for valley- and exciton-based optoelectronic applications. Tuning those properties is desirable to further exploit their potentials, for which deterministic doping is a viable technique that has proven suitable for bulk semiconductors. Here, implantation with low energy ions is explored as a method to introduce dopant atoms into TMDC MLs, with the prototypical system of Se-implanted MoS_2. Isoelectronic substitution of Se for S in MoS_2 converts the material into $MoSe_{2x}S_{2(1-x)}$ without creating free carriers. For the optimal compromise between Se incorporation and defect formation, different implantation conditions were investigated, including treatment for healing defects. Structural and electronic effects of implantation on MLs were studied using Raman, reflectance and photoluminescence spectroscopies. Implantation levels much higher than required for doping, up to 20%, were achieved. Results of $MoSe_2$ implanted with P for p-type dopants, and Cr for substitution in Mo sites are also discussed.

HL 74.21 Thu 15:00 P2/2OG

2D van der Waals heterostructures for electronic devices — •Phanish Chava[1], Vivek Koladi[1], Himani Arora[1], Kenji Wanatnabe[2], Takashi Taniguchi[2], Manfred Helm[1], and Artur Erbe[1] — [1]Helmholtz Zentrum Dresden Rossendorf, Bautzner Landstrasse 400, 01328 — [2]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

The interlayer van der Waals(vdWs) interaction allows 2D materials to be easily stacked to form various heterostructures with unique and

novel features. Layer dependent electronic band structure and the absence of surface dangling bonds make them promising candidates for electronic devices. In this study, we focus particularly on devices that enable lower operating voltages thereby forming a basis for energy efficient circuits. This is done by investigating the idea of a Tunnel Field Effect Transistor (TFET) based on vdWs hetrostructures.

HL 74.22 Thu 15:00 P2/2OG

Optical phonon mediated valley depolarization in monolayer WSe2 — •Robin Bernhardt, Julian Wagner, Jingyi Zhu, and Paul van Loosdrecht — Universität zu Köln, II. Physikalisches Institut, D-50937 Köln, Germany

The valley degree of freedom in semiconducting transition metal dichalcogenide monolayers is considered as a potential basis for novel information technology. Key to this is the degree and lifetime of an induced valley polarization. We investigated the temperature dependent transient valley polarization using circularly polarized and femtosecond time-resolved photoluminescence spectroscopy on exfoliated WSe2. Using these data, the intervalley scattering rate is evaluated over a broad temperature range, showing that optical-phonon assisted scattering is the dominant intervalley scattering mechanism.

HL 74.23 Thu 15:00 P2/2OG

Optical characterization of $MoTe_2$-based monolayer-monolayer heterostructures — •Mohammed Adel Aly[1], Shachi Machchhar[1], Manan Shah[1], Lorenz Maximilian Schneider[1], Saeideh Edalati Boostan[2], Claudia Draxl[2], Wolfram Heimbrodt[1], and Arash Rahimi-Iman[1] — [1]Faculty of Physics and Materials Sciences Center, Philipps-Universität, Marburg, 35032 Germany — [2]Theoretical solid state physics, Institute for Physics, Humboldt-Universität Berlin, 12489 Berlin, Germany

Van-der-Waals heterostructures (vdW-HSs) based on 2D layered materials have received huge attention due to their strong light matter interaction and the promise of bandgap engineering capabilities. Owing to the strong out-of-plane quantum confinement and electronic interaction between the layers, the HSs can exhibit exotic properties. Moreover, the strain effect is recognized as an effective parameter in the modulation of electronic properties. Although in recent years a few reports on $MoTe_2/WSe_2$ HS have emerged, a comprehensive study exploring their properties is still lacking. Here, we present our cooperative theoretical/experimental work on $MoTe_2/WSe_2$ type-I and $MoTe_2/MoSe_2$ type-II vdW-HSs. We have investigated our specimen using μ–PL and reflection contrast, shedding light on exciton physics in such structures, band alignment and possible charge transfer between type-II layers. We performed μ–Raman spectroscopy to determine the characteristic phonon modes and their separation to extract possible strain values. Our overall strain estimation is derived from the variation in the excitonic peaks and Raman modes' positions.

HL 74.24 Thu 15:00 P2/2OG

Small angle twisted bilayer graphene — Simon Wagner[1], Tobias Rockinger[1], Kenji Watanabe[2], Takashi Taniguchi[2], Dieter Weiss[1], and •Jonathan Eroms[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

One recent observation in graphene is the appearance of interaction effects in twisted bilayer graphene (TBG) with a twist angle of about 1.1°, which is called magic angle. Depending on the angle between the two layers the band structure changes and can show flat bands. At the magic angle, the band width is minimal. This leads to enhanced carrier-carrier interaction resulting in both Mott-like insulating behavior and superconductivity. Both effects were recently discovered by Cao *et al.* in magic angle bilayer graphene. We fabricated TBG by van der Waals stacking of two parts of a single graphene monolayer (the tear and stack-technique), which we encapsulate in hexagonal boron nitride. During fabrication the twist angle is controlled in a dedicated setup and can be verified afterwards by the position of secondary Dirac peaks and flux-dependent features in a Landau fan diagram. In a sample with a twist angle of about 0.9°, we observe those signatures of a superlattice potential, and also detect additional insulating states at gate voltages corresponding to filling 1, 2 or 3 electrons per moire unit cell.

Y. Cao, *et al.*, Nature **556**, 80 (2018), *ibid.* 43

HL 75: Poster IIIB

This poster session includes contributions from the following topics:

- Functional semiconductors for renewable energy solutions - Materials and devices for quantum technology - Optical properties - Thermal properties - Focus Session: Tailored Nonlinear Photonics

Please put up your poster at the beginning of the session and remove the poster immediately after the session. The person peresenting the poster should attend it for at least half of the session duration and indicate the time when to find him/her at the poster.

Time: Thursday 15:00–17:30 Location: P2/3OG

HL 75.1 Thu 15:00 P2/3OG

Classification of Silicon Carbide for Maser Application by Electron Paramagnetic Resonance — •S. Scherbel, A. Gottscholl, C. Kasper, V. Soltamov, V. Dyakonov, and A. Sperlich — Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg

Although masers have been known for decades, their application as low noise amplifier is still limited due to their operating conditions, requiring vacuum and cryogenic temperatures. Hence, our aim is to build a room-temperature maser based on spin-carrying defects in the technologically advanced material silicon carbide (SiC). To generate such spin-carrying defects, in our case the negatively charged silicon vacancies (V_{Si}), the SiC crystal was exposed to high-energy particles (electrons or neutrons). To obtain population inversion we optically pumped the ground state spin sublevels of V_{Si}. By applying an external magnetic field we tuned the Zeeman splitting into resonance with an applied microwave frequency of 10 GHz [1]. Using magnetic resonance techniques, we quantified the population inversion within V_{Si} spin sublevels for different SiC polytypes (4H, 6H) and irradiation methods for a wide range of irradiation doses. Finally, we studied the influence of optical pump power, temperature and samples orientation with respect to the external magnetic field on the population inversion. Our systematic study specifies the parameters, necessary for SiC to become a suitable maser system with a wide-ranging applicability.

[1] H. Kraus et al., Nat. Phys. **10**, 152 (2014)

HL 75.2 Thu 15:00 P2/3OG

Temperature dependent optical properties of CuI thin film — •Jan Kremkow, Vitaly Zviagin, Evgeny Krüger, Chang Yang, Chris Sturm, and Marius Grundmann — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik

We present the optical properties of copper iodide (CuI) thin film fabricated by reactive sputtering at 360 °C on c-sapphire substrate. The dielectric function (DF) was determined by the means of spectroscopic ellipsometry in a wide spectral range (0.5 eV - 8.5 eV) and in the temperature range from 10 K to 300 K. The DF line-shape was initially determined numerically and consequently parametrized by a series of model functions. The DF spectra was found to be dominated by electronic transitions involving the Γ- and L- symmetry points of the CuI Brillouin zone.[1] Their evolution with temperature is investigated with respect to the Bose-Einstein model approximation. The results show a general agreement with literature and give insight into the temperature dependence of CuI electronic structure. [1] E. Krüger *et al.*, Appl. Phys. Lett. **113**, 172102 (2018).

HL 75.3 Thu 15:00 P2/3OG

Raman spectroscopy on anisotropic media — •Ron

Hildebrandt[1], Chris Sturm[1], Matthias Wieneke[2], Armin Dadgar[2], and Marius Grundmann[1] — [1]Universität Leipzig, Felix Bloch Institute for Solid State Physics, Germany — [2]Otto-von-Guericke Universität Magdeburg, Institute for Physics, Germany

Raman spectroscopy is a widely used technique e.g. for the determination of the phonon modes, alloy composition, crystalline orientation or characterization of crystalline quality. In optically anisotropic materials, the polarization of the incident and scattered light changes along the propagation within the crystal due to birefringence. Thus the "standard" Raman tensor formalism cannot be applied there. Recently we presented a modified Raman tensor formalism which allows to model the Raman intensity in dependence on the polarization configuration for any crystal symmetry [1,2]. For an optically uniaxial crystal with the optical axis in the surface plane, the effective standard Raman formalism is recovered except an additional phase factor needs to be added to the Raman tensor elements. This phase factor depends only on the material's birefringence and the penetration depth.

Here we investigated exemplarily on a-plane GaN the phase factor as a function of the penetration depth by varying the film thickness from 0.7 to 12 μm. The experimentally determined phase factors agree very well with predictions by the modified Raman formalism.

[1] C. Kranert *et al.*, Phys. Rev. Lett., **116**, 127401, 2016.
[2] C. Kranert *et al.*, Sci. Rep., **6**, 35964, 2016.

HL 75.4 Thu 15:00 P2/3OG

On the calculation of the band gap of periodic solids with MGGA functionals using the total energy — •Fabien Tran — Vienna University of Technology, Vienna, Austria

During the last few years, it has become more and more clear that functionals of the meta generalized gradient approximation (MGGA) are more accurate than GGA functionals for the geometry and energetics of electronic systems. However, MGGA functionals are also potentially more interesting for the electronic structure, in particular when the potential is non-multiplicative (i.e., when MGGAs are implemented in the generalized Kohn-Sham framework), which may help to get more accurate band gaps. Here, we show that the calculation of band gap of solids with MGGA functionals can be done very accurately also in a non-self-consistent manner. This scheme uses only the total energy and can, therefore, be very useful when the self-consistent implementation of a particular MGGA functional is not available. Since self-consistent MGGA calculations may be difficult to converge, the non-self-consistent scheme may also help to speed-up the calculations. Furthermore, it can be applied to any other types of functionals, for which the implementation of the corresponding potential is not trivial.

HL 75.5 Thu 15:00 P2/3OG

In-situ Fabrication of Magnetic Topological Insulator Devices — •Max Vassen-Carl[1], Michael Schleenvoigt[1], Tobias W. Schmitt[2], Abdur R. Jalil[1], Stefan Trellenkamp[3], Florian Lentz[3], Gregor Mussler[1], Peter Schüffelgen[1], and Detlev Grützmacher[1] — [1]Peter Grünberg Institute, Forschungszentrum Jülich & JARA Jülich-Aachen Research Alliance, 52425 Jülich, Germany — [2]JARA-FIT Institute Green IT, RWTH Aachen University, 52062 Aachen, Germany — [3]Helmholtz Nano Facility, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

Magnetic topological insulators (MTIs), which have their Fermi level in the exchange gap exhibit the quantum anomalous Hall (QAH) effect with chiral edge states. The latter are of high interest to spintronic applications. Moreover, by proximity coupling the MTI to a superconductor (SC), chiral Majorana edge modes are expected to arise. To access the QAH regime in MTIs, it is beneficial to avoid ambient conditions or chemicals during device fabrication, which may disturb the sensitive surface states. This makes ultra-high vacuum (UHV) fabrication techniques highly interesting for these materials. I will present a UHV technique that enables molecular beam epitaxy (MBE) growth of MTIs ((Cr)z(Bi,Sb)2-z(Te,Se)3) in selected areas on silicon substrates. In a second step, a normal conductor or SC can be deposited in-situ onto the MTI utilizing an angular arrangement, effectively creating MTI devices in the MBE without breaking the vacuum.

HL 75.6 Thu 15:00 P2/3OG

Raman spectra under hydrostatic pressure: a first principles investigation — •Jan M. Waack[1,2], Marcel Giar[1], and Christian Heiliger[1,2] — [1]Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Gießen — [2]Zentrum für Materialforschung (LaMa), Justus-Liebig-Universität Gießen, Gießen

In a first principles investigations the vibrational properties of Cu_4O_3 (paramelaconite) under hydrostatic pressure were derived from DFT calculations. With increasing hydrostatic pressure on the system, imaginary phonon frequencies occur. These determine the limit of the stability of the tetragonal Cu_4O_3 in respect to hydrostatic pressure. It became recognizable, that the influence on intensities of Raman peaks strongly depends on the laser wavelength. The resulting effects on Raman spectra are discussed. Additionally, a change of the lattice parameters leads to a clear shift of the Raman peak positions. The impact on the calculations of Raman spectra are explained.

HL 75.7 Thu 15:00 P2/3OG

Open-gate junction field effect transistors as cryogenic charge detectors with attoampere leakage — •Tom Risse, Hüseyin Azazoglu, Kornelia Huba, Hermann Nienhaus, and Rolf Möller — Faculty of Physics/Cenide, University of Duisburg-Essen, Germany

Open-gate junction field effect transistors (JFET) at cryogenic temperatures can be employed as almost perfect charge detectors with leakage currents of less than 0.1 aA [1]. The minimum detectable charge is primarily determined by the leakage current between the source and gate terminals. The intrinsic leakage current is due to a generation of charge carriers in the pn-depletion zone and may be well described by the Shockley-Reed-Hall model. The extrinsic leakage current occurs through parasitic resistive current paths outside the JFET, e.g. due to contaminations. Both contributions can be precisely distinguished by measuring the variation of a gate discharge current with time. The study reports on the intrisic leakage current in the JFET BF545B at 220 K and at room temperature. By reducing the parasitic resistances a leakage current of 2.1 aA is achieved and charges of only 14 aC can be determined. The gate contact of the cryogenic device is successfully connected to an external electrode which allows sensitive charge detection in setups at room temperature. Examples of low charge detection due to UV- , alpha- and beta radiation as well as of detection of moving charged droplets by electrostatic induction are demonstrated. [1] A. Kavangary et al. AIP Advances 9, 025104 (2019).

HL 75.8 Thu 15:00 P2/3OG

Simulating the influence of spectral jitter and phonons on four-wave mixing signals of single quantum dots — •Thilo Hahn, Daniel Wigger, and Tilmann Kuhn — Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Four-wave mixing (FWM) micro-spectroscopy is a powerful technique to investigate the dynamics of charge carriers in semiconductor nanostructures. By using a heterodyne interferometry technique one is able to detect coherence as well as occupation dynamics of a single quantum dot [1]. We model the QD exciton as a two-level system, excited by a series of ultrafast pulses. Additionally we take the pure dephasing coupling to a discrete phonon mode into account. By introducing characteristic functions the dynamics of the entire exciton-phonon system can be calculated analytically in the limit of ultrafast optical excitation [2]. We will present photon echo formation as a consequence of a randomization of the transition energy due to for example charge fluctuations [3]. Then we take the coupling to a discrete phonon mode into account and discuss its impact on FWM signals.

[1] W. Langbein, *Rivista Del Nuovo Cimento* **33**, 5 (2010)
[2] A. Vagov, et al., *Phys. Rev. B* **66**, 165312 (2002)
[3] T. Jakubczyk, et al., *ACS Photonics* **3**, 2461-2466 (2016)

HL 75.9 Thu 15:00 P2/3OG

Four-Wave-Mixing Spectroscopy of a Quantum Dot Microcavity System at Large Pulse Areas — •Daniel Groll[1], Daniel Wigger[1], Jacek Kasprzak[2,3], and Tilmann Kuhn[1] — [1]Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [2]Univ. Grenoble Alpes, F-38000 Grenoble, France — [3]CNRS, Institut Néel, "Nanophysique et Semiconducteurs" Group, F-38000 Grenoble, France

We use four-wave-mixing (FWM) spectroscopy to investigate a single quantum dot (QD) strongly coupled to a microcavity, which we model by the usual Jaynes Cummings (JC) Hamiltonian. The corresponding spectrum is called the JC ladder and consists of doublets of dressed states with a splitting that depends nonlinearly on the number of photons present in the cavity. The inevitable coupling between the QD exciton and the phonons of the surrounding medium is treated using a master equation approach. In our study special emphasis is laid on the behavior of the system, when a large number of photons, up to ∼50,

is excited inside the cavity. Reaching large pulse areas, where such an amount of photons drives the dynamics, we observe a quasiperiodic behavior of the cavity polarization which gives rise to characteristic features in the measured FWM signals. We find good agreement between experiment and theory for the entire range of considered pulse areas.

HL 75.10 Thu 15:00 P2/3OG

Open optical microcavities for tunable light–matter coupling with 2D semiconductors — •Chirag Palekar, Franziska Wall, Oliver Mey, Lorenz Maximilian Schneider, and Arash Rahimi-Iman — Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, Marburg, 35032, Germany

Light–matter coupling experiments with 2D semiconductors such as transition-metal dichalcogenides in optical microcavities are very attractive due to the strong excitonic binding energies, spin–valley locking and the overall prospect of polariton Bose condensation at elevated temperatures. In this context, microcavities with tunable length, low mode volume and open resonator configuration can be very useful for the systematic variation of the system's parameters [1]. Moreover, tuning between the weak and strong coupling regime becomes feasible, as discussed here based on our simulations. We use the transfer-matrix method to show how to tailor and alter the coupling strength actively by varying the relative field strength at the excitons' position. Therefore, a transparent PMMA spacer layer and angle-dependencies of optical resonances are exploited [2]. The adjustable polariton energy levels could be interesting for polariton chemistry or optical sensing. In addition, cavities that allow working at the exceptional point promise the exploration of topological properties of that point. [1] P. Qing et al., *APL* 114, 021106 (2019). [2] F. Wall et al., *arXiv* (2019).

HL 75.11 Thu 15:00 P2/3OG

Transient four-wave-mixing in semiconductors with half-gap pulses — •Alexander Trautmann[1], Wolf-Rüdiger Hannes[1], Markus Stein[2], Felix Schäfer[2], Martin Koch[2], and Torsten Meier[1] — [1]Department of Physics and CeOPP, University of Paderborn, Warburger Straße 100, D-33098 Paderborn, Germany — [2]Department of Physics and Materials Science Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany

Transient four-wave-mixing (FWM) is demonstrated to occur in bulk semiconductors when excited by two spatiotemporally overlapping strongly off-resonant pulses. This $\chi^{(3)}$-process can be analyzed theoretically by means of the semiconductor Bloch equations including inter- and intraband excitations [1]. As a result of the interference of different excitation pathways, characteristic multi-peak structures may appear in the FWM spectra. The spectra are also significantly broadened compared to the width of the incident pulses. These theoretical findings are qualitatively confirmed by spectrally-resolved FWM experiments on bulk CdTe and bulk GaAs samples with excitation wavelengths near half the band gap.

[1] W.-R. Hannes and T. Meier, Phys. Rev. B **99**, 125301 (2019).

HL 75.12 Thu 15:00 P2/3OG

Cesium-Vapor-Based Delay of Single Photons Emitted by Deterministically Fabricated Quantum Dot Microlenses — •Lucas Bremer[1], Sarah Fischbach[1], Suk-In Park[2], Sven Rodt[1], Jin-Dong Song[2], Tobias Heindel[1], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany — [2]Center for Opto-Electronic Materials and Devices, Korea Institute of Science and Technology, Seoul 02792, Republic of Korea

Controlling the propagation of single photons is highly relevant for the implementation of large-scale quantum networks. We report on the realization of a hybrid interconnection of a high-performance quantum dot (QD) microlens with hot cesium (Cs) vapor, allowing to control the time delay of the emitted photons [1]. The QD microlens with excellent optical properties was realized by a deterministic 3D in-situ electron beam lithography process [2]. By numerical simulations of the light-matter interaction in realistic QD-Cs vapor configurations, the influence of the Cs vapor temperature and the spectral QD-atom detuning is investigated in detail in order to maximize the achievable delay in experimental studies. Thus, our hybrid quantum system enables us to delay the emission pulses by up to (15.71 ± 0.01) ns for an effective Cs cell length of 150 mm.

[1] L. Bremer et al., Adv. Quantum Technol., 1900071 (2019).
[2] M. Gschrey et al., Appl. Phys. Lett. 102, 251113 (2013).

HL 75.13 Thu 15:00 P2/3OG

Optical properties of TiN based superlattices: applicability of the effective medium approximation — •Felix-Florian Delatowski, Chris Sturm, Oliver Herrfurth, Florian Jung, and Marius Grundmann — Felix-Bloch-Institut für Festkörperphysik, Universität Leipzig, Linnéstraße 5, 04103Leipzig

Superlattices based on MgO and TiN are promising for the realization of optical hyperbolic metamaterials [1]. In order to show such hyperbolic behavior, it is possible to describe a superlattice by an uniaxial anisotropic effective medium [2]. The effective medium approximation (EMA) allows a simplified description of the optical properties of the entire superlattice.

In this study, we discuss the applicability of the EMA for TiN/MgO superlattices as a function of the number of layer pairs and thickness of each individual layer. The obtained results are compared to experimental TiN/MgO superlattices grown by pulsed laser deposition and investigated by spectroscopic ellipsometry.

[1] G. Naik *et al.*, PNAS **111**, 7546 (2014).
[2] S. Rytov, Soviet Physics JETP **2**, 466 (1956).

HL 75.14 Thu 15:00 P2/3OG

Applying infrared thermography for thermal interface analysis — •Steven Becker and Manfred Bayer — TU Dortmund University, Dortmund, Germany

Combining μLEDs to array-structures enables the manufacturing of high-resolution light sources in a small form factor. Thermal interface analyses are crucial to improve these devices, but chip-level electronics limit the pixel-wise accessibility of the required junction temperature. Here we present an approach to overcome this limitation by using thermal images as data for the JEDEC 51-14 standard's calculation. Thermal imaging cameras are promising candidates due to their spatially resolved and contactless measurement of the μLED array temperature.

HL 75.15 Thu 15:00 P2/3OG

Novel Concepts for Angle-Resolved Photoemission Spectroscopy and Transport Characterization of 1-Dimensional Topological Insulator/Superconductor Heterostructures — •Kevin Janssen[1,2,4], Abdur Rehman Jalil[2,4], Tristan Heider[1,4], Michael Schleenvoigt[2,4], Tobias Schmitt[3,4], Gregor Mussler[2,4], Peter Schüffelgen[2,4], Claus-Michael Schneider[1,4], Detlef Grützmacher[2,4], Lukasz Plucinski[1,4], and Thomas Schäpers[2,4] — [1]Peter Grünberg Institute (PGI-6), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [3]Peter Grünberg Institute (PGI-10), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [4]JARA-FIT, RWTH Aachen University and FZ-Jülich GmbH

Heterostructures formed by topological insulators (TI's) and superconductors are the main basis for topological quantum computing. Quantum processors employing Majorana fermions demand high purity and one dimensionality of these structures. With our integrated approach we aim to characterize these heterostructures of TI nanoribbons and superconductors by comparing angle-resolved photoemission spectroscopy (ARPES) and transport measurements. Here, we present a novel in-situ fabrication scheme to realize one dimensional heterostructures of TI and superconductor for transport characterization by combining selective area growth and a newly developed shadow technique. Additionally, we show indications of the Dirac cone by ARPES from an array of TI nanoribbons.

HL 75.16 Thu 15:00 P2/3OG

Multi-probe electrical characterization of pn-GaAs-based nanowires under illumination — •Juliane Koch, Andreas Nägelein, Matthias Steidl, Peter Kleinschmidt, and Thomas Hannappel — TU Ilmenau, Institute for Physics, Fundamentals of Energy Materials, Ilmenau, Germany

Semiconducting nanowires (NW) are known as promising candidates for a large variety of future optoelectronic devices, such as for solar energy conversion devices. For their beneficial use it is essential to control doping profiles along the NW with abrupt charge-separating contacts and to assess their optoelectronic performance. This can be achieved by appropriate electronic and optoelectronic characterization. In this work, a multi-tip scanning tunneling microscope (MT-STM), which is equipped with a scanning electron microscope (SEM), enables the independent control of four tungsten-tips, which are employed to perform 2- and 4-point I-V-measurements on individual, freestanding

NWs with high spatial resolution. We were able to to record measurements on NW comprising pn-junctions, both with and without illumination. The resulting resistance profiles without illumination provide direct access to the doping profiles, so that the doping concentration of the p- and the n-doped region can be determined as well as the position of the charge-separating contact. Measurements under illumination yields the photocurrent as well as the fill factor associated with the I-V characteristic of the illuminated NW. In addition, the charge-separating contact can be visualized in the SEM by detection of the electron beam induced current.

HL 75.17 Thu 15:00 P2/3OG

Ab initio study on structural and electronic properties of carbon defects in SiC(0001)/SiO_2 systems — •Takuma Kobayashi[1,2] and Yu-ichiro Matsushita[1] — [1]Tokyo Institute of Technology, Yokohama, Japan — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Silicon Carbide (SiC) has been regarded as a promising material for power devices owing to its superior physical properties, such as wide bandgap and high critical field strength. SiC metal-oxide-semiconductor field effect transistors (MOSFETs) have, however, suffered from their unexpectedly low channel mobility due to the high interface state density of SiC/SiO_2 systems. So far, carbon byproducts created during the oxidation of SiC were pointed out as a strong candidate for the interface states. In the present study, we report the stable atomic structures of carbon defects in SiC, silicon dioxide (SiO_2), and those at their interface, depending on the oxidation environment. We also discuss their impact on the device performance based on the calculated defect levels.

HL 75.18 Thu 15:00 P2/3OG

Development of ab initio equations describing optical properties in solids — •Nicolas Schüler, Tobias Zier, and Martin Garcia — Theoretische Physik, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

Optical properties of materials are crucial to describe femtosecond-laser pulse excitations properly, since they determine the absorbed energy by the system. However, in regular density functional theory these properties are not included. In order to extend our density functional theory code CHIVES, we seek to develop an analytical theory that describes optical properties in solids and is compatible to our code. In CHIVES the valence electrons are described by atom-centered Gaussian basis sets, which needs a different description than available theories using plane waves, e.g., implemented in WIEN2k. In order to develop such theory, we start from textbook description using Maxwell's equations. This path enables us to understand the nature of optical properties and allow us to derive first equations for metals, which then will be extended to semiconductors. Parallel to this path we consider a different approach, which uses the Berry phase to obtain optical properties of systems. Besides the more precise description of femtosecond-laser excitations in general, this important extension of our code will allow us to directly compare our simulations to optical measurements like time-resolved reflectivity measurements.

HL 75.19 Thu 15:00 P2/3OG

Towards a fully electrically tunable entangled photon source — •Zheng Zeng[1], Arne Ludwig[2], Marcel Schmidt[2], Beata Kardynał[1], and Feng Liu[3] — [1]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany — [3]JARA-Institute for Quantum Information, RWTH Aachen University, 52074 Aachen, Germany

An entangled photon source (EPS) is one of the key components for optical quantum computing and quantum network. Bright sources of entangled photon pairs have already demonstrated using In(Ga)As self-assembled quantum dots (QDs). However, their scalability and entanglement fidelity are limited by the broad energy distribution and energy splitting between bright exciton states (fine structure splitting (FSS)). In this work, we aim to develop a fully electrical tunable on-demand EPS based on InAs QDs. Simultaneous tuning of the QD transition energy and FSS is essential to achieve this goal. To this end, we fabricated devices with a full back gate and split front gates. We measured the tuning of the QD transition energy by electric field along the QD growth direction via the quantum Stark effect and the tuning of the FSS by the in-plane electric field. Our results strongly indicate that our device can be potentially used as a fully electrically tunable EPS.

HL 75.20 Thu 15:00 P2/3OG

Exceptional Points in optical anisotropic semiconductors — •Sebastian Henn[1], Evgeny Krüger[1], Chris Sturm[1], Armin Dadgar[2], Matthias Wieneke[2], Rüdiger Schmidt-Grund[1,3], and Marius Grundmann[1] — [1]Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Linnéstr. 5, Leipzig — [2]Otto-von-Guericke-Universität Magdeburg, Institut für Physik — [3]now at: Technische Universität Ilmenau, Institut für Physik, Weimarerstr. 25, Ilmenau

We investigate exceptional points (EP) in optically anisotropic transparent thin films both experimentally and theoretically. EP represent degeneracies in k-space and were already observed in absorptive biaxial crystals [1] and microcavities [2,3]. At the degeneracy the eigenvalues and eigenstates of the system, i.e. the complex energy and polarization, *coalesce*. This is reflected by a complex square root topology around the EP [2]. Promising systems for the realization of EP are optically anisotropic thin films, providing symmetry breaking and dissipation through losses at the interfaces. We demonstrate the presence of EP in GaN and ZnO thin films using spectroscopic Müller Matrix ellipsometry and presenting rigorous Maxwell-based calculations. We discuss ways to control the occurrence and direction of the EP by altering the design of the system. [1] W. Voigt*et al.*, Ann. Phys **314**, 367 (1902) [2] S. Richter*et al.*, Phys. Rev. Lett. **123**, 227401 (2019) [3] J. Wiersig, Phys. Rev. Lett. **112**, 203901 (2014)

HL 75.21 Thu 15:00 P2/3OG

Confocal microscopy of irradiation induced defects in silicon carbide — •Yuan Gao[2], Michael Hollenbach[1,2], Yonder Berencen[1], Gregor Hlawacek[1], Manfred Helm[1,2], and Georgy Astakhov[1] — [1]Institute of Ion Beam Physics and Material Research, Helmholz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany

Photons, as the information carrier in quantum technology, can be generated from point defects in crystal structures. Silicon carbide is a promising host material for such defects that can be created by ion implantation of different types [1]. Compared to other ions, helium ions can create defects with less crystal damages and high coherence. For further applications, defects need to be integrated with nanostructures. This can be done by focused ion beam technology [2]. However, the achieved resolution using protons is not sufficient for nanometer range. Here, we present an approach to create defects locally. In this approach, silicon vacancies are fabricated with a Helium Ion Microscope using different fluences at an energy of 25keV. Upon irradiation, defects are systematically characterized by confocal spectroscopy. It is shown that the defects can be created near the surface by this approach. Moreover, the fluence dependence of the count rate and the lateral resolution are investigated. We demonstrate that this approach holds promises for fabricating silicon carbide based quantum nanostructures.

[1] J. F. Wang, et. al, ACS Photonics 6(7),1736-1743(2019). [2] H. Kraus, et. al, Nano Lett. 17(5),2865-2870(2017).

HL 75.22 Thu 15:00 P2/3OG

Identification of defect properties by positron annihilation in heavily doped n-type GaAs — •juanmei duan[1,2], maciej oskar liedke[1], manfred helm[1,2], shengqiang zhou[1], and slawomir prucnal[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, D-01328 Dresden, Germany — [2]Technische Universität Dresden, D-01062 Dresden, Germany

The electron concentration limits for GaAs are a universal feature existing in group VI donors and Si doping, which limits the carrier concentration to 1e19 cm-3. In our work, we can use ion implantation method beyond the equilibrium solid solubility limits to achieve heavy doped GaAs with Zn, S and Te. We can use millisecond-range flash lamp annealing (FLA) or nanosecond-range pulsed laser annealing (PLA) to reactive and recrystallize the as-implanted samples. The carrier concentration for n-type GaAs can reach up to 5 e19 cm-3. , which is much above the solid solubility of S in GaAs (~1019 cm-3) prepared by MBE. From Positron annihilation spectroscopy (PAS) results, It shows the positron lifetime from heavily n-type doped GaAs has a longer lifetime (above 500ps) and lower intensity I2 than virgin GaAs, which indicates open-volume defects become bigger, defect evolving from monovacancy to multi-vacancy with decreasing the intensity after doping and annealing process.

HL 75.23 Thu 15:00 P2/3OG

Auger Electron Detected Magnetic Resonance — •David

Vogl, Paul Steinacker, and Martin S. Brandt — Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4, 85478 Garching, Germany

For plausible quantum storage applications, long coherence times are required. As Silicon is one of the purest and best-understood materials in the world, it is a natural candidate for such implementations. We investigate and set up a measurement technique for the initialization, manipulation, and readout of electron and nuclear spins of shallow Phosphorus donors in highly isotopically purified ^{28}Si utilizing the spin-dependent and resonant excitation of donor-bound excitons and their successive Auger decay. This method was first implemented by the Thewalt group, who were able to demonstrate coherence times in the order of tens of minutes for the ionized donors at room temperature. In our work, we explore this spin system in detail, applying typical pulsed microwave sequences to measure Rabi oscillations, Ramsey fringes, and Hahn echo decays. We observe beatings in the electron spin Rabi oscillation and are able to selectively generate spin hyperpolarization of the ^{31}P nuclei via a cross relaxation. This technique is also applicable to donors with nuclear spin higher than 1/2, which opens up the possibility of examining the quadrupolar spin interaction in more detail.

HL 75.24 Thu 15:00 P2/3OG

Time-resolved micro-photoluminescence of CuI microwires — •A. Müller[1], E. Krüger[1], G. Benndorf[1], S. Blaurock[2], V. Gottschalch[2], H. Krautscheid[2], C. Sturm[1], and M. Grundmann[1] — [1]Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik — [2]Universität Leipzig, Institut für Anorganische Chemie

The intrinsically p-type conducting copper iodide (CuI) with a direct band gap of 2.95 eV @ 300 K [1] and high exciton binding energy is a promising material for a variety of applications like in transparent semiconductor devices. In particular, CuI micro and nanostructures with high optical quality are well suited candidates for building blocks in integrated optoelectronic circuits. Although photoluminescence emission properties of such CuI crystals have been recently reported [2], the dynamical aspects remain almost unexplored. We report on spectral and dynamical properties of the near band gap emission of CuI microwires, grown by vapor-phase transport method [2]. At low temperatures (10 K) several excitonic emission lines are observed, proving high optical quality of the investigated microwires. The decay of the observed transitions can be modeled by biexponential decay indicating different recombination channels. Here, we focus on the dependence of the decay characteristics on the excitation conditions at low temperature (10 K) as well as their temperature dependence in the range between 10 K and 300 K.

[1] M. Grundmann *et al.*, Phys. Status Solidi A **210**, 1671 (2013)
[2] M. Wille *et al.*, Appl. Phys. Lett. **111**, 031105 (2017)

HL 75.25 Thu 15:00 P2/3OG

Surface modification and charge carrier dynamics of materials and structures for semiconductor-based solar water splitting applications under operation conditions — •Elena Vedel[1], Dani Olfa[1], Mario Kurniawan[2], Theo Pflug[3], Sascha Kürth[1], Noah Hill[1], Shirly Espinoza[4], Mateusz Rebarz[4], Markus Olbrich[3], Oliver Herrfurth[5], Stefan Krischok[1], Alexander Horn[3], Jakob Andreasson[4], Rüdiger Schmidt-Grund[1], Andreas Bund[2], and Thomas Hannappel[1] — [1]Institut für Physik, TU Ilmenau, Weimarer Straße 25, 98693 Ilmenau, Germany — [2]Institut für Werkstofftechnik, TU Ilmenau, Weimarer Straße 25, 98693 Ilmenau, Germany — [3]Laserinstitut Hochschule Mittweida, Technikumplatz 17, 09648 Mittweida, Germany — [4]ELI Beamlines/Fyzikální ústav AV CR, v.v.i., Za Radnicí 835, 25241 Dolní Břežany, Czech Republic — [5]Felix-Bloch-Institut für Festkörperphysik, Uni Leipzig, Linnéstr. 5, 04103 Leipzig, Germany

We present investigations on InP-based materials and heterostructures for applications in photo-chemical water splitting by (fs-time resolved) spectroscopic ellipsometry and real-structure methods. i) We sensitively monitored the modification/corrosion of the semiconductor surfaces under operation in aqueous environment in dependence on the strength and duration of the photo-current flow. ii) The dynamics of the dielectric functions provides access on the dynamics of both, photoexcited electrons and holes in dependence on the carriers' excess energy [1,2] as well as on their transport to the active interface.

[1] APL **115**, 212103 (2019). [2] arXiv:org/abs/1902.05832v2 (2019).

HL 75.26 Thu 15:00 P2/3OG

Dielectric function tensor of ZnO microwires determined by spatially resolved spectroscopic ellipsometry — •Noha Hill[1], Matthias Duwe[2], Sebastian Funke[2], Chris Sturm[3], Lukas Trefflich[3], Marius Grundmann[3], Stefan Krischok[1], and Rüdiger Schmidt-Grund[1] — [1]Institut für Physik, Technische Universität Ilmenau, Weimarer Straße 25, 98693 Ilmenau, Germany — [2]Accurion GmbH, Stresemannstr. 30, 37079 Göttingen, Germany — [3]Felix-Bloch-Institut für Festkörperphysik, Universität Leipzig, Linnéstr. 5, 04103 Leipzig, Germany

ZnO-based nano- and microwire microcavities are very promising systems for room-temperature lasing and quantum-optical applications [1]. But up to know, the optical dispersion functions are not known exactly, there is much evidence that they differ from that of single crystalline bulk material. We have obtained the dielectric function tensor from a single microwire by imaging ellipsometry. The measurements and geometrical conditions provide us with data from three different experimental configurations simultaneously: i) signals from reflection at the top facet of the wire, ii) the same but superimposed with reflections from the wires backside, iii) signals where the light is normally transmitted through the wire and reflected at the substrate. All those were measured for two types of substrates which are SiO_2/Si as well as gold. Especially the transmitted signal, in configuration perpendicular to the wires axis and thus to the crystals *c*- or optic axis, gives us a very sensitive access to the materials birefringence.

[1] R. Schmidt-Grund *et al.*, phys stat sol b, **256**, 1800462 (2019).

HL 75.27 Thu 15:00 P2/3OG

Electrical readout of NV- centers — •Lina Todenhagen and Martin S. Brandt — Walter Schottky Institut and Physik-Department, Technische Universität München, Garching, Germany

The charged nitrogen-vacancy center (NV- center) in diamond is a remarkable option for various quantum technologies. The recently demonstrated, electrical readout dramatically reduces the complexity of NV-based sensing setups compared to the currently more widely used optical readout. Here, we report on the optimization of the electrical readout, in particular by improving the laser pulse sequences used for excitation, photoionization and reset of the NV- center, maximizing the electrically detected contrast.

HL 75.28 Thu 15:00 P2/3OG

Investigation of charge carrier dynamics in Z-scheme water splitting systems — •Nathalie Schmid, Yiou Wang, Jochen Feldmann, and Jacek Stolarczyk — Chair for Photonics and Optoelectronics, Nano-Institute Munich and Department of Physics, Ludwig-Maximilians-Universität (LMU), Königinstr. 10, 80539 Munich, Germany

The so-called "Z-scheme", mimicking the photosystem II - photosystem I in natural photosynthesis, has emerged as a cutting-edge system for efficient photocatalytic water splitting. It consists of two narrow-bandgap semiconductors and is therefore capable of absorbing light in the visible range. One semiconductor acts as oxygen evolution photocatalyst and the other as hydrogen evolution photocatalyst, connected by recycled redox pairs[1,2]. Although the trial-and-error development of materials has boosted the performance over the last two decades, the efficiencies are still far from economically satisfactory. This is mainly due to the lack of fundamental physical knowledge of a Z-scheme photosystem. Therefore, we apply transient absorption spectroscopy to investigate the charge carrier dynamics in an organic/inorganic Z-scheme system, Pt-CN/I-/IO3-/PtOx-WO3 and Pt-CN/Fe2+/Fe3+/BiVO4.

[1] Y. Wang et al., Mimicking Natural Photosynthesis: Solar to Renewable H2 Fuel Synthesis by Z-Scheme Water Splitting Systems. Chem. Rev. 118, 5201 (2018)
[2] J. Stolarczyk et al., Challenges and Prospects in Solar Water Splitting and CO2 Reduction with Inorganic and Hybrid Nanostructures, ACS Catal. 8, 3602 (2018)

HL 75.29 Thu 15:00 P2/3OG

Energieabhängigkeit der Schwellen von Polaritonen-Bistabilität — •Fabian Herbst[1], Daniel Schmidt[1], Manfred Bayer[1,2] und Marc Assmann[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, Dortmund, Germany — [2]Ioffe Institute, St. Petersburg, 194021 Russia

Auf Exziton-Polariton basierende Optikexperimente finden in den letzten Jahren Aufmerksamkeit, unter anderem durch die Entdeckung der Bistabilität von Polaritonen in Mikrokavitäts-Quantentrögen. Diese Bistabilität wird durch eine Blauverschiebung der Polaritonenmode bei

höherer Population hervorgerufen. Wir untersuchen die Energieabhängigkeit ebendieser Bistabilitätsschwellen in einer (In)GaAs-Probe mittels Transmissionsmessung bei resonanter Anregung mit einem CW-Laser.

Bisherige Messungen ließen einen Anstieg der Schwellen mit steigender Laserenergie vermuten. Neue Messungen zeigen jedoch ein anderes Verhalten. Die Bistabilitätsschwelle zeigt, für gewisse Anregungsenergien im Bereich der Polaritonen, Minima der Bistabilitätsschwellen. Dies lässt darauf schließen, dass die Blauverschiebung der Polaritonmode nicht nur abhängig von der Laserleistung ist, sondern auch von der Population eines langlebigen, nicht-radiativ zerfallenden Reservoirs. Bisherige Messungen lassen vermuten, dass es sich hierbei um das Reservoir der Biexzitonen handelt, jedoch muss dies noch hinreichend nachgewiesen werden.

HL 76: Poster IIIC

This poster session includes contributions from the following topics:

- Perovskites and photovoltaics - Organic semiconductors - Ultra-fast phenomena

Please put up your poster at the beginning of the session and remove the poster immediately after the session. The person peresenting the poster should attend it for at least half of the session duration and indicate the time when to find him/her at the poster.

Time: Thursday 15:00–17:30 Location: P2/4OG

HL 76.1 Thu 15:00 P2/4OG

Collective effects of polyaromatitc molecules embedded in rare gas matrices — •Moritz Michelbach, Matthias Bohlen, Rupert Michiels, and Frank Stienkemeier — Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany

Polyaromatic molecules, such as oligoacenens, are promising candidates for organic solar cells. These solar cells can achieve photon-to-current conversion efficiencies beyond the 30% Shockley-Queisser [1] limit. The underlying process responsible for creating multiple charge carriers from a single photon is called singlet fission. In this process, an excited molecule can partially transfer energy to a neighboring ground-state molecule, and thereby create a correlated triplet pair [2]. To investigate collective processes especially singlet fission, we have measured the lifetime of the excited molecule embedded in rare gas matrices. A significant lifetime reduction is observed in the presence of neighboring molecules [3]. As a comparison to isolated molecules on solid cluster surfaces, we use the artificially bound bis-TIPS pentacene molecule [4], which is embedded in superfluid helium nanodroplets.

[1] W. Shockley and H. J. Queisser, J. Appl. Phys. 32, 510 (1961).
[2] M. B. Smith, J. Michl, Chem. Rev. 110, 6891-6936, (2010).
[3] S. Izadnia et al., J. Phys. Chem. Lett. 8, 2068 (2017).
[4] S. R. Reddy, J. Phys. Chem. Lett., 9, 5979-5986, (2018).

HL 76.2 Thu 15:00 P2/4OG

Laser-induced nonthermal diffusion of impurities and vacancies in Silicon — •Christelle Inès Kana Mebou, Tobias Zier, and Martin Garcia — Institut für Physik, Universität Kassel, Germany

Laser-induced disordering processes have been studied intensively during the last decades. In this work, we present investigations of a laser induced ordering process which consists in the controlled mobility of crystal defects. In order to study the possibility to guide vacancies by femtosecond-laser pulses we performed ab initio molecular dynamics simulations of laser-excited Silicon with different defect densities using our code CHIVES (Code for Highly Excited Valence Electron Systems). The objective of this study is to determine the impact of laser excitation on defects (vacancies and impurity atoms) migration in Silicon (Si). Starting from initially randomly distributed defects, we simulated the ultrashort time dynamics of the system after laser heating. As a preliminary results we observed the changed mobility of the vacancies.

HL 76.3 Thu 15:00 P2/4OG

Electrochemical and Spectroelectrochemical Characterization of Methoxylated and Fluorinated $Bis(bis(8-quinolinyl)amide)_2metal(II)$ **Complexes** — •Sophie Göbel[1], Thi Hai Quyen Nguyen[1], Harald Locke[2], Peter R. Schreiner[2], and Derck Schlettwein[1] — [1]Justus Liebig University Gießen, Institute of Applied Physics — [2]Justus Liebig University Gießen, Institute of Organic Chemistry

Organic semiconductors are targeted for applications in flexible electronic devices such as organic transistors. Intermolecular coupling is strongly influenced by the arrangement of molecules in solid state. In this work, well-stacking $bis(bis(8-quinolinyl)amide)_2metal(II)$ molecules with different central cations (Fe, Cr, Zn, and Mn) as well as their corresponding methoxylated and fluorinated derivates were analysed in their electronic and optical properties. Cyclic voltammetry of the molecules in solution was performed in a three-electrode setup to estimate the HOMO- and LUMO level of each molecule. Supporting spectroelectrochemical studies were carried out by in situ UV/Vis spectroscopy for a clear assignment of the redox and oxidation waves. By comparing the unsubstituted with the substituted complexes, a down-shift of the energy levels was observed revealing the inductive and mesomeric effects of the methoxy- and fluoro groups altering the effective electron density in the aromatic core. The obtained values for the energy levels of the different molecules allow good estimations for future investigations of their electrical contact behaviour in devices and performances in thin films.

HL 76.4 Thu 15:00 P2/4OG

Lanthanide Doping of the Double Perovskite $Cs_2AgBiBr_6$ — •Gioele Conforto[1,2], Jonas Horn[1], Fabian Schmitz[2], Teresa Gatti[2], and Derck Schlettwein[1] — [1]Justus Liebig University Gießen, Institute of Applied Physics — [2]Justus Liebig University Gießen, Institute of Physical Chemistry

Studies on inorganic halide perovskite solar cells showed remarkable improvement of the power conversion efficiency in recent years. An alternative to the extensively studied lead perovskites are double perovskites where Pb^{2+} is replaced by a monovalent and a trivalent cation, e. g. $Cs_2AgBiBr_6$. This material is not toxic and very stable. However, it has a large indirect band gap, low charge carrier mobility and weak absorption of visible light that decrease their efficiency. In this work, doping of this double perovskite with lanthanide atoms is studied in order to investigate options to decrease the band gap, improve absorption of visible light and enhance photoluminescence. The material is prepared either by a hydrothermal method in HBr or is used directly from a solution in dimethyl sulfoxide ($DMSO$). Thin films are deposited by spin-coating the (doped) double perovskite on fluorine doped tin oxide (FTO) or quartz glass substrates. Structure and composition are characterized by XRD, Raman and SEM-EDX analysis. In addition, optical properties are investigated by the use of UV-Vis absorption and photoluminescence spectroscopy. Small amounts of Eu led to the expected changes of the lattice constant but do not substantially change the absorption characteristics.

HL 76.5 Thu 15:00 P2/4OG

Light and electron beam induced current analysis of perovskite solar cells — •Felix Müller, Tobias Westphal, and Michael Seibt — University of Göttingen, IV. Physical Institute, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

As perovskite solar cells showing promising properties for future photovoltaics it is of interest to investigate their electronic properties. Light beam induced current (LBIC) or electron beam induced current (EBIC) are well-established techniques to study excess carrier recombination, i.e. to measure their diffusion length and to investigate recombination at extended defects. Both methods locally generate excess charge carriers in a certain generation volume beneath the spot where the beam (electron or light) hits the sample resulting in a short circuit current in a charge-separating junction. A current map is generated

by scanning the beam over the sample.

As the spot size of an electron beam is typically smaller than the spot size of a laser, EBIC has a potentially higher spatial resolution. Some perovskites, however, suffer from beam damage produced by high energy electrons inside the SEM which is nearly no problem using LBIC. Despite a reduced spatial resolution of LBIC the excitation energy can be varied by using laser diodes with different wavelengths, to be sensitive to different band gaps.

In our present work we have measured LBIC and EBIC maps of the same perovskite samples to compare them regarding the mentioned properties of both methods. Combining the results of both we achieve a more complete picture of the sample's electronic characteristics.

HL 76.6 Thu 15:00 P2/4OG

Temperature-Depandent Impedance Spectroscopy of a Transition Metal Oxide Perovskite Heterojunction — Michael Seibt[1], Christian Jooss[2], Tobias Meyer[1], Birte Kressdorf[2], and •Mucun Yang[1] — [1]IV. Physical Institute, Uni-Goettingen, Goettingen, Germany — [2]Institute of Material Physics, Uni-Goettingen, Goettingen, Germany

Some organic perovskite materials are recently more frequently used for sollar cells because of their high efficiency of photovoltaic behaviours. In this work, capacitance-voltage (C-V) characteristics of $Pr_{0.66}$$Ca_{0.34}MnO_{3}$-Sr$Ti_{0.998}$$Nb_{0.002}$$O_{3}$ perovskite heterojunction is studied by using impedance analyzer, which can calculate the capacitance with the help of impedance spectroscopy. The temperature dependence of C-V measurements is examined in a tmeperature range between 300 K and 40 K. The frequency dependence of capacitance is also observed in the range from 10^{2} Hz up to 10^{7} Hz under AC condition. In addition, an another factor which might greatly affect the capacitance are the electron's deep level states, which might be partially formed by interface states induced by mismatch of lattice structures at the interface of heterojunction. The deep level states can be charged and discharged only at low frequencies, thus the properties and behaviours of deep level states are investigated under low frequency condition in the range between 10^{2} Hz and 10^{3} Hz.

HL 76.7 Thu 15:00 P2/4OG

Optical properties of metal-organic-bis(8-quinolinyl)amide complexes — •Nicolas Broda[1,4], Harald Locke[2,4], Pascal Schweitzer[3,4], Detlev Hofmann[1,4], Peter Schreiner[2,4], Derck Schlettwein[3,4], and Sangam Chatterjee[1,4] — [1]I. Physikalisches Institut, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany — [2]Institut für Organische Chemie, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany — [3]Institut für Angewandte Physik, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany — [4]Zentrum für Materialforschung (ZfM), Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

Organic semiconductors are advanced functional materials, for nextgeneration optoelectronic devices. Here, we report the optical properties of neutral metal-organic complexes with two pincer-type bis(8- quinolinyl)amide (BQA) ligands. In particular, we analyse a series of transition-metal-BQA-complexes where the central metal atom is varied by photoluminescence and absorption spectroscopies. Prominent optical transitions are observed in the spectral range between 350nm and 900nm. The transition energies depend on the central metal atom of the BQA complexes, namely Zn, Fe, Mn or Cr. The measurements are analysed in the frame of configuration coordinate models. Our results show that the materials are suitable for organic semiconductors and organic solar cell application.

HL 76.8 Thu 15:00 P2/4OG

Nano-floating gate memory based on lead halide perovskite nanocrystals — •Tianhao Jiang[1,2], Martin Stutzmann[1], Xiujuan Zhang[2], and Jiansheng Jie[2] — [1]Walter Schottky Institut, TUM, Munich, Germany — [2]Institute of Functional Nano & Soft Materials, Suzhou, China

Lead halide perovskites have been extensively investigated in a host of optoelectronic devices, such as solar cells, light-emitting diodes, and photodetectors. The halogen vacancy defects arising from halogen-poor growth environment are normally regarded as an unfavorable factor to restrict the device performance. Here,for the first time, we demonstrate the utilization of the vacancy defects in lead halide perovskite nanostructures for achieving high-performance nano-floating gate memories (NFGMs). CH3NH3PbBr3 nanocrystals (NCs) were uniformly decorated on CdS nanoribbon (NR) surface via a facile dip-coating process, forming a CdS NR-CH3NH3PbBr3 NCs core-shell structure. Significantly, owing to the existence of sufficient carrier trapping states in CH3NH3PbBr3 NCs, the hybrid device possessed an ultra-large memory window up to 77.4 V, a long retention time of 12 000 s, a high current ON/OFF ratio of 7*107, and a long-term air stability for 50 days. This work paves the way toward the fabrication of new-generation, high-capacity nonvolatile memories using lead halide perovskite nanostructures.

HL 76.9 Thu 15:00 P2/4OG

Electrical characterization of deep levels inside sulfur hyperdoped silicon based on graded junction calculations — •Erica F. Warth Pérez Arias[1], Arne Ahrens[1], Anna L. Baumann[2], Wolfgang Schade[2], and Michael Seibt[1] — [1]University of Goettingen, IV. Physical Institute, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Fraunhofer Heinrich Hertz Institute HHI, Am Stollen 19H, 38640 Goslar, Germany

Semiconductor devices are the constituent of a considerable amount of technologies such as transistors, solar cells and LEDs. The performance of such devices can be changed by deep defects inside the material, which can lead on one hand to a decreased diffusion length of charge carriers and increased current leakages [1]. On the other hand, deep levels at very high concentrations may form intermediate bands, which is well established for sulfur hyperdoped silicon [2], leading to an increased infrared absorption in the case of solar cells or photodetectors. Nearly exponential sulfur concentration depth profiles have been observed in such materials [3], giving rise to graded p-n junctions.

Therefore, this work analyses the depth profile of deep traps inside sulfur hyperdoped silicon using CV and DLTS measurements, under the implementation of a graded p-n junction model.

[1] K. A. Jackson et. al.; Handbook of Semiconductor Technology, Deep Centers in Semiconductors Vol. 1. WILEY-VCH (2000)

[2] M.T. Winkler et al.; Phys. Rev. Lett. 106, 178701 (2011)

[3] P. Saring, et. al. ; Appl. Phys. Lett. 103, 061904 (2013)

HL 76.10 Thu 15:00 P2/4OG

Thermally evaporated two dimensional perovskites for photovoltaic applications — •Zongbao Zhang, Ran Ji, Martin Kroll, Changsoon Cho, Tim Schramm, Frederik Nehm, Yana Vaynzof, and Karl Leo — Dresden Integrated Center for Applied Physics and Photonic Materials, Dresden,Germany

Organic-inorganic hybrid perovskite solar cells have demonstrated remarkable progress recently. Despite their excellent photovoltaic performance, their instability upon exposure to oxygen and moisture remains a critical challenge that needs to be mitigated prior to their commercialization. It has been recently shown that two-dimensional (2D) perovskites exhibit excellent stability, far surpassing that of traditional 3D perovskites. Solar cells with 2D perovskite have recently reached a high efficiency of over 18%. Most commonly, these devices are fabricated via solution processing, which has yet to prove feasibility for industrial mass production, with only very few reports of vacuum evaporated 2D perovskites. Here, we fabricate 2D perovskites ((PEA)2(MA)n-1PbnI3n+1, (PEA)2Csn-1PbnI3n+1) via thermal evaporation and analyze their microstructure, crystallinity and optical properties. We find that the crystal structure of evaporated 2D perovskites is in excellent agreement with previous results reported for solution-processed fabrication. Similarly, the optical properties of the evaporated and solution-processed 2D perovskites are very similar. Our results highlight the efficacy of thermal evaporation as a tool for the formation of 2D perovskites of high electronic quality - a promising route for their integration into a range of optoelectronic applications.

HL 76.11 Thu 15:00 P2/4OG

Multistable circular currents of polariton condensates trapped in ring potentials — •Franziska Barkhausen[1], Stefan Schumacher[1,2], and Xuekai Ma[1] — [1]Department of Physics and CeOPP, Universität Paderborn, Paderborn, Germany — [2]College of Optical Sciences, University of Arizona, Tucson, AZ 85721, USA

Vortices occur in a broad range of nonlinear systems. They have been widely investigated in many physical systems and different materials for their fundamental interest and for applications in data storage and information processing. In polariton condensates in planar semiconductor microcavities vortices can be supported and trapped by a ring-shaped potential, for example optically induced using spatially structured non-resonant excitation [1,2]. Here we theoretically study vortices excited non-resonantly in a fabricated ring-shaped external

potential. This kind of potential traps the polariton condensate such that different steady-state solutions, oscillating or rotating solutions can be formed, depending on the width and depth of the potential. For a narrow and shallow potential, multistable ring solutions can be stabilized carrying different orbital angular momenta (OAM) but the same ring-shaped density structure. By increasing the confinement of the potential, a higher mode together with the fundamental mode can be excited. Their beating generates an oscillating solution if they have the same OAM or a spatially rotating solution if they have different OAM.

[1] X. Ma and S. Schumacher, Phys. Rev. Lett. 121, 227404 (2018).
[2] X. Ma et al., arXiv: 1907.03171 (2019).

HL 76.12 Thu 15:00 P2/4OG

Photoluminescence studies of organic microcrystals with π-conjugated core/shell molecule — Aswin Asaithambi[1], Kohei Iwai[2], •Guenther Prinz[1], Hiroshi Yamagishi[2], Yohei Yamamoto[2], and Axel Lorke[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Duisburg, Germany — [2]Division of Material Science, Faculty of Pure and Applied Sciences, University of Tsukuba, Tsukuba, Japan

Organic crystals in optoelectronic devices such as LEDs or solar cells have drawn a lot of attention in the last years. Oligo(p-phenylene vinylene) (OPV) molecules have many interesting properties such as a well-defined architecture and the ability to be modified with functionalized endgroups opening up an exciting number of functional assemblies. π-conjugated core/shell molecules can be grown into crystalline solids.

Here, we report on photoluminescence studies of eye-shaped crystals synthesized from fluorescent π-conjugated core/shell molecules. These crystals emit light in the green spectral range under 405 nm excitation. The spatial profile of the emission is not completely symmetric and depends on the excitation spot within the crystal. This already indicates a special orientation of the molecules within the crystal. XRD data also shows distinct diffraction peaks for these crystals, showing that the molecules are well ordered. Polarization dependent absorption and emission studies show an angle dependent characteristic of the light emission of these crystals, which will be discussed regarding the crystal and molecular orientation.

HL 76.13 Thu 15:00 P2/4OG

Universal short-time response and formation of correlations after quantum quenches — •Klaus Morawetz — Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil

The short-time evolutions of two distinct systems, the pump and probe experiments with a semiconductor and the sudden quench of cold atoms in an optical lattice, are found to be described by the same universal response function. This analytic formula at short time scales is derived from the quantum kinetic-theory approach observing that correlations need time to form. The demand of density conservation leads to a reduction of the relaxation time by a factor of 4 in quench setups. The influence of the finite-trapping potential is derived and discussed along with Singwi-Sjølander local-field corrections including the proof of sum rules. The quantum kinetic equation allows to understand how two-particle correlations are formed and how the screening and collective modes are build up.
Phys. Rev. B 90 (2014) 075303, Phys. Rev. E 66 (2002) 022103, Phys. Rev. E 63 (2001) 20102, Phys. Lett. A 246 (1998) 311

HL 76.14 Thu 15:00 P2/4OG

Organic field effect transistors based on PNDIT2 polymers — •Annika Morgenstern[1], Apoorva Sharma[1], Georgeta Salvan[1], Dietrich R. T. Zahn[1], and Michael Sommer[2] — [1]Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz — [2]Polymer Chemistry, Chemnitz University of Technology, D-09107 Chemnitz

Organic field effect transistors (OFETs) based on polymers have attracted significant attention thanks to the availability of high-mobility polymers. Polymers are cost-efficient in production and can be deposited on almost any substrate. There are already numerous studies dedicated top-gate geometry OFETs and p-type polymers. These studies showed that the mobility is highly influenced by the chain length and the crystallinity of the polymer. Studies of n-type polymers in bottom-gate geometry are scarce. Here we present the characterization of bottom-gate OFETs based on the n-type polymer PNDIT2. This geometry is useful, for example, for further measurements of the photoinduced charge transport by light irradiation. The PNDIT2 films were deposited by spin coating onto prestructured substrates having Au source and drain electrodes on top of a 232,4 nm SiO2 gate dielectric layer. An additional PMMA layer was required to prevent the oxidation of the polymer film. The influence of the molar mass of the polymer, of the crystalline order of the films and of the channel length on the transistor characteristics and the electron mobility was determined.

HL 76.15 Thu 15:00 P2/4OG

Synthesis and nanoscale characterization of perovskite single crystals using scanning probe techniques — •Andrei Karabanov, Marianela Escobar, Vladimir V. Shvartsman, and Doru C. Lupascu — Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Universitätsstraße 15, 45141 Essen, Germany

In the last ten years enormous efforts have been put into the research of hybrid perovskites as an absorbing material for solar cells. These materials show excellent photovoltaic properties not only in single, but also in tandem devices. However, the physical nature and the underlying mechanisms of such excellent photovoltaic performance are still unclear.

Here we report on solution growth of MAPbBr3 single crystals. We studied the effect of the precursor concentration and temperature on the crystal quality. We found that the high concentrations of precursor in dimethylformamide solvent (0.9-1 g/ml) and the temperature range of 40-50 °C are optimal to get good quality cubic-shaped MAPbBr3 crystals with the (110) orientation. The dielectric, ferroelectric, and photovoltaic properties of the crystals are studied in details both macroscopically and locally.

HL 76.16 Thu 15:00 P2/4OG

Analysis of semitransparent top contact induced Voc losses and their influences on long term stability in tandem solar cells — •Bor Li, Amran Al-Ashouri, Marko Jošt, Eike Köhnen, Marlene Härtel, Hans Köbler, and Steve Albrecht — HZB, Berlin, Germany

Semitransparent top contact layers are a key element for high efficiency perovskite based tandem solar cells. In addition, these layers, namely atomic layer deposited (ALD) tin oxide (SnO2) and sputtered indium zinc oxide (IZO) protect the perovskite solar cells against decomposition reactions in humid air and at high temperature, thus improving long term stability. However, they often induce fill factor (FF) and open circuit voltage (Voc) losses due to e.g. improper energetic alignment and/or defect generation during deposition. In this work, these effects are quantified and it is shown how Voc losses can be mitigated by using different additives and ultrathin interlayers between the perovskite absorber and the n-type top contact. By introducing modifications such as LiF interlayer or phenyl ethylammonium iodide (PEAI) additive, the non-radiative recombination losses can be reduced. This is proven by an increased steady-state photoluminescence yield and improvements in Voc. The successful absorber and interface modifications, together with the evaluation of stability and efficiency enhancement, were integrated into monolithic perovskite/silicon tandem solar cells. These modifications aim to increase the performance and stability of perovskite solar cell structures and to get one step closer towards commercial availability of this tandem solar cell technology.

HL 76.17 Thu 15:00 P2/4OG

Coherent Dynamics in Rhenium Disulphide Studied by Ultrafast Electron Diffraction — •Ahmed Hassanien, Arne Ungeheuer, Mashood Tariq Mir, Arne Senftleben, and Thomas Baumert — Institute of Physics and CINSaT, University of Kassel, Heinrich-Plett-Strasse 40, D-34132 Kassel, Germany

Coherent phonons are interesting phenomenona where lattice vibrations are coherently excited by the impact of an ultrashort laser pulse. While pump-probe-based reflectometry experiments provide an indirect visualization for such coherent phenomena [1], Ultrafast electron diffraction represents a direct visualization of the coherent atomic oscillations providing an insight into the electron-phonon coupling strength [2]. Using a highly compact femtosecond electron diffractometer developed in our group [3], we were able to probe the coherent structural dynamics of mechanically-exfoliated few-layers ReS2 revealed on a picosecond time scale, following the photoexcitation by femtosecond laser pulses. ReS2 shows highly anisotropic structure due to which its optical properties showed significant polarization-dependence compared

to TMDCs of hexagonal structure [4]. In this work we also concluded about the dependence of the electron-phonon coupling strength on the polarization state of the excitation pulse.

References: [1] Ishioka, Kunie, et al. Journal of Physics:Condensed Matter 31.9 (2019):094003. [2] Chatelain, Robert P., et al. Physical review letters 113.23 (2014):235502. [3] Gerbig, C., et al. New J. Phys. 17.4 (2015):043050. [4] Cui, Yudong, et al. Scientific Reports 7 (2017):40080.

HL 76.18 Thu 15:00 P2/4OG

Progress in the Vapour Deposition of Organic-inorganic Hybrid Metal-halide Perovskite Thin-films — •Juliane Borchert[1], Ievgen Levchuk[2], Lavina C. Snoek[1], Mathias Uller Rothmann[1], Henry J. Snaith[1], Laura M. Herz[1], Christoph J. Brabec[2], and Michael B. Johnston[1] — [1]Clarendon Laboratory, Department of Physics, University of Oxford — [2]Materials for Electronics and Energy Technology (i-MEET), FAU Erlangen-Nürnberg, Erlangen, Germany

Hybrid metal-halide perovskites are promising semiconductors for use in solar cells, LEDs and other optoelectronic devices. Especially their application in solar cells has attracted a lot of research attention in recent years, due to the rapid rise of solar cell efficiencies for these materials. Record efficiencies have now reached to above 24%. Co-evaporation of perovskite thin-films for solar cells offers many advantages such as precise thickness control, pinhole free planar films and compatibility with a large range of different substrates. The very planar films achieved with co-evaporation have enabled in-depth optoelectronic studies of perovskite materials. Furthermore co-evaporation is a promising technique for the upscaling of perovskite solar cells to commercial scales. Some challenges remain, including optimisation of the process control and relatively small crystallites in the deposited films. Additionally, it is more challenging to achieve mixed compositions with co-evaporation than with solution processing. Here we present recent progress made to address these challenges.

HL 76.19 Thu 15:00 P2/4OG

Transient negative thermal expansion in HgTe/CdTe heterostructures by heating transverse phonons — •Matthias Rössle[1], Marc Herzog[2], Jan Pudell[2], Wolfram Leitenberger[2], Maximilian Mattern[1,2], Lukas Lunczer[3], Claus Schumacher[3], Harmut Buhmann[3], Laurens Molenkamp[3], and Matias Bargheer[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Germany — [2]Institut für Physik und Astronomie, Universität Potsdam, Germany — [3]Physikalisches Institut EP3, Universität Würzburg, Germany

We investigate the transient negative thermal expansion of semimetallic HgTe and semiconducting CdTe by using synchrotron-based time-resolved X-ray diffraction. At $T = 20\,\mathrm{K}$, far below the Debye temperature of both materials, the selective optical excitation of the HgTe top layer with an ultrashort near-infrared laser pulse leads to a rapid expansion of HgTe that is followed by a long lasting contraction. The CdTe substrate is compressed by the HgTe thin film expansion, and subsequently CdTe contracts due to thermally excited transverse phonon modes. This shows that negative thermal expansion is manifest on ultrafast timescales, consistent with the negative Grüneisen coefficient for transverse phonons in semiconducting materials with sphalerite crystal structure. At $T = 200\,\mathrm{K}$, far above the Debye temperature of both materials, the expansion driven by longitudinal acoustic phonons is prevalent. We simulate the lattice dynamics in an elastic model where transient thermal stresses are calculated via heat diffusion based on equilibrium thermoacoustic properties.

HL 76.20 Thu 15:00 P2/4OG

Coupling dynamics of coherent acoustic phonons in a Graphite−MoS_2 heterostructure observed by ultrafast electron diffraction — •Arne Ungeheuer, Ahmed Hassanien, Arne Senftleben, Mashood Mir, and Thomas Baumert — University of Kassel, Institute of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), D-34132 Kassel, Germany

We investigate the coupling dynamics of coherent acoustic phonons in a Graphite−MoS_2 heterostructure, excited with a femtosecond laser pulse. Since the MoS_2 layer is transparent at our excitation wavelength of 785 nm, the coherent acoustic phonons are first excited exclusively in the Graphite layer. The subsequent coupling dynamics between the two materials are then probed with an ultrashort electron pulse imaging the transient by varying the delay time between pump- and probe-pulse. Furthermore we aim to coherently control these dynamics by using a double-pulse sequence for excitation. Amplification or annihilation of the coherent acoustic phonons in the Graphite layer can be achieved by adjusting the time-delay between the two excitation pulses.

HL 76.21 Thu 15:00 P2/4OG

Investigating 2D block array for OLED light outcoupling — •Dinara Samigullina[1], Paul-Anton Will[1], Simone Lenk[1], Lydia Galle[2], Stefan Kaskel[2], and Sebastian Reineke[1] — [1]Integrated Center for Applied Physics and Photonic Materials, TU Dresden — [2]Chair of Inorganic Chemistry I, TU Dresden

Organic Light-Emitting Diodes (OLEDs) have already been established in the industry and have a high potential in the future in backlight-free displays, portable displays and lighting applications. However, to achieve high efficiency, the light outcoupling needs to be improved because the high refractive index of organic materials limits light extraction. Some of the generated light remains trapped in the OLED due to total internal reflection. For this reason, light outcoupling structures are used to extract light from the OLED and increase the External Quantum Efficiency (EQE).

In this work, 2D TiO_2 block arrays were implemented to the bottom-emitting OLEDs to increase the amount of extracted light by scattering. Different periods of the blocks were investigated with an ultimate goal to achieve maximum EQE improvement. All the samples with the outcoupling structures showed an efficiency increase. The highest EQE is 23.6% for the blocks with a period of 700 nm and height of 90 nm. The enhancement is 16.3%. Additionally, the effectiveness of the structures, i.e. the fraction of extracted photons, was calculated according to reference [P.-A. Will et al., Adv.Fun.Mat., 29, 1901748 (2019)].

HL 76.22 Thu 15:00 P2/4OG

irradiance dependent photoresponse organic near infrared photodetectors for distance measurement — •yazhong wang[1], christoph lungenschmied[2], karl leo[1], and donato spoltore[1] — [1]iapp, tu dresden, dresden, germany — [2]trinamix gmbh, industriestrasse 35, 67063 ludwigshafen am rhein, germany

Focus-Induced Photoresponse (FIP) technique is a new and elegant optical distance measurement solution. Organic near infrared (NIR) optical distance photodetectors based on FIP technique are irradiance dependent which is realized by inserting an extraction barrier for holes within the photodetectors. In this work, the barrier is introduced by replacing the normal hole transporting layer (HTL) material with a deeper highest occupied molecular orbital (HOMO) HTL material into an organic solar cell device. Holes are piled up by the extraction barrier, which increases the probability of charge recombination. With increasing irradiance, which can be achieved by decreasing the illumination spot area on the photodetector, the probability of charge recombination is becoming higher and higher. We demonstrate the organic NIR optical distance photodetectors with detection area up to 2.52 cm2 and detection wavelengths at 850 nm and 1060 nm. Such NIR photodetectors have highly potential to be utilized as robust, low-cost and simple optical distance measurement setup.

HL 76.23 Thu 15:00 P2/4OG

Transient negative thermal expansion and Poisson effect — •Marc Herzog[1], Alexander von Reppert[1], and Matias Bargheer[1,2] — [1]Institut für Physik und Astronomie, Universität Potsdam — [2]Helmholtz-Zentrum Berlin für Materialien und Energie

Negative thermal expansion (NTE) and the Poisson effect have been mainly studied in thermal equilibrium. Here we discuss the two phenomena in the context of strain waves generated by ultrafast excitation of various material systems that exhibit NTE in thermal equilibrium. These materials range from simple semiconductors to various spin- or charge ordered phases such as (anti-)ferromagnets and ferroelectrics. As NTE can be generally understood from increasing entropy with decreasing volume, we discuss ultrafast entropic stresses as the driver of lattice dynamics.

HL 76.24 Thu 15:00 P2/4OG

Effects of controlled slot-die-printing on halide perovskite films — •Meike Kuhn, Christopher Greve, and Eva M. Herzig — Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany

Perovskite solar cells gained a lot of interest because of their steeply increasing efficiency in the last years. But Perovskite materials in

general are of strong interest due to their transport properties which are strongly linked to their nanostructure. There are different ways to deposit perovskite films, but for fabrication of large-area films methods like spin coating are hard to realize. So it is important to improve the fabrication of films by printing. By using a slot-die-printing system, we test different environmental control parameters and solvents to get a homogeneous perovskite layer. These parameters determine the structure of the perovskite layer [1] and thus the transport performance.

References

[1] Filonik, Oliver; Thordardottir, Margret E.; Lebert, Jenny; Pröller, Stephan; Weiß, Sebastian; Haur, Lew J.; Priyadarshi, Anish; Fontaine, Philippe; Müller-Buschbaum, Peter; Mathews, Nripan; Herzig, Eva M., Energy Technology, 7(10), 1900343, 2019

HL 76.25 Thu 15:00 P2/4OG

Surface charge-carrier dynamics of $CsPbBr_3$ inorganic perovskite — •Felix Trunk, Janek Rieger, Thomas Fauster, and Daniel Niesner — Lehrstuhl für Festkörperphysik, Friedrich-Alexander University Erlangen-Nürnberg (FAU), Staudtstr. 7, D-91058 Erlangen, Germany

Several models have been proposed to understand the outstanding long lifetimes of charge carriers in lead-halide perovskites. Amongst others, there is an ongoing debate about the role of the organic ion on the charge-carrier cooling. We investigated the femto- to picosecond dynamics of conduction-band electrons at the surface of the purely inorganic perovskite $CsPbBr_3$.

Time-resolved bichromatic two-photon photoelectron spectroscopy with femtosecond time-resolution was carried out on epitaxially grown films with well-defined crystalline surfaces. The position of the conduction-band minimum indicates that our samples are intrinsic. Therefore, the carrier dynamics is dominated by electron-phonon scattering rather than electron-electron scattering.

In a systematic study, we could identify three different time regimes. After the initial cooling we can detect a second time constant before the charge carriers recombine.

The poster will focus on a comparison of carrier dynamics for different sample temperatures and thicknesses. From the latter we can distinguish carrier recombination at the surface from their diffusion into the bulk.

HL 76.26 Thu 15:00 P2/4OG

Universal Pure Aromatic Hydrocarbon Hosts for High-Efficiency Phosphorescent Organic Light-Emitting Diodes — •Qiang Wang[2,3], Fabien Lucas[1], Cassandre Quinton[1], Liang-Sheng Liao[2], Zuo-Quan Jiang[2], and Cyril Poriel[1] — [1]Univ Rennes, CNRS, ISCR- UMR 6226 35000 Rennes, France — [2]Institute of Functional Nano & Soft Materials, Soochow University Suzhou 215123, P. R. China — [3]Institut für Physik & IRIS Adlershof Humboldt-Universität zu Berlin 12489 Berlin, Germany

In the field of phosphorescent organic light-emitting diodes (PhOLEDs), heteroatoms are prescriptively used to design host materials with controlled optoelectronic properties. To date, all the very high-efficiency universal hosts reported incorporate heteroatoms. However, one of the inherent issues of heteroatom-based hosts is the fragile heteroatom bonds, which causes instability in device performance. Here, we show that pure aromatic hydrocarbons hosts designed with the spirobifluorene scaffold are highly efficient and versatile hosts for PhOLEDs. With external quantum efficiencies of 27.1%, 26.0% and 27.3% for red, green and blue PhOLEDs respectively, this work not only reports the first example of high-efficiency pure hydrocarbon host in RGB PhOLEDs but also among the highest performance reported universal host. The overall performance demonstrates that pure aromatic hydrocarbons can provide new perspectives in the design of functional materials for PhOLEDs.

HL 77: Annual General Meeting of the Semiconductor Physics Division

Time: Thursday 18:00–19:00 Location: POT 81

Duration 60 min.

HL 78: Nano- and Optomechanics (jointly with CPP, DS, DY, BP) (joint session TT/HL/CPP)

Time: Friday 9:30–10:30 Location: HSZ 03

Invited Talk HL 78.1 Fri 9:30 HSZ 03

Microwave Optomechanics with Superconducting Quantum Interference Cavities — •Daniel Bothner, Ines C. Rodrigues, and Gary A. Steele — Kavli Institute of Nanoscience, Delft University of Technology, PO Box 5046, 2600GA Delft, The Netherlands

Within the recent decade, cavity optomechanics has achieved tremendous breakthroughs regarding the detection and control of macroscopic mechanical oscillators with electromagnetic radiation. Among the most groundbreaking results are displacement sensing beyond the standard quantum limit, quantum ground-state sideband cooling and the generation of non-classical states of motion in massive mechanical objects. With most current approaches for optomechanical systems, however, the nonlinear single-photon regime seems still far out of reach.

Here, I will introduce a recently realized, novel approach for coupling microwave fields in a superconducting circuit to mechanical motion: flux-mediated microwave optomechanics. In this approach, mechanical motion is transduced to magnetic flux, which couples into a superconducting quantum interference device (SQUID). The SQUID forms the inductor of a superconducting microwave circuit and the coupling strength between the microwave circuit and the mechanical displacement is tunable and scales with the magnitude of the magnetic transduction field. Due to the linear scaling behavior, this flux-mediated approach has been predicted to have the realistic potential to reach the fully nonlinear regime of the optomechanical coupling, opening the door for the preparation of mechanical quantum states and a new generation of optomechanical devices.

HL 78.2 Fri 10:00 HSZ 03

Magnetoelastic readout concepts — •Daniel Schwienbacher[1,2,3], Nynke Vlietstra[1,2], Thomas Luschmann[1,2,3], Rudolf Gross[1,2,3], and Hans Huebl[1,2,3] — [1]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, Technische Universität München, Garching, Germany — [3]Munich Center for Quantum Science and Technologies, München, Germany

Nanostring resonators are prime candidates for mechanical sensing applications. Typically, they are used for mass and force sensing. However, it is also possible to use these resonators for the investigation of solid state properties of materials, like magnetoelastics. We investigated the mechanical motion of a 60 μm long SiN/Co bi-layer nanostring resonator with a resonance frequency in the MHz range. Here, we simultaneously use optical and electrical readout techniques. We observe the well known impact of the magnetoelastics, due to the presence of Co, on the resonance frequency of the nanostring. In addition, we study the impact of electrical transport through the string resonator on the mechanical properties of the system.

HL 78.3 Fri 10:15 HSZ 03

Magnetomechanical Crystals — •T. Luschmann[1,2,3], D. Schwienbacher[1,2,3], J. Graf[4], F. Engelhardt[4], S. Viola Kusminskiy[4], R. Gross[1,2,3], and H. Huebl[1,2,3] — [1]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, Technische Universität München, Garching, Germany — [3]Munich Center for Quantum Science and Technologies, München, Germany — [4]Max Planck Institute for the Science of Light, Erlangen, Germany

Optomechanical crystals have become an established platform for the investigation of light-matter interaction, specifically in the context of optomechanical interaction. The success of this concept is founded in the simultaneous localization of GHz frequency phonons alongside THz photons in a suspended nanostructure [1]. We expand this concept with the introduction of magnetic materials capable of supporting spin-wave resonances in the GHz frequency range. We present finite element studies of phononic crystal cavities alongside micromagnetic simulations of spin-waves in nanostructured magnetic materials to tailor the geometries towards the realization of resonant, artificial magnon-phonon coupling. In addition, we will quantitatively compare numerical simulations with early experimental data.

[1] Eichenfield et al. Nature **462**, 7882 (2009).

HL 79: Quantum dots and wires IV

Time: Friday 9:30–12:00 Location: POT 151

HL 79.1 Fri 9:30 POT 151

Controlling entanglement in different realms — •Kisa Barkemeyer[1], Samir Bounouar[2], Stephan Reitzenstein[2], Andreas Knorr[1], and Alexander Carmele[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Entanglement lies at the heart of many applications in the field of quantum information processing. As a platform for their implementation, photonic degrees of freedom are promising candidates. Thus, the ability to efficiently control and tailor quantum optical properties is a central goal.

Photon pairs entangled in their polarization degrees of freedom are, for example, generated in a quantum dot biexciton cascade. We study how the measured degree of entanglement is influenced by the properties of the quantum dot as well as by the measurement setup itself [1]. For this system, it is possible to control the entanglement properties using coherent time-delayed feedback [2]. We aim to extend this scheme to a new realm by focussing on energy-time entanglement inspired by the paradigmatic Franson interferometer [3].

[1] S. Bounouar et al., manuscript in preparation.
[2] K. Barkemeyer, R. Finsterhölzl, A. Knorr, and A. Carmele, Adv. Quantum Technol. 1900078 (2019).
[3] J. D. Franson, Phys. Rev. Lett. 62, 2205 (1989).

HL 79.2 Fri 9:45 POT 151

Polarization Resolved Excitation Spectroscopy on GaAs Quantum Dots — •Caspar Hopfmann[1], Robert Keil[1], Nand Lal Sharma[1], Fei Ding[2], and Oliver Schmidt[1,3] — [1]Institute for Integrative Nanosciences, Leibniz IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [2]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstraße 2, 30167 Hannover, Germany — [3]Material Systems for Nanoelectronics, Technische Universität Chemnitz, 09107 Chemnitz, Germany

Entangled photon sources based on Aluminum droplet etched GaAs quantum dots embedded in a AlGaAs matrix have attracted considerable research interest for applications such as quantum entanglement swapping [1]. In order to use these devices for more advanced quantum optical experiments - such as photonic cluster states [2] - a keen understanding of the quantum dot electronic structure of both fundamental and excited states is essential. We employ combined quasi-resonant and polarization resolved photo excitation spectroscopy in order to investigate the electronic structure of GaAs quantum dots comprehensively.

[1] Zopf et. al. PRL 123, 160502 (2019)
[2] Schwartz et. al. Science, 354.6311 (2016)

HL 79.3 Fri 10:00 POT 151

Towards photocurrent monitoring of single photon emitters — •Sebastian Krehs, Björn Jonas, Alex Widhalm, Kai Spychala, Timo Langer, Dirk Reuter, and Artur Zrenner — Physics Department, Paderborn University, Warburger Straße 100, 33098 Paderborn, Germany

In the past photocurrent (PC) detection of single quantum dot excitons was limited to the regime of high tunnelling rates and elevated excitation powers, which results for π-pulse excitation in currents in the 10 pA-range. Refined PC detection enabled us to improve the sensitivity down to the fA-range. This allows for ultrasensitive photocurrent detection in the regime of single photon emission and leads to a new concept for the frequency stabilization of single photon emitters.

In this work we have fabricated Schottky photodiodes with embedded high quality MBE grown InAs/GaAs QDs. We have been able to demonstrate exciton ground state linewidths as low as 1.62 μeV by electrically detected laser spectroscopy. Our results are close to the Fourier transform limit of QD systems [1]. Extremely weak electric detection of the resonance position of a single photon emitter is possible down to a regime, where only 0.2% of the excitation is extracted by charge separation. To utilize this, we need to realize a seamless electric field induced transition from the PC- to the PL-regime, which avoids the formation of charged states. To achieve this, we performed band structure engineering for the symmetrisation of electron and hole tunnelling rates.

[1] A.V. Kuhlmann et al. Nature Physics 9, 570-575 (2013)

HL 79.4 Fri 10:15 POT 151

Importance of the effect of correlation on the response of weakly confining QDs to applied magnetic field — •Petr Klenovský[1,2,3], Diana Csontosová[1,2], Daniel Huber[4,5], and Armando Rastelli[4] — [1]Department of Condensed Matter Physics, Faculty of Science, Masaryk University, Kotlářská 267/2, 61137 Brno, Czech Republic — [2]Central European Institute of Technology, Masaryk University, Kamenice 753/5, 62500 Brno, Czech Republic — [3]Czech Metrology Institute, Okružní 31, 63800 Brno, Czech Republic — [4]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, Altenbergerstr. 69, 4040 Linz, Austria — [5]Secure and Correct Systems Lab, Linz Institute of Technology, Altenbergerstr. 69, 4040 Linz, Austria

We study magnetic field response of the charged and neutral excitonic states weakly confined in single GaAs/AlGaAs quantum dots obtained by the Al droplet-etching method. [1] Using direct comparison of the results of single-particle theory and the configuration interaction method, we show that the widely used single-particle Zeeman Hamiltonian cannot be used to extract reliable values of the g-factors and diamagnetic coefficients, nor to single out those for individual electrons and holes. The results are supported by extensive μ-photoluminescence measurements in Voigt and Faraday configurations of the applied magnetic field.

[1] Huber, D., *et al.*, arXiv:1909.04906 (2019).

15 min. break.

HL 79.5 Fri 10:45 POT 151

Radiative Auger Process in the Single Photon Limit on a Quantum Dot — •Matthias C. Löbl[1], Clemens Spinnler[1], Alisa Javadi[1], Liang Zhai[1], Giang N. Nguyen[1,2], Julian Ritzmann[2], Leonardo Midolo[3], Peter Lodahl[3], Andreas D. Wieck[2], Arne Ludwig[2], and Richard J. Warburton[1] — [1]University of Basel, Switzerland — [2]Ruhr-Universität Bochum, Germany — [3]Niels Bohr Institute Copenhagen, Denmark

In a quantum dot (QD), an electron can decay by emitting a photon. In a radiative Auger process, the leftover carriers are in an excited state, and a red-shifted photon is created [1]. Here, we report radiative Auger on trions in individual QDs [2]. For the trion, just one electron is left after the optical recombination. The radiative Auger process promotes this electron to a higher shell of the QD; the emitted photon is red-shifted. We show that radiative Auger directly measures the quantization energies of the single electron. Using resonant excitation, we measure the radiative Auger process on two types of charge-tuneable QDs: InGaAs, GaAs QDs [3]. We rigorously prove the radiative Auger mechanism by measuring the photon statistics and the magnetic field dispersion of the emission. We show how quantum optics applied to the Auger photons gives access to the single-electron dynamics, notably relaxation and tunnelling rates. All these properties of radiative Auger can be exploited on other semiconductor nanostructures. [1] T.

Åberg *et al.*, Phys. Rev. Lett. **22**, 1346-1348 (1969). [2] M. C. Löbl *et al.*, arxiv:1911.11784 (2019) [3] Y. H. Huo *et al.*, Appl. Phys. Lett. **102**, 152105 (2013).

HL 79.6 Fri 11:00 POT 151

Semiconductor-based single-photon source for quantum radiometry — •Hristina Georgieva[1], Marco López[1], Beatrice Rodiek[1], Helmuth Hofer[1], Justus Christinck[1], Peter Schnauber[2], Arsenty Kaganskiy[2], Tobias Heindel[2], Sven Rodt[2], Stephan Reitzenstein[2], and Stefan Kück[1] — [1]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany — [2]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany

Single-photon sources find application in many fields of quantum information processing. Therefore, there is an increasing need to ensure high accuracy and metrological traceability of measurements involving small photon fluxes. In quantum radiometry, the discrete nature of light in principle enables a direct realization of the radiometric quantities by counting photons. The narrow emission bandwidth of semiconductor quantum dots makes them perfect candidates for the detection efficiency calibration of non-photon-number-resolving detectors. We aim for a high photon flux reaching the detector area by means of an efficient quantum emitter combined with a low-loss optical setup, which uses two ultra-narrow bandpass filters instead of a monochromator to reach fluxes up to 370 kphotons/s. The optical power is determined by an unbroken calibration chain to the primary standards. Furthermore, the ratio of detection efficiencies of two single-photon avalanche photodiodes of the same type has been determined to be 1.061 ± 0.008 using a single quantum dot as a light source. This result is validated by a comparison with a standard calibration using an attenuated laser.

HL 79.7 Fri 11:15 POT 151

Least biased steady state of open quantum systems — •Boris Melcher, Boris Gulyak, and Jan Wiersig — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Postfach 4120, D-39016 Magdeburg, Germany

By applying the principle of maximum entropy [1] we develop a standalone approach to conclude a reasonable guess for the full density matrix of an open quantum system in a steady state. It is centered around the obvious perception that in the steady state all observables are constant in time. This is used as a constraint to deduce the least biased density matrix self-consistently.

In doing so, we circumvent the many-particle hierarchy problem that arises in conventional equation of motion techniques [2]. Furthermore, our approach gives access to the full density matrix and thus all relevant expectation values and correlation functions as well as the full statistics of the investigated system.

We employ the maximum entropy method for quantum dot microcavity lasers and demonstrate excellent agreement with conventional approaches [3]. Beyond that, we study the systems in terms of entropy, mean photon number, autocorrelation functions as well as the full photon statistics, giving insight into the fundamental physical processes operating in these systems.

[1] E. T. Jaynes, Phys. Rev. 106, 620 (1957), 108, 171 (1957)
[2] H. A. M. Leymann et al., Phys. Rev. B 89, 085308 (2014)
[3] B. Melcher et al., Phys. Rev. A 100, 013854 (2019)

HL 79.8 Fri 11:30 POT 151

High-bandwith in an all-optical read-out scheme for quantum events — •Jens Kerski[1], Hendrik Mannel[1], Annika Kurzmann[1,2], Arne Ludwig[3], Andreas D. Wieck[3], Axel Lorke[1], and Martin Geller[1] — [1]Faculty of Physics and CENIDE, University Duisburg-Essen, Germany — [2]Solid State Physics Laboratory, ETH Zurich, Switzerland — [3]Chair of Applied Solid State Physics, Ruhr-University Bochum, Germany

The maximum information about a dynamic quantum system can be drawn from real-time measurements of every single quantum event (random telegraph signal). Such studies are performed on single quantum dots (QDs) to investigate electron transport in an all-electrical measurement [1]. Unfortunately, these methods are either invasive or limited in bandwidth. However, it became recently possible to measure the random telegraph signal in a non-invasive all-optical scheme, using resonance fluorescence and a single self-assembled QD coupled to an electron reservoir [2].

This is a promising approach, as the bandwidth of this technique is given by the averaged number of emitted photons per second, limited ultimately by the spontaneous emission rate ($\sim 1 - 10\,\mathrm{GHz}$). In this contribution, we demonstrate this behavior by evaluating the random telegraph signal with full counting statistics and intensities up to 2.6 MCounts/second leading to bandwidths of more than 100 kHz.

[1] S. L. Rudge et al. J. Chem. Phys. 151, 034107 (2019).
[2] A. Kurzmann et al., Phys. Rev. Lett. 122, 247403 (2019).

HL 79.9 Fri 11:45 POT 151

Quantum Dot Optomechanics In Suspended Nanophononic Strings — •BENJAMIN MAYER[1], ANJA VOGELE[1], MAXIMILIAN M. SONNER[1], XUEYONG YUAN[1,2], MATTHIAS WEISS[1], EMELINE D. S. NYSTEN[1], SAIMON F. COVRE DA SILVA[2], ARMANDO RASTELLI[2], and HUBERT J. KRENNER[1] — [1]Lehrstuhl für Experimentalphysik 1, Universität Augsburg, 86159 Augsburg, Germany — [2]Institute of Semiconductor and Solid State Physics, Johannes Kepler Universität Linz, 4040 Linz, Austria

The optomechanical coupling of quantum dots and flexural mechanical modes is studied in suspended nanophononic strings. The investigated devices are designed and monolithically fabricated on an (Al)GaAs heterostructure. Radio frequency elastic waves with frequencies ranging between $f = 250$ and 400 MHz are generated as Rayleigh surface acoustic waves (SAW) on the unpatterned substrate and injected as Lamb waves in the nanophononic string. Quantum dots inside the nanophononic string exhibit a 15-fold enhanced optomechanical modulation compared to those dynamically strained by the SAW. Finite element simulations of the phononic mode spectrum of the nanophononic string confirm that the observed modulation arises from valence band deformation potential coupling via shear strain. The corresponding optomechanical coupling parameter is quantified to 0.15 meV nm^{-1}. Using this value, a derived vertical displacement in the range of 10 nm is deduced from the experimental data. (Vogele et al., Adv. Quantum Tech. early view (2019). doi: 10.1002/qute.201900102)

HL 80: Quantum transport and quantum Hall effects

Time: Friday 9:30–12:00 Location: POT 51

HL 80.1 Fri 9:30 POT 51

Resolution of the "exponent puzzle" for the Anderson transition in doped semiconductors — Edoardo Carnio[1], •Rudolf Römer[2,3], and Nicholas Hine[2] — [1]Albert-Ludwigs-Universität Freiburg, 79104 Freiburg, Germany — [2]University of Warwick, Coventry, UK — [3]Université de Cergy-Pontoise, Institut d'Études Avancées, and LPTM (UMR8089 of CNRS), F-95302 Cergy-Pontoise, France

The Anderson metal-insulator transition (MIT) is central to our understanding of the quantum mechanical nature of disordered materials. Despite extensive efforts by theory and experiment, there is still no agreement on the value of the critical exponent ν describing the universality of the transition*the so-called *exponent puzzle.* In this Rapid Communication, going beyond the standard Anderson model, we employ ab initio methods to study the MIT in a realistic model of a doped semiconductor. We use linear-scaling density functional theory to simulate prototypes of sulfur-doped silicon (Si:S). From these we build larger tight-binding models close to the critical concentration of the MIT. When the dopant concentration is increased, an impurity band forms and eventually delocalizes. We characterize the MIT via multifractal finite-size scaling, obtaining the phase diagram and estimates of ν. Our results suggest an explanation of the long-standing exponent puzzle, which we link to the hybridization of conduction and impurity bands.

HL 80.2 Fri 9:45 POT 51

Model wavefunctions for interfaces between lattice Laughlin states — •Blazej Jaworowski and Anne Nielsen — Max Planck Institut für Physik Komplexer Systeme, 01187 Dresden, Germany

Interfaces between different topological orders, e.g. different fractional

quantum Hall states, are predicted to exhibit nontrivial phenomena, such as anyonic Andreev reflection or parafermion zero modes. However, microscopic descriptions of such systems are quite rare, as they are difficult to study using exact diagonalization. In this work we use conformal field theory to construct microscopic model wavefunctions for interfaces between lattice Laughlin states, describing both the ground states and quasihole excitations [1]. We find that requiring trivial mutual statistics of particles on different sides puts a restriction on possible fillings, coinciding with a similar condition based on K-matrices known in the literature. Next, using the Monte Carlo methods, we show that the entanglement entropy at the interface is higher than in the bulk on the either side, which is expected if some quasiparticles are not able to cross through the interface. This is indeed the case * we find that although all quasiholes remain well-localized when crossing the interface, the statistics of some of them become ill-defined in such a process. Although our work is partly numerical, the closed-form expressions for the wavefunctions allow us to study systems too large for exact diagonalization.

[1] B. Jaworowski, A. E. B. Nielsen, *Model wavefunctions for interfaces between lattice Laughlin states*, submitted to *Physical Review B*

HL 80.3 Fri 10:00 POT 51

Magnetotunnelspectroscopy of Double-Quantum-Wells in GaAs/AlGaAs Heterostructures — •Maximillian Mischke[1], Gunnar Schneider[1], Werner Dietsche[2], and Rolf J. Haug[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, Germany — [2]Max-Planck Institut für Festkörperforschung, Stuttgart, Germany

In order to investigate the influence of a parallel magnetic field on bilayer phenomena, we performed magnetotunnel measurements on GaAs/AlGaAs double quantum wells. Therefore the tunneling current between the two quantum wells was measured dependent on applied bias voltage, electron densities in the individual wells and a magnetic field oriented parallel to the 2D layers. We observe a systematic dependence of the tunneling resonance on the energetic difference of the two wells due to imbalanced densities. The applied bias compensates the mismatch. The parallel magnetic field introduces an additional term to the wave vector of the electrons, leading to a shift of the Fermi circles of the two quantum wells against each other [1]. This shift has an influence on the tunneling resonance since 2D-2D-tunneling requires not only energy conservation but also conservation of momentum [2]. Our measurements reveal an energetic splitting of the tunneling conductance with magnetic field. This splitting starts at a certain magnetic field depending on the density ratio. We expect many-particle-effects to influence this offset field.

[1] G.S. Boebinger et al, Phys. Rev. B 43, 12673 (1991)
[2] J.P. Eisenstein et al, Appl. Phys. Lett. 58, 1497 (1991)

HL 80.4 Fri 10:15 POT 51

Helical quantum Hall phase in graphene on SrTiO3 — •Louis Veyrat[1,7], Corentin Deprez[1], Alexis Coissard[1], Xiaoxi Li[2,3,4], Frédéric Gay[1], Kenji Watanbe[5], Takashi Taniguchi[5], Zheng Vitto Han[2,3,4], Benjamin Piot[6], Hermann Sellier[1], and Benjamin Sacépé[1] — [1]Univ. Grenoble Alpes, CNRS, Grenoble INP, Institut Néel, Grenoble, France — [2]SYNL, Chinese Academy of Sciences, P.R. China — [3]SMSE, University of Science and Technology of China, P.R. China — [4]State Key Laboratory of Quantum Optics and Quantum Optics Devices, SXU, P.R. China — [5]NIMS, Tsukuba, Japan — [6]LNCMI-CNRS-UGA-UPS-INSA-EMFL, Grenoble, France — [7]Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Univ. Würzburg, Germany

The ground state of charge neutral graphene under perpendicular magnetic field was predicted to be a quantum Hall topological insulator with a ferromagnetic order and spin-filtered, helical edge channels. In most experiments, however, an otherwise insulating state is observed and is accounted for by lattice-scale interactions that promote a broken-symmetry state with gapped bulk and edge excitations. We tuned the ground state of the graphene zeroth Landau level to the topological phase via a suitable screening of the Coulomb interaction with a SrTiO3 high-k dielectric substrate. We observed robust helical edge transport emerging at a magnetic field as low as 1T and withstanding temperatures up to 110K over micron-long distances [1]. This new and versatile graphene platform opens new avenues for spintronics and topological quantum computation. [1] Veyrat et al., arXiv:1907:02299

30 min. break

HL 80.5 Fri 11:00 POT 51

2-dimensional superconductivity in the Weyl Semi-metal trigonal-PtBi2 — •Arthur Veyrat — IFW, Dresden, Germany

PtBi2 has attracted attention in recent years with the discovery of the unsaturated Extremely Large Magnetoresistance (XMR) (11.2M % at 33T) in its pyrite structure. In this talk, I will report on our study of quantum transport in exfoliated microstructures of trigonal-PtBi2, patterned using usual e-beam lithography techniques. I will report on the discovery of superconductivity at very low temperatures (~300mK) in this compound, as well as the fitting of our measurements of the microsctructures by a 2D superconductivity model.

HL 80.6 Fri 11:15 POT 51

Anomalous Floquet Anderson Insulators in Quantum Hall Systems — •Hui Liu[1], Ion Cosma Fulga[1], and Janos Asboth[2] — [1]IFW Dresden and Wrzburg-Dresden Cluster of Excellence ct.qmat, Helmholtzstrasse 20, 01069 Dresden, Germany — [2]Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungarian Academy of Sciences, H-1525 Budapest P.O. Box 49, Hungary

Recently, the anomalous Floquet Anderson insulator (AFAI) has attracted significant attention due to its coexistence of chiral edge modes and fully localized bulk. Here we study how an AFAI may be obtained by periodically kicking a quantum Hall system, without using multiple-step, periodic driving procotol. By computing the conductance and topological invariant of the system, we find that the AFAI phase survives even in the strong disorder limit. Our results are general, and therefore applicable to a variety Floquet topological systems, and may provide a more accessible way to construct AFAIs in cold atom experiments.

HL 80.7 Fri 11:30 POT 51

Proximity-Induced Superconductivity in top-down fabricated bulk-insulating TI nanowires — •Matthias Rössler, Dingxun Fan, Junya Feng, Andrea Bliesener, Gertjan Lippertz, Alexey Taskin, and Yoichi Ando — II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln, Germany

With proximity-induced superconductivity, bulk-insulating topological insulator nanowires (TINWs) are expected to serve as a robust platform for realizing Majorana bound states (MBSs). Thanks to their predicted non-Abelian exchange statistics, MBSs could enable realizations of topological quantum computation schemes. In previous reports, TINWs grown by the usual vapour-liquid-solid (VLS) method offer limited possibilities for device layouts and their finite bulk transport contribution yet showed potential for improvements.

We have been performing fabrication of TINWs based on an alternative and scalable approach, namely, etching of bulk-insulating MBE-grown high-quality $(Bi_{1-x}Sb_x)_2Te_3$ thin films. So far, we have been able to prepare such top-down TINWs with a quality close to that of the pristine films and to achieve high gate tuneability. However, proximity-induced superconductivity was never achieved in such systems. In this presentation, we report our success in observing proximity-induced superconductivity in these TINWs and present our characterizations based on Josephson junctions. These results enable further studies on narrower TINWs with quantized 1D surface subbands, which could potentially host MBS when proximitized.

HL 80.8 Fri 11:45 POT 51

Measurements of large density of states in 2D systems: case of narrow HgTe quantum wells — •Aleksandr Kuntsevich[1], Grigorii Minkov[2], Nikolai Mikhailov[3], and Sergei Dvoretsky[3] — [1]P.N. Lebedev Physical Institute, Moscow, Russia — [2]Ural Federal University,Ekaterinburg, Russia — [3]Institute of Semiconductor Physics, Novosibirsk, Russia

For heavy carriers, mobility and cyclotron splitting are small, magneto-oscillations are damped, and it is hard to access experimentally the density of states or effective mass. Narrow HgTe quantum wells serve as a model system. The valence band in such structures contains well-conductive Dirac-like light holes at the Γ point and poorly conductive heavy hole subband located in the local valleys.

We propose and employ two methods to measure the density of states for these heavy holes. The first method uses a gate-recharging technique to measure thermodynamical entropy per particle. As the Fermi level is tuned with gate voltage from light to heavy subband, the entropy increases dramatically, and the value of this increase gives an estimate for the density of states. The second method determines the density of states for heavy holes indirectly from the gate voltage

dependence of the period of the Shubnikov-de Haas oscillations for light holes. The results obtained by both methods are in the reasonable agreement with each other. Our approaches can be applied to measure large effective carrier masses in other two-dimensional gated systems.[To be published in PRB]

HL 81: Semiconductor lasers II

Time: Friday 9:30–11:45 Location: POT 81

Invited Talk HL 81.1 Fri 9:30 POT 81

Ultrafast Spin-Lasers — Markus Lindemann[1], Natalie Jung[1], Tobias Pusch[2], Gaofeng Xu[3], Pascal Stadler[1], Igor Zutic[3], Rainer Michalzik[2], Martin R. Hofmann[1], and •Nils C. Gerhardt[1] — [1]Photonics and Terahertz Technology, Ruhr-University Bochum, 44780 Bochum, Germany — [2]Institute of Functional Nanosystems, Ulm University, 89081 Ulm, Germany — [3]Department of Physics, University at Buffalo, State University of New York, Buffalo, New York 14260, USA

Current-driven intensity modulated semiconductor lasers are key devices for optical transmitters in short-distance data transmission, but their modulation bandwidth is usually limited to values below 50 GHz. By exploiting the coupling between carrier spin and light polarization in semiconductor spin-lasers, the modulation frequencies in such lasers can be increased to values above 200 GHz [1]. These high frequencies are achievable by increasing the resonance frequency of the coupled spin-photon system using strong birefringence in the laser cavity. Birefringent spin-lasers are capable to provide polarization modulation bandwidths and digital data transmission rates of more than 240 GHz and 240 Gbit/s respectively [1]. In contrast to intensity modulation in conventional lasers, polarization modulation in spin-lasers is largely independent of the pumping level. This makes spin-lasers perfect candidates for future ultrafast communication systems with extraordinarily low power consumption.

[1] M. Lindemann et al., Nature 568, 212 (2019).

HL 81.2 Fri 10:00 POT 81

Fabrication of spectrally homogeneous microlaser arrays as a nanophotonic hardware for reservoir computing — •Tobias Heuser[1], Jan Grosse[1], Daniel Brunner[2], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universiät Berlin, D-10623 Berlin, Germany — [2]FEMTO-ST, 15B Avenue des Montboucons, 25030 Besançon, France

Reservoir computing is a powerful machine learning concept for a new kind of neural inspired data processing. In this concept an interacting network of nodes is evaluated by a trained readout for applications like fast pattern recognition. To further improve the performance of this concept, a photonic hardware implementation is of particular interest. Here, we report on our newest developements in the fabrication process, lasing performance and polarisation characteristics of large 2D arrays of microlasers, specifically quantum dot micropillars [1]. These arrays will serve as a nonlinear network via diffractive optical coupling [2]. For this spectral alignment of the involved lasers is crucial. To achieve this with a spectral homogeneity better than 200μeV throughout the array of up to 900 lasers, shifts of the emission energy are compensated by precisely adjusting the radius of the fabricated micropillars based on the local sample emission[3, 4].

References

[1] S.Reitzenstein, A.Forchel, J.Phys.D.Appl.Phys. 43, 033001 (2010)
[2] D.Brunner, I.Fischer, Opt. Lett. 40, 3854-3857 (2015)
[3] T.Heuser et al., APL Photonics 3, 116103 (2018)
[4] T.Heuser et al., IEEE JSTQ 26, 1, (2020)

HL 81.3 Fri 10:15 POT 81

Dynamic instabilities in gain-folded mode-locked VECSELs — •Marius Grossmann[1], Roman Bek[2], Michael Jetter[1], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQST) and Research Center SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]Twenty-One Semiconductors, Kiefernweg 4, 72654 Neckartenzlingen, Germany

Since the first demonstration of mode-locked vertical external-cavity surface-emitting lasers (VECSELs) using semiconductor saturable absorbers (SESAMs) in the year 2000, these lasers have shown to provide a diffraction-limited beam quality as well as high output powers across multiple emission wavelengths. These ultrashort pulse lasers offer interesting dynamics, which are often linked to semiconductor properties and can be influenced by the exact cavity design. A cavity geometry often used is the z-shaped cavity, which provides further flexibilities concerning mode area ratios, cavity lengths and additional intra-cavity elements like etalons and nonlinear crystals.

We present the mode-locked emission characteristics of a red-emitting SESAM mode-locked VECSEL with an average output power up to 2 mW. We put the focus on the temporal dynamics recorded upon wavelength tuning of the pulsed emission and discuss the emission dynamics based on numerical modelling.

15 min. break

HL 81.4 Fri 10:45 POT 81

Dynamical properties of quantum dot lasers with and without p-doping and tunneling injection quantum wells in the active region — •Sven Bauer[1], Vitalii Sichkovskyi[1], Florian Schnabel[1], Anna Sengül[1], Ori Eyal[2], Igor Khanonkin[2], Gadi Eisenstein[2], and Johann Peter Reithmaier[1] — [1]Technische Physik, Institute of Nanostructure Technologies and Analytics (INA), CINSaT, University of Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany — [2]Electrical Engineering Department and Russell Berrie Nanotechnology Institute, Technion, Haifa 32000, Israel

The performance of directly modulated quantum dot (QD) lasers, used for 1.55 μm telecommunication, is limited by the intraband carrier relaxation time as well as thermally broadened hole distribution effects. These properties could be improved by using a so-called tunnel injection (TI) scheme or the introduction of p-type doping into the active region of a high-speed laser design. Conventional QD lasers are directly compared to QD lasers with TI, p-type doping and both. The QD density and uniformity are nominally the same for all devices. Small signal modulation measurements yielded higher bandwidths for the QD lasers in comparison to the TI QD lasers. P-type doping greatly improved the performance of TI QD lasers and more refined doping profiles are promising to further enhance the modulation properties. Large signal modulation measurements showed a maximum data rate of more than 25 Gbit/s for both laser types, which is already suitable for telecom applications.

HL 81.5 Fri 11:00 POT 81

Wave front analysis of monolithic passively mode locked semiconductor quantum well lasers — •Clemens Adler[1], Christoph Weber[2], Inga-Maria Eichentopf[1], Andreas Klehr[3], Andrea Knigge[3], Stefan Breuer[2], and Martin Reufer[1] — [1]Hochschule Ruhr West, Institute of Natural Sciences, Duisburger Str. 100, 45479 Mülheim an der Ruhr — [2]Institute of Applied Physics, Technische Universität Darmstadt, Schlossgartenstraße 7, 64289 Darmstadt, Germany — [3]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Gustav-Kirchhoff-Straße 4, 12489 Berlin, Germany

Mode-locked semiconductor diode lasers are well established photon sources. Their temperature and charge carrier distributions within the active layer depends on the injection conditions and are expected to change with the process of mode locking. Higher optical modes are supported by the resonator potentially impacting the modal composition and emitted laser beam properties. We experimentally study the bias dependent modal composition of a passively mode-locked quantum well laser emitting at 1070 nm [1]. A Shack-Hartmann sensor detects the local gradients of the Poynting vector of the laser beam. Deviations in the wave front are identified by decomposition into Zernike polynomials [2]. Our near and far field measurement results suggest a dependence of the wave front properties on the laser operation mode.

[1] Weber et al, IEEE J. Quantum Electron. 54 (3), 2000609 (2018)
[2] Schäfer et al, Applied Optics 41, 2809 (2002)

HL 81.6 Fri 11:15 POT 81

Nonlinear lensing in optically-pumped semiconductor disk lasers — Christian Kriso[1], Sascha Kress[1], Tasnim Munshi[1],

Marius Grossmann[2], Roman Bek[3], Michael Jetter[2], Peter Michler[2], Wolfgang Stolz[1], Martin Koch[1], and •Arash Rahimi-Iman[1] — [1]Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integraed Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart — [3]Twenty-One Semiconductors GmbH, Kiefernweg 4, 72654 Neckartenzlingen

Semiconductor disk lasers or vertical-external-cavity surface-emitting-lasers (VECSELs) have been highlighted in recent years as promising sources for ultrashort pulses. Particularly, saturable-absorber-free "self-mode-locked" operation of VECSELs has raised considerable attention. The origin of this phenomenon is still not well-enough understood to effectively utilize it for future mode-locking device concepts. Currently, nonlinear lensing in the VECSEL chip itself, which has been indicated to be sufficiently strong to enable Kerr-lens-like mode-locking, is suspected to be one driving mechanism behind self-mode-locking [Kriso et al., *Opt. Express* (2019)]. Here, we summarize a systematical characterization of the effective nonlinear refractive index and nonlinear absorption coefficient of an optically-pumped gain chip, having probed the complex, effective third-order susceptibility of the chip for excited charge-carrier densities similar to that of laser operation [Kriso et al., *Phot. Tech. Lett.* (in press)].

HL 81.7 Fri 11:30 POT 81

Pulse generation and emission dynamics of Fabry-Pérot multisection passively mode-locked lasers on an InP photonic integrated circuit — •Abishek Vibhaker[1], Christoph Weber[1], Dominik Auth[1], Luke F. Lester[2], and Stefan Breuer[1] — [1]Institute of Applied Physics, Technische Universität Darmstadt, 64289 Darmstadt, Germany — [2]Bradley Department of Electrical and Computer Engineering, Virginia Polytechnic Institute and State University, Blacksburg, Virginia, 24061, USA

Passively mode-locked lasers on photonic integrated circuits based on InP material are low footprint light sources emitting picosecond short pulses in the C- or L-band for telecommunication applications. Recent investigations on photonic integrated circuit symmetric ring structures [Lo et al, Optics Letters 44 (14), 3566 (2019)] are now followed by investigations on multimode interference reflectors based Fabry-Perot cavity designs consisting of gain and saturable absorber sections for short pulse generation at high repetition rates. Multiple designs are realized to study the optical frequency comb generation and the pulse train stability in terms of timing jitter and amplitude stability.