Semiconductor Physics Division
Fachverband Halbleiterphysik (HL)

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Overview of Invited Talks and Sessions

(Lecture halls POT 6, POT 81, POT 112, POT 151, POT 251, and POT 361; Poster P1 and P2/EG)

Plenary Talks of the Semiconductor Physics Division

PLV I	Mon	8:30– 9:15	HSZ 01	**Spin-Photon Interfaces and Their Applications** — •Mete Atatuere
PLV VIII	Thu	8:30– 9:15	HSZ 01	**Nanomechanics: Tunes of the nanoguitar** — •Eva Weig
PLV IX	Thu	14:00–14:45	HSZ 01	**Metal Halide Perovskites for Photovoltaic Applications** — •Laura Herz

Invited Talks

HL 3.1	Mon	9:30–10:00	POT 151	**Schrödinger cat states of a 16-microgram mechanical oscillator** — •Yiwen Chu, Marius Bild, Matteo Fadel, Yu Yang, Uwe von Lüpke, Phillip Martin, Alessandro Bruno
HL 3.2	Mon	10:00–10:30	POT 151	**High-fidelity quantum information processing with spins and phonons** — •Peter Rabl
HL 3.5	Mon	11:30–12:00	POT 151	**Control of spin centers in silicon carbide using acoustic fields** — •Alberto Hernández-Mínguez
HL 8.9	Mon	17:30–18:00	POT 81	**Time-resolved optical spectroscopy of 3R-stacked MoS_2** — •Swarup Deb, Michael Kempf, Rico Schwartz, Tobias Korn
HL 9.1	Mon	15:00–15:30	POT 361	**Spin and valley lifetime in graphene quantum dots** — •Guido Burkard
HL 9.2	Mon	15:30–16:00	POT 361	**Microscopic modelling of electrostatically induced bilayer graphene quantum dots** — •Angelika Knothe
HL 9.4	Mon	16:45–17:15	POT 361	**Single-shot spin and valley Pauli blockade read-out in bilayer graphene quantum dots** — •Chuyao Tong, Rebekka Garreis, Wister Wei Huang, Annika Kurzmann, Jocelyn Terle, Samuel Jele, Kenji Watanabe, Takashi Taniguchi, Thomas Ihn, Klaus Ensslin
HL 9.5	Mon	17:15–17:45	POT 361	**Particle-hole symmetry protects spin-valley blockade in graphene quantum dots** — •Christian Volk, Luca Banszerus, Samuel Möller, Katrin Hecker, Eike Icking, Kenji Watanabe, Takashi Taniguchi, Fabian Hassler, Christoph Stampfer
HL 10.1	Mon	15:00–15:30	POT 151	**Surface Acoustic Wave Cavity Optomechanics with 2D Materials** — •Galan Moody
HL 10.2	Mon	15:30–16:00	POT 151	**Phononic Microresonators Coupled by Surface Acoustic Waves** — •Sarah Benchabane, Maciej Baranski, Feng Gao, Olivier Gaiffe, Valérie Soumann, Roland Salut, Abdelkrim Khelif
HL 23.1	Wed	9:30–10:00	POT 361	**Vertical-cavity surface-emitting lasers – this is the way** — •Å. Haglund, G. Cardinali, L. Persson, F. Hjort, J. Enslin, E. Torres, C. Kuhn, S. Graupeter, M. Grigoletto, M. A. Bergmann, N. Prokop, M. Guttmann, L. Sulmoni, N. Lobo Ploch, M. Cobet, T. Kolbe, J. Gustavsson, F. Nippert, I. Häusler, M. R. Wagner, J. Ciers, T. Wernicke, M. Kneisl

HL 23.2	Wed	10:00–10:30	POT 361	**Towards GaN-based diode lasers with narrow linewidth and high reliability** — •Sven Einfeldt, Erik Freier, Ji-Hye Kang, Hans Wenzel, Anna Mogilatenko, Johannes Glaab, Asmaa Abou-Shewarib, Veit Hoffmann, Johannes Enslin, Martin Guttmann, Saad Makhladi, Jörg Fricke, Olaf Brox, Mathias Matalla, Maria Norman-Reiner, Christoph Stölmacker, Markus Weyers, Luca Sulmoni, Michael Kneissl, Lukas Uhlig, Ulrich T. Schwarz
HL 23.3	Wed	10:30–11:00	POT 361	**Use of wafer patterning for new functionalities of InGaN light emitters** — •Anna Kafar, Ryota Ishii, Atsushi Sakaki, Kiran Saba, Conny Becht, Szymon Grzanka, Ulrich Schwarz, Mitsuru Funato, Yoichi Kawakami, Piotr Perlin
HL 25.1	Wed	9:30–10:00	POT 251	**Interfaces in perovskite optoelectronics: role of energy level alignment and interface chemistry** — •Selina Olthof
HL 27.1	Wed	15:00–15:30	POT 81	**experimentamus! Forschendes Lernen von Physik und Chemie in der Grundschule** — •Sebastian Schlücker
HL 27.4	Wed	16:00–16:30	POT 81	**Under the Microscope – spotlighting materials and nano science** — •Svenja Lohmann, Pranoti Kshirsagar
HL 27.5	Wed	17:00–17:30	POT 81	**Phyphox – A pocketful of physics** — •Christoph Stampfer
HL 27.8	Wed	18:00–18:30	POT 81	**Physics for school and the public at the LMU** — •Dr. Cecilia Scorza-Lesch
HL 28.1	Wed	15:00–15:30	POT 361	**Fabrication of AlGaN-based UV-B laser diodes on lattice-relaxed high-quality AlGaN** — •Motoaki Iwaya, Sho Iwayama, Tetsuya Takeuchi, Satoshi Kamiyama, Hideto Miyake
HL 28.2	Wed	15:30–16:00	POT 361	**Breakthrough technologies to realize room-temperature continuous-wave deep-ultraviolet laser diodes** — •Maki Kushimoto
HL 35.1	Thu	9:30–10:00	POT 361	**Quantum Dynamics of Polarons in Doped Semiconductor Monolayers** — •Xiaoqin Elaine Li, Di Huang
HL 35.2	Thu	10:00–10:30	POT 361	**Impact of phonons on time-resolved optical signals from excitons** — •Doris E. Reiter
HL 35.3	Thu	10:30–11:00	POT 361	**Hot-Exciton Quantum Dynamics in Zero-Dimensional Structures** — •Alfred Leitenstorfer
HL 35.6	Thu	12:00–12:30	POT 361	**Ultrafast dynamics and wave mixing at excitonic resonances in atomically thin semiconductors** — •Andreas Knorr, Dominik Christiansen, Florian Katsch, Manuel Katzer, Malte Selig
HL 35.7	Thu	12:30–13:00	POT 361	**Spontaneous parametric down-conversion in semiconductor metasurfaces** — •Maria Chekhova
HL 43.1	Thu	15:00–15:30	POT 251	**Superradiance as a witness to multipartite entanglement** — •Frederik Lohof, Christopher Gies

Invited Talks of the joint Symposium SKM Dissertation Prize 2023 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	HSZ 04	**Diffusion of antibodies in solution: from individual proteins to phase separation domains** — •Anita Girelli
SYSD 1.2	Mon	10:00–10:30	HSZ 04	**Intermediate Filament Mechanics Across Scales** — •Anna V. Schepers
SYSD 1.3	Mon	10:30–11:00	HSZ 04	**Ultrafast Probing and Coherent Vibrational Control of a Surface Structural Phase Transition** — •Jan Gerrit Horstmann
SYSD 1.4	Mon	11:00–11:30	HSZ 04	**Electro-active metasurfaces employing metal-to-insulator phase transitions** — •Julian Karst
SYSD 1.5	Mon	11:30–12:00	HSZ 04	**The role of unconventional symmetries in the dynamics of many-body systems** — •Pablo Sala

Invited Talks of the joint Symposium Real-Time Measurements of Quantum Dynamics (SYQD)

See SYQD for the full program of the symposium.

SYQD 1.1	Thu	9:30–10:00	HSZ 01	**Real-time measurement and control of spin dynamics in quantum dots** — •Seigo Tarucha

SYQD 1.2	Thu	10:00–10:30	HSZ 01	**Quantum Dot arrays for Quantum Information Transfer** — •Gloria Platero, David Fernandez-Fernandez, Juan Zurita
SYQD 1.3	Thu	10:30–11:00	HSZ 01	**Optical Detection of Real-Time Quantum Dynamics in Quantum Dots** — •Martin Geller, Jens Kerski, Eric Kleinherbers, Jürgen König, Annika Kurzmann, Pia Lochner, Axel Lorke, Arne Ludwig, Hendrik Mannel, Philipp Stegmann, Andreas Wieck, Marcel Zöllner
SYQD 1.4	Thu	11:30–12:00	HSZ 01	**Cooper Pair Splitting in Real-Time** — •Christian Flindt
SYQD 1.5	Thu	12:00–12:30	HSZ 01	**Trajectory-based detection in stochastic and quantum thermodynamics** — •Jukka Pekola

Invited Talks of the joint Symposium Physics of van der Waals 2D Heterostructures (SYHS)

See SYHS for the full program of the symposium.

SYHS 1.1	Fri	9:30–10:00	HSZ 01	**Novel moiré excitons and ultrafast optical dynamics in van der Waals 2D heterostructures** — •Steven G. Louie
SYHS 1.2	Fri	10:00–10:30	HSZ 01	**Interaction induced magnetism in 2D semiconductor moiré superlattices** — •Xiaodong Xu
SYHS 1.3	Fri	10:30–11:00	HSZ 01	**Ions in tight places: intercalation and transport of ions in van der Waals heterostructures** — •Irina Grigorieva
SYHS 1.4	Fri	11:15–11:45	HSZ 01	**Spin-orbit proximity in van der Waals heterostructures** — •Felix Casanova
SYHS 1.5	Fri	11:45–12:15	HSZ 01	**Plethora of many-body ground states in magic angle twisted bilayer graphene** — •Dmitri Efetov

Sessions

HL 1.1–1.10	Mon	9:30–12:30	POT 81	**2D Materials I (joint session HL/CPP)**
HL 2.1–2.6	Mon	9:30–11:15	POT 361	**Organic Semiconductors (joint session HL/CPP)**
HL 3.1–3.9	Mon	9:30–13:00	POT 151	**Focus Session: Progress in Hybrid Phononic Quantum Technologies I**
HL 4.1–4.10	Mon	9:30–12:30	POT 251	**Perovskite and photovoltaics I (joint session HL/CPP)**
HL 5.1–5.5	Mon	10:00–11:15	POT 112	**Heterostructures, interfaces and surfaces**
HL 6.1–6.8	Mon	10:30–13:00	TRE Ma	**Focus Session: Frontiers of Electronic-Structure Theory III (joint session O/HL)**
HL 7.1–7.66	Mon	13:00–15:00	P2/EG	**Poster I**
HL 8.1–8.10	Mon	15:00–18:15	POT 81	**2D Materials II (joint session HL/CPP)**
HL 9.1–9.5	Mon	15:00–17:45	POT 361	**Focus Session: Graphene quantum dots (joint session HL/TT)**
HL 10.1–10.10	Mon	15:00–18:30	POT 151	**Focus Session: Progress in Hybrid Phononic Quantum Technologies II**
HL 11.1–11.7	Mon	15:00–17:15	POT 251	**Quantum transport and quantum Hall effects I (joint session HL/TT)**
HL 12.1–12.7	Mon	15:00–17:15	POT 112	**Semiconductor lasers I**
HL 13.1–13.7	Mon	15:00–17:15	TRE Ma	**Focus Session: Frontiers of Electronic-Structure Theory II (joint session O/HL)**
HL 14.1–14.10	Tue	9:30–12:15	POT 81	**2D Materials III (joint session HL/CPP)**
HL 15.1–15.4	Tue	9:30–10:30	POT 361	**Spin phenomena in semiconductors**
HL 16.1–16.9	Tue	9:30–12:15	POT 151	**Quantum dots: Transport (joint session HL/TT)**
HL 17.1–17.11	Tue	9:30–12:45	POT 251	**THz and MIR physics in semiconductors**
HL 18.1–18.12	Tue	9:30–13:00	POT 112	**Optical Properties (joint session HL/CPP)**
HL 19.1–19.13	Tue	9:30–13:00	GÖR 226	**Organic Electronics and Photovoltaics I (joint session CPP/HL)**
HL 20.1–20.7	Tue	10:30–12:45	TRE Ma	**Focus Session: Frontiers of Electronic-Structure Theory I (joint session O/HL)**
HL 21.1–21.3	Tue	11:00–11:45	POT 361	**Thermal properties**
HL 22.1–22.10	Wed	9:30–12:30	POT 81	**2D Materials IV (joint session HL/CPP)**
HL 23.1–23.6	Wed	9:30–12:15	POT 361	**Focus Session: Breakthroughs in wide-bandgap semiconductor laser diodes I**
HL 24.1–24.13	Wed	9:30–13:15	POT 151	**Quantum dots: Optics**

HL 25.1–25.11	Wed	9:30–13:00	POT 251	**Perovskite and photovoltaics II (joint session HL/CPP)**
HL 26.1–26.8	Wed	10:30–13:00	TRE Ma	**Focus Session: Frontiers of Electronic-Structure Theory IV (joint session O/HL)**
HL 27.1–27.8	Wed	15:00–18:30	POT 81	**Focus Session: Wissenschaftskommunikation / Outreach (joint session HL/O/TT)**
HL 28.1–28.5	Wed	15:00–16:45	POT 361	**Focus Session: Breakthroughs in wide-bandgap semiconductor laser diodes II**
HL 29.1–29.10	Wed	15:00–18:00	POT 151	**Materials and devices for quantum technology I**
HL 30.1–30.6	Wed	15:00–17:00	POT 251	**Quantum transport and quantum Hall effects II (joint session HL/TT)**
HL 31.1–31.8	Wed	15:00–17:30	TRE Ma	**Focus Session: Frontiers of Electronic-Structure Theory V (joint session O/HL)**
HL 32.1–32.9	Wed	15:00–17:30	GÖR 226	**Organic Electronics and Photovoltaics II (joint session CPP/HL)**
HL 33.1–33.62	Wed	17:00–19:00	P1	**Poster II**
HL 34.1–34.9	Thu	9:30–12:00	POT 81	**2D Materials V (joint session HL/CPP)**
HL 35.1–35.9	Thu	9:30–13:30	POT 361	**Focus Session: Transient multi-wave mixing on excitonic resonances**
HL 36.1–36.7	Thu	9:30–11:45	POT 151	**Transport properties**
HL 37.1–37.9	Thu	9:30–12:15	POT 251	**Materials and devices for quantum technology II**
HL 38.1–38.7	Thu	9:30–11:45	POT 6	**Functional semiconductors for renewable energy solutions I**
HL 39.1–39.11	Thu	9:30–12:30	GÖR 226	**Organic Electronics and Photovoltaics III (joint session CPP/HL)**
HL 40.1–40.7	Thu	10:30–12:45	TRE Ma	**Focus Session: Frontiers of Electronic-Structure Theory VI (joint session O/HL)**
HL 41.1–41.7	Thu	15:00–17:00	POT 81	**Oxide Semiconductors I: Ga_2O_3**
HL 42.1–42.7	Thu	15:00–17:15	POT 151	**Quantum dots: Growth**
HL 43.1–43.6	Thu	15:00–16:45	POT 251	**Semiconductor lasers II**
HL 44.1–44.7	Thu	15:00–17:00	POT 112	**Nitrides: Devices**
HL 45.1–45.7	Thu	15:00–17:15	POT 6	**Functional semiconductors for renewable energy solutions II**
HL 46	Thu	18:00–19:00	POT 6	**Members' Assembly**
HL 47.1–47.7	Fri	9:30–11:30	POT 81	**Oxide Semiconductors II**
HL 48.1–48.9	Fri	9:30–12:00	POT 361	**Ultra-fast Phenomena**
HL 49.1–49.7	Fri	9:30–11:45	POT 151	**Quantum dots: Devices**
HL 50.1–50.12	Fri	9:30–13:00	POT 251	**Materials and devices for quantum technology III**
HL 51.1–51.10	Fri	9:30–12:15	POT 112	**Nitrides: Preparation and Characterization**
HL 52.1–52.8	Fri	9:30–12:30	GÖR 226	**Focus: Self-Assembly of Plasmonic Nanostructures (joint session CPP/HL)**

Mitgliederversammlung / Members' Assembly of the Semiconductor Physics Division

Donnerstag 18:00–19:00 POT6

Alle Mitglieder des Fachverbands Halbleiterphysik sind herzlich willkommen / All members of the Semiconductor Physics Division are invited to participate.

- Bericht
- Wahl der Fachverbandsleitung
- Informationen zur Frühjahrstagung 2024
- Verschiedenes

HL 1: 2D Materials I (joint session HL/CPP)

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

HL 1.1 Mon 9:30 POT 81

Spin-valley physics in strained transition metal dichalcogenides monolayers — •Paulo E. Faria Junior[1], Klaus Zollner[1], Tomasz Woźniak[2], Marcin Kurpas[3], Martin Gmitra[4], and Jaroslav Fabian[1] — [1]University of Regensburg, Regensburg, Germany — [2]Wroclaw University of Science and Technology, Wroclaw, Poland — [3]University of Silesia, Chorzów, Poland — [4]Pavol Jozef Šafárik University in Košice, Košice, Slovakia

Transition metal dichalcogenides (TMDCs) are ideal candidates to explore the manifestation of spin-valley physics under external stimuli. Here, we investigate the influence of strain on the spin, orbital angular momenta and g-factors of monolayer TMDCs within first principles[1]. Our calculations reveal the behavior of direct exciton g-factors under the isolated impact of strain: tensile (compressive) strain increases (decreases) the absolute value of g-factors. Strain variations of 1% modify the bright (A and B) exciton g-factors by 0.3 (0.2) for W (Mo) based compounds and the dark exciton g-factors by 0.5 (0.3) for W (Mo) compounds, suggesting that strain can be responsible for g-factor fluctuations observed experimentally. We complete our analysis for the Gamma and Q valleys, revealing that the spin degree of freedom dominates. This fundamental microscopic insight into the role of strain in the spin-valley physics of TMDCs is crucial to understand recent experiments[2,3]. [1] Faria Junior et al., NJP 24, 083004 (2022). [2] Covre, Faria Junior et al., Nanoscale 14, 5758 (2022). [3] Blundo, Faria Junior et al., PRL 129, 067402 (2022). Funding: DFG SFB 1277, SPP 2244.

HL 1.2 Mon 9:45 POT 81

A bright single-photon source based on a WSe_2 monolayer in an open cavity — •Victor Mitryakhin[1], Hangyong Shan[1], Jens-Christian Drawer[1], Sven Stephan[1], Martin Silies[2], Falk Eilenberger[3], Carlos Antón-Solanas[1], Martin Esmann[1], and Christian Schneider[1] — [1]Carl von Ossietzky Universität Oldenburg, 26129 Oldenburg, Germany — [2]Hochschule Emden/Leer, 26723 Emden, Germany — [3]Friedrich-Schiller-Universität Jena, 07745 Jena, Germany

Single photon sources based on crystalline defects present in transition-metal dichalcogenide monolayers, 2D atomically thin direct-bandgap semiconductors, have recently emerged as a promising platform for realization of and use in quantum communication and information processing.

In this work, we investigate the properties of single photon emission from a single exciton in a WSe_2 monolayer weakly coupled to an asymmetric plano-concave microcavity consisting of freely movable mirrors in 3 directions. In this regard, it enables us for an in-situ control of the properties of the emission and the extraction efficiency of single photons in the device.

We report a highly bright and linearly polarized single photon source with source brightness exceeding 70 % under saturation conditions, polarization degree of 98.4±1.3 % and high photon purity noted by the second-order correlation $g^{(2)}(0)$ value of 0.047±0.007, measured in Hanbury-Brown-Twist type of a setup.

HL 1.3 Mon 10:00 POT 81

Strong coupling of excitons in a WS2-monolayer coupled to a silver nanogroove array — •Yuhao Zhang[1], Hans-Joachim Schill[1,2], Stephan Irsen[2], and Stefan Linden[1] — [1]Physikalisches Institut, Universität Bonn — [2]Center of Advanced European Studies and Research (caesar)

In this work, we report on room-temperature interaction of a WS2 monolayer with a tapered nanogroove array milled into monocrystalline silver flake. The bare nanogroove array features three polariton branches resulting from the coupling of localized surface plasmon modes (LSPR) in the nanogrooves and propagation surface plasmon modes (SPP). The linewidth of the lower plasmon polariton branch critically depends on the geometry of the nanogrooves. When a WS2 monolayer is deposited on the nanogroove array with optimized damping, the reflection spectra show an avoided crossing of the exciton mode and the lower plasmon polariton branch with a Rabi splitting of 38.7 meV indicating strong exciton-plasmon polariton coupling.

HL 1.4 Mon 10:15 POT 81

Theory of exciton localization in TMDCs using metal nanoparticles — •Robert Salzwedel[1], Lara Greten[1], Stefan Schmidt[1], Chelsea Carlson[2], Stephen Hughes[2], Malte Selig[1], and Andreas Knorr[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Berlin, Germany — [2]Department of Physics, Queen's University, Kingston, Ontario, Canada

In recent years, monolayers of transition metal dichalcogenides (TMDCs) have attracted considerable attention due to their strong Coulomb and light-matter interactions, leading to tightly bound excitons with large optical oscillator strength. Due to the finite thickness of the monolayers, these excitons are very sensitive to the environment, which allows their properties to be tailored, e.g., by functionalization with molecules or metal nanoparticles (MNPs) [1,2].

We present a theory based on a self-consistent solution of Maxwell's and Bloch equations to analytically study a coupled system of MNP plasmons and TMDC excitons. For the combined system, we identify an effective eigenvalue equation that governs the center of mass motion of the dressed excitons in a plasmon-induced potential. Examination of the ensuing plexcitonic equation reveals the existence of bound states, which we interpret as excitons localized in the external potential. The appearance of these bound states in this potential is an indicator of strong coupling between excitons and plasmons.

[1] Carlson et al. (2021). PRB, 104(12), 125424.
[2] Denning et al. (2022). PRB, 105(8), 085306.

15 min. break

HL 1.5 Mon 10:45 POT 81

Electronic effects of non-uniformly strained 2D TMDCs — •Mohammadreza Daqiqshirazi and Thomas Brumme — Chair of Theoretical Chemistry, Technische Universität Dresden, Bergstraße 66c, 01069 Dresden, Germany

Strain plays an important role in most 2D materials since there is a strong influence of the strain state on the relative band alignment of different valleys in the electronic band structure. The effects of non-uniform strain on the properties of 2D materials are scarcely studied theoretically, even if in experiments a lot of different structures can be found in which a spatial varying strain state is present such as wrinkles or folds. Here, we are investigating how such non-uniform strain influences the electronic properties of the prototypical 2D materials WSe2 and MoS2.We study nanoscale wrinkles and nanotubes in detail and discuss important differences in the strain distribution and magnitude, also to understand if nanotubes could be used as a model system for non-uniformly strained systems. Using Density Functional Theory we find that the inclusion of spin-orbit interaction is crucial to correctly predict the changes in the band structure of wrinkled 2D materials as the non-uniform strain changes the symmetry compared to a flat layer. This introduces a strong Rashba-like splitting of the valence-band maximum near the Γ point. The situation complicates even more with the addition of an extra layer forming a bilayer or a hetrobilayer. The spatial varying band alignments in wrinkled multilayers can lead to new interlayer excitons which are confined to certain regions of the system.

HL 1.6 Mon 11:00 POT 81

Optical properties of monolayer $ReSe_2$ and ReS_2 — •Thorsten Deilmann — Institute of Solid State Theory, University of Münster, Germany

Rhenium-based transition metal dichalcogenides unite the fascinating characteristics of the confined in-plane physics with their reduced crystal symmetry. This paves the way for polarization-sensitive applications, such as optical logic circuits operating in the infrared spectral region.

Here, we investigate the doping-dependent optical properties of $ReSe_2$ and ReS_2 from first principles. Besides strong excitonic effects, recent experimental studies have reported three-particle states (i.e. trions) with trion binding energies of more than 100 meV [1,2]. Using our ab initio methods we are able to predict neutral and charged properties and find much smaller binding energies compared to experiment.

[1] Advanced Functional Materials, 10, 1905961 (2019)
[2] Applied Physics Letters 119, 113103 (2021)

HL 1.7 Mon 11:15 POT 81

Evaluating Atomically Thin Single-Photon Sources for Quantum Key Distribution — •Timm Gao[1], Martin v. Helversen[1], Carlos Anton-Solanas[2], Christian Schneider[2], and Tobias Heindel[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany — [2]Institut für Physik, Carl von Ossietzky Universität Oldenburg, 26111 Oldenburg, Germany

Quantum light sources are considered key building blocks for future quantum communication networks. In recent years, atomic monolayers of transition metal dichalcogenides (TMDCs) emerged as a promising material platform for the development of compact quantum light sources. In this work, we evaluate for the first time the performance of a single-photon source (SPS) based on a strain engineered WSe_2 monolayer [1] for applications in quantum key distribution (QKD) [2]. Employed in a QKD-testbed emulating the BB84 protocol, an antibunching of $g^{(2)}(0) = 0.127 \pm 0.001$ and a raw key rate of up to (66.95 ± 0.10)kHz make this source competitive with previous SPS based QKD experiments using quantum dot based SPSs. Furthermore, we exploit routines for the performance optimization previously applied to quantum dot based single-photon sources [2]. Our work represents an important step towards the application of TMDC-based devices in quantum technologies.

[1] L. Tripathi et al., ACS Photonics 5, 1919-1926 (2018)
[2] T. Gao et al., arXiv:2204.06427 (2022)
[3] T. Kupko et al., npj Quantum Information 6, 29 (2020)

HL 1.8 Mon 11:30 POT 81

Theory of Thermalization of Excitons at Elevated Densities in Atomically Thin Semiconductors — •Manuel Katzer, Andreas Knorr, and Malte Selig — Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Atomically thin semiconductors exhibit tightly bound electron-hole pairs which stimulated exciton research in recent years [1]. So far, many studies focused on the understanding of exciton dynamics in the limit of very dilute systems. Recent experimental findings [2] raised the question of the excitonic thermalization behaviour for densities above this dilute, classical limit. Due to the co-bosonic nature of excitons [3], we find both bosonic but also fermionic contributions to the thermalization, with the fermionic Pauli blocking effects being dominant for a broad range of parameters. Based on a Heisenberg equation of motion ansatz [4], we discuss the first order of non-linear exciton-phonon interaction exceeding the classical Boltzmann scattering limit, in order to analyze the character of the exciton thermalization at elevated excitation densities.

[1] Wang et al. RMP 90, 021001 (2018). [2] Sigl et al. PRR 2 (4), 042044 (2020). [3] Katsch et al., PRL 124 25 257402 (2020). [4] Selig et al. PRR, 1, 022007 (2019).

15 min. break

HL 1.9 Mon 12:00 POT 81

Strong exciton-plasmon coupling in hybrids of 2D semiconductors and plasmonic crystals — •Lara Greten[1], Robert Salzwedel[1], Stephen Hughes[2], Malte Selig[1], and Andreas Knorr[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany — [2]Department of Physics, Queen's University, Kingston, Canada

Monolayers of transition metal dichalcogenides (TMDCs) are direct-gap semiconductors that exhibit tightly bound excitons with pronounced optical amplitudes. Thus, they are promising for various optoelectronic applications and an excellent material to investigate excitons. Another material with a large optical amplitude is a plasmonic crystal - arrays of metal nanoparticles - which supports collective plasmon modes, and yields amplification of the electric fields on the nanoscale.

Here, we theoretically consider exciton-plasmon coupling in a hybrid structure of a TMDC layer interacting with a plasmonic crystal with a 2d lattice. Our study reveals a hybridization of plasmons and initially momentum dark excitons. In addition, we find an excitonic mode with negligible coupling to the plasmonic near field, emitting undisturbed radiation into the far field. To connect to related experiments, we compute the scattered light in the near- and far-field explicitly and identify signatures of strong exciton-plasmon coupling with a Rabi splitting of more than 100 meV. We also find that the uncoupled exciton mode results in a third peak at the undisturbed exciton energy.

HL 1.10 Mon 12:15 POT 81

Enhancement of Light Emission in Hexagonal Boron Nitride Structures — •Felix Schaumburg, Marcel Zöllner, Vasilis Dergianlis, Stephan Sleziona, Marika Schleberger, Axel Lorke, Martin Geller, and Günther Prinz — Faculty of Physics and CENIDE, University Duisburg-Essen, Germany

Optical spectroscopy, especially Raman- and photoluminescence (PL)-spectroscopy, is commonly used to study the optical properties of 2D materials. In order to obtain the highest Raman/PL-signals, it is important to reduce the reflection of the excitation laser.

We studied a number of exfoliated hexagonal Boron Nitride (hBN) flakes with different thicknesses on a Si substrate with a 300 nm SiO_2 top layer. By changing the hBN layer thickness, we found a specific thickness, where all Raman signals (from Si, SiO_2 and hBN) showed maximum intensity, whereas the backscattered laser light was suppressed. To explain the increased intensities, we calculated the reflectivity and transmissivity of the full layer system (air, hBN, SiO_2, Si) for different hBN layer thicknesses and for different excitation wavelengths (457 nm, 532 nm, 633 nm), using the transfer-matrix-algorithm. To compare theory with experiment, we performed Raman measurements with the 3 different wavelengths on different flakes and determined their thicknesses with AFM-measurements.

Our results are in good agreement with theory and show that it is possible to choose the best flakes for spectroscopy, just by looking at their color in an optical microscope. This also allows us to easily find good flakes for observation of efficient single defect emission.

HL 2: Organic Semiconductors (joint session HL/CPP)

Time: Monday 9:30–11:15 Location: POT 361

HL 2.1 Mon 9:30 POT 361

Field-induced Seebeck voltage in disordered semiconductors — •Anton Kompatscher and Martijn Kemerink — IMSEAM, University Heidelberg

For disordered semiconductors it is theorized that finite electric fields can heat up the charge carrier distribution to effective temperatures that can significantly exceed the lattice temperature. Here, we argue that this effective temperature should be able to efficiently drive a thermoelectric generator (TEG) based on the Seebeck effect.(1) Utilizing kinetic Monte-Carlo simulations we were able to show similar results when driving a TEG with temperature or field. As a model system we choose the Seebeck ratchet introduced by Büttiker, replacing temperature- with field-driven effective temperature modulation. This allowed us to compare the current predicted by theory with the simulation currents resulting in good functional agreement. Effective temperature drive offers interesting advantages. Since only the electron distribution but not the lattice itself is heated, one of the mayor loss channels in TEG, lattice thermal conductivity, can be suppressed. Additionally, there is no need for n- and p-type materials (nor for heat exchangers) and a single material is sufficient. The main issue for concrete realization lies in the very high necessary field strengths at which effective temperature becomes relevant and that somehow need to be coupled into the TEG.

1. "On the concept of an effective temperature Seebeck ratchet", Appl. Phys. Lett. 119, 023303 (2021) https://doi.org/10.1063/5.0052116

HL 2.2 Mon 9:45 POT 361

Momentum dependent investigation of electronic excitations in β-metal-phthalocyanines — •Louis Philip Doctor and Martin Knupfer — Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, Helmholtzstraße 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 2.3 Mon 10:00 POT 361

Photovoltaic and nonlinear optical properties of complex self-assembled liquid crystal structures — •Ahmad Murad[1], Alexey Eremin[1], Martin Feneberg[1], Maximilian Baumann[2], Matthias Lehmann[2], and Mohamed Alaasar[3] — [1]Otto-von-guericke-Universität, Magdeburg,Deutchland — [2]Julius- Maximilians - Universität Würzburg — [3]Martin Luther University Halle-Wittenberg, Halle (Saale),

We explore conducting and photovoltaic properties in a series of two classes of semiconducting liquid crystals. BTBT-derived polycatenary mesogens doped with fullerenes show helical network phases exhibiting a strong photovoltaic effect in a broad range of light spectrum from UV to VIS. The second class is star-shaped mesogens with subphthalocyanine core that forms self-assembled ferroelectric columnar phases. We characterise the polar order using polarisation-resolved measurements of Second Harmonic Generation (SHG). Dynamical SHG studies provide information about the switching rates and the stability of the ferroelectric states. The photovoltaic effect is demonstrated under UV exposure.

HL 2.4 Mon 10:15 POT 361

What's special about Y6; working mechanism of Neat Y6 organic solar cell — •Elifnaz Saglamkaya[1], Artem Musiienko[2], Mohammad Saeed Shadabrooa[1], Bowen Sun[1], Sreelakshmi Chandrabose[3], Giulia Lo Gerfo M.[4], Niek F. van Hulst[4], Dieter Neher[3], and Safa Shoaee[1] — [1]University of Potsdam Disordered Semiconductor Optoelectronics Karl-Liebknecht-Strasse 24-25 14476 Potsdam-Golm — [2]Department Novel Materials and Interfaces for Photovoltaic Solar Cells, Helmholtz-Zentrum Berlin für Materialien und Energie, Kekuléstraße 5, 12489 Berlin, Germany — [3]University of Potsdam Physik und Optoelektronik weicher Materie Karl-Liebknecht-Straße 24-25 14476 Potsdam-Golm — [4]Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels, Barcelona, Spain

In this study, we analyse the working mechanism of single component small molecule acceptor Y6 solar cells with power conversion efficiencies reaching up to 4.5% and short circuit currents up to 8.4 mAcm-2.Using Hall effect, photo-Hall, and photoinduced absorption (PIA) measurements, we show that the charge photo-generation occurs in the bulk of Y6. With the aid of space charge limited current (SCLC) measurements we show that Y6 has an ambipolar charge carrier mobility. Our data shows that the limiting factor for the power conversion efficiency is fast charge recombination, which can be suppressed in presence of the transport layers, or modifying the morphology with a solvent additive.

15 min. break

HL 2.5 Mon 10:45 POT 361

Ultrastrong light-matter coupling of J-aggregated squaraine in a room temperature open cavity — •Christoph Bennenhei[1], Lukas Lackner[1], Moritz Gittinger[1], Heiko Knopf[2], Falk Eilenberger[2], Jennifer Zablocki[3], Arne Lützen[3], Martin Silies[1], Christoph Lienau[1], Martin Esmann[1], and Christian Schneider[1] — [1]Institute of Physics, University of Oldenburg — [2]Fraunhofer-Institute for Applied Optics and Precision Engineering IOF, Jena — [3]Kekulé Institute of Organic Chemistry and Biochemistry, University of Bonn

Organic molecule exciton-polaritons in artificial lattices are an emerging platform to emulate complex electronic Hamiltonians at ambient conditions. We present J-aggregated squaraine dye (SQ) thin films [1] as a promising candidate for exciton-polaritons in optical cavities due to the high oscillator strength and tunable resonance. Using white light reflection spectroscopy, we demonstrate tunable ultrastrong coupling of light to the SQ thin film in an open cavity at room temperature [2] which we support by transfer matrix calculations. In ongoing experiments, we introduce structured photonic lattices to the open cavity to investigate the coupling of the polaritons to tailored potential landscapes. [1] M. Schulz, et al., Nat Commun 9, 2413 (2018). [2] L. Lackner, et al., Nat Commun 12, 4933 (2021).

HL 2.6 Mon 11:00 POT 361

Room-temperature polariton lasing in anisotropic optical microcavities — •Christoph Bennenhei[1], Nils Kunte[1], Marti Struve[1], Heiko Knopf[2], Falk Eilenberger[2], Jürgen Ohmer[3], Utz Fischer[3], Martin Esmann[1], and Christian Schneider[1] — [1]Institute for Physics, Universität Oldenburg, Germany — [2]Fraunhofer-Institute for Applied Optics and Precision Engineering IOF, Jena, Germany — [3]Department of Biochemistry, Universität Würzburg, Germany

Organic molecule exciton-polaritons in artificial photonic potentials are an emerging platform to emulate electronic Hamiltonians at ambient conditions and for realizing low-threshold microlasers. In this work, we probe the polarization of polariton lasing in microcavities composed of dielectric Bragg reflectors with anisotropic indentations, enclosing the fluorescent protein mCherry. This material has been previously presented as a promising material for room-temperature polariton condensation [1,2]. Here, we experimentally show that lasing above the threshold differs distinctly for the two linearly polarized, energetically non-degenerate cavity eigenmodes. This effect leads to a drastic increase in the degree of linear polarization for the coherent photoluminescence emitted from the cavity. Our devices have relevant applications both for new types of polarized coherent light sources on chip and for accessing additional degrees of freedom in the emulation

of topological electronic lattice Hamiltonians at room temperature.

[1] S. Betzold et al. ACS Photonics 7, 384 (2020).

[2] M. Dusel et al. Nano Lett. 21, 6398 (2021).

HL 3: Focus Session: Progress in Hybrid Phononic Quantum Technologies I

Phonons, the quanta of lattice vibrations, are the fundamental excitations in a crystal and couple to literally any type of excitation in a solid. This universal coupling makes them ideally suited for hybrid quantum architectures which synergistically harness the strengths of its components and at the same time mitigate individual shortcomings. For chip-based hybrid quantum devices, phonons are particularly attractive because they can be routed in integrated circuits with very little dissipation over macroscopic distances in the solid state or confined in small mode volume phononic cavities. Although the research of phonons has a long-lasting history, only recently important breakthroughs were made that will unleash the full potential of acoustic waves in quantum technologies. For example, the rapid progress in the development of surface acoustic wave resonators now allows to generate desired phonon quantum states which promotes the field of quantum acoustics.

Organized by Hubert J. Krenner and Daniel Wigger

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

Invited Talk HL 3.1 Mon 9:30 POT 151

Schrödinger cat states of a 16-microgram mechanical oscillator — •Yiwen Chu[1,2], Marius Bild[1,2], Matteo Fadel[1,2], Yu Yang[1,2], Uwe von Lüpke[1,2], Phillip Martin[1,2], and Alessandro Bruno[1,2] — [1]Department of Physics, ETH Zürich — [2]Quantum Center, ETH Zürich

While the principle of superposition in quantum physics is routinely validated for microscopic systems, it is still unclear why we do not observe macroscopic objects to be in superpositions of states that can be distinguished by some classical property. I will present our experiments that harness the resonant Jaynes-Cummings interaction between a high overtone resonator mode of a bulk acoustic wave resonator and a superconducting qubit to demonstrate the preparation of Schrödinger cat states of motion. In such a state, the constituent atoms oscillate in a superposition of two opposite phases with an effective oscillating mass of 16 micrograms. Making use of the circuit quantum acoustodynamics toolbox we have developed, we furthermore show control over amplitudes and phases of the created Schrödinger cat states, and investigate their decoherence dynamics by observing the disappearance of Wigner negativities. Our results can find applications in continuous variable quantum information processing and in fundamental investigations of quantum mechanics in massive systems.

Invited Talk HL 3.2 Mon 10:00 POT 151

High-fidelity quantum information processing with spins and phonons — •Peter Rabl — Atominstitut, TU Wien, Stadionallee 2, 1020 Wien, Austria — Physik-Department, Technische Universität München, 85748 Garching, Germany — Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany

Phonons in solids are usually uncontrolled and therefore represent one of the main sources of decoherence for many solid-state quantum systems. However, when appropriately designed, isolated mechanical modes offer fascinating new opportunities for engineering coherent interactions between systems that cannot be coupled efficiently otherwise. In this talk, I will discuss the prospects of this approach for engineering phonon-mediated quantum gate operations between spin qubits associated with SiV defect centers in a diamond phononic crystal. Specifically, I will show how the application of continuous spin-echo techniques can substantially boost the coherence times in this system and suppress gate errors below 10^{-4} for experimentally realistic noise parameters. Therefore, although the field is still in its infancy, this analysis outlines a realistic path toward moderate- and large-scale quantum devices with spins and phonons, at a level of control that is comparable to other leading quantum-technology platforms.

HL 3.3 Mon 10:30 POT 151

Acoustically-induced pseudo-gauge fields and anomalous transport phenomena in graphene — •Pai Zhao[1], Lars Tiemann[1], Lev Mourokh[2], Vadim M. Kovalev[3], and Robert H. Blick[1] — [1]University of Hamburg, Germany — [2]Department of Physics, Queens College, New York, USA — [3]Novosibirsk, Russia

One of many remarkable consequences of the low-energy Dirac description of graphene is the emergence of synthetic gauge fields under lattice deformation that affect the carrier dynamics. We show that acoustically stimulated carrier transport in graphene at 4 Kelvin signals the presence of artificial gauge fields through the build-up of a transversal voltage at zero magnetic field. We fabricated a gate-tunable, large-scale CVD graphene Hall bar on a hybrid piezoelectric $LiNbO_3$ on insulator substrate. An interdigitated transducer launches a surface acoustic wave (SAW) that acoustically accelerates the carriers in the graphene. At zero magnetic field, we observe large anomalous acoustically-induced synthetic Hall voltages up to 200 μV, depending on the carrier type, concentration and SAW power. The synthetic Hall voltage can modulate a conventional Hall voltage arising in a large external magnetic field [1]. Our observation is consistent with studies of strain-induced pseudo-gauge fields [2-4].

[1] P. Zhao et al., Phys. Rev. Lett. 128, 256601 (2022); [2] N. Levy et al., Science 329, 544 (2010); [3] F. Guinea, M. I. Katsnelson and A. K. Geim, Nat. Phys. 6, 30 (2010); [4] M. Oliva-Leyva and G. G. Naumis, J. Phys.: Condens. Matter 28, 025301 (2015).

HL 3.4 Mon 10:45 POT 151

On-chip waveguides for hypersound with planar semiconductor optical microcavities — Antonio Crespo-Poveda, •Alexander Kuznetsov, Alberto Hernández-Mínguez, Abbes Tahraoui, Klaus Biermann, and Paulo Santos — Paul Drude Institute for Solid State Electronics, Berlin, Germany

In solid-state systems, coherent oscillations of the atomic lattice (phonons) couple to the majority of elementary excitations. This motivates studies that aim at creating phonon-based interfaces between photons and quantum systems. In this work, we show piezoelectric excitation of 6 GHz hypersound in a buried (Al,Ga)As planar waveguide. Acoustic echo spectroscopy reveals that phonons propagate over mm-long distances. Furthermore, the waveguide contains quantum wells and is embedded into an optical microcavity. The strong-coupling between nIR photons and excitons leads to the formation of light-matter quasiparticles – polaritons. Due to the excitonic component, polaritons act as a sensitive local optical probe for gAPs. Thus, we demonstrated a conversion of microwave signals to guided hypersound with the subsequent polariton-mediated transduction to photons. In a broad context, the results are important for the remote coherent control of optoelectronic resonances and the realization of the on-chip phonon circuitry and a microwave-to-optical interface.

30 min. break

Invited Talk HL 3.5 Mon 11:30 POT 151

Control of spin centers in silicon carbide using acoustic fields — •Alberto Hernández-Mínguez — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany

Atom-like color centers in solids are attractive for applications in quantum technologies because their spin states exhibit long coherence times and can be controlled by optical, microwave and acoustic fields. In this contribution, we report on acoustically driven spin transitions in sil-

icon vacancy centers in SiC. Specifically, we use the dynamic strain of surface acoustic waves to selectively excite room-temperature spin transitions with magnetic quantum number differences of ± 1 and ± 2 in the absence of external microwave fields [1]. Compared to the ground states, spin levels in the optically accessible excited states possess even stronger interaction with acoustic vibrations, thus giving rise to novel and, so far, largely unexploited physical phenomena. A remarkable example is the acoustically induced coherent spin trapping [2], which consists in the quenching of the optically detected spin resonance due to the precession of the spin around the same axis in both ground and excited states. Our findings provide new opportunities for the coherent control of spin qubits with dynamic strain fields that can lead towards the realization of future spin-acoustic quantum devices.

[1] A. Hernández-Mínguez *et al.*, Phys. Rev. Lett. **125**, 107702 (2020)

[2] A. Hernández-Mínguez *et al.*, Sci. Adv. **7**, eabj5030 (2021)

HL 3.6 Mon 12:00 POT 151

Storage and retrieval of telecom single photons from a semiconductor quantum dot in a rubidium ORCA memory — •Lukas Wagner[1], Sarah Thomas[2], Cornelius Nawrath[1], Simone Luca Portalupi[1], Patrick Ledingham[3], Ian Walmsley[2], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen (IHFG), Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]Faculty of Natural Sciences, Department of Physics, Imperial College London, Imperial College Rd, South Kensington Campus, London SW7 2AZ, United Kingdom — [3]Department of Physics and Astronomy, University of Southampton, Southampton SO17 1BJ, United Kingdom

Photons are highly attractive as carriers of information thanks to their propagation at the speed of light and their low interaction with matter. Furthermore, various implementations of photonic quantum technologies will strongly benefit from the possibility of storing quantum information. Indeed, quantum memories would allow synchronizing the arrival time of multiple photons. Semiconductor quantum dots (QDs) are highly attractive as sources of quantum light. Atomic vapors are known as a very powerful platform to realize on-demand storage and retrieval of light. For these reasons a hybrid quantum system combining these two elements was for long sought after. Here, we will report on our progress to interface single photons from an In(Ga)As QD emitting at telecom wavelength with a rubidium off-resonance cascaded absorption (ORCA) quantum memory.

HL 3.7 Mon 12:15 POT 151

Excitation and read-out of macroscopic mechanical motion by phase-modulated optical driving of a single-photon emitter — •Thilo Hahn[1], Jacek Kasprzak[2], Ortwin Hess[3], Tilmann Kuhn[1], and Daniel Wigger[3] — [1]Institute of Solid State Theory, University of Münster, Germany — [2]Université Grenoble Alpes, CNRS, France — [3]School of Physics, Trinity College Dublin, Ireland

Resonance phenomena provide an access to drive inert systems out of equilibrium by applying a periodic force. In this contribution we will investigate a hybrid quantum system consisting of a single photon emitter (SPE) that is on the one hand coupled to a single phonon mode, e.g., in the form of a mechanic resonator, and on the other hand driven by a laser field. To convert a series of laser pulses into a measurable displacement of the phonon mode, originally a synchronization between the pulse repetition and the mode frequency was suggested [2] and demonstrated. Here, we discuss a different excitation scheme that is adapted from the heterodyne four-wave mixing (FWM) technique: We consider a series of pulse pairs which drives the phonons into a far displaced quasi-coherent state by tuning the harmonically oscillating phase relation within the pulse pairs in resonance with the phonons. Conversely, the optical properties of the SPE are dynamically affected by the phonon motion. Conveniently this can directly be measured by the FWM signal emitted by the SPE in order to detect the mechanical motion. Consequently, we combine resonant driving and read-out in a single method.

[1] Phys. Rev. A 90, 023818 (2014) [2] Nat. Nanotechnol. 16, 283 (2021)

HL 3.8 Mon 12:30 POT 151

Imaging surface acoustic waves on 2D materials using atomic force microscopy — •Mingyun Yuan[1], Alberto Hernández-Mínguez[1], Igor Aharonovich[2], and Paulo V. Santos[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany — [2]School of Mathematical and Physical Sciences, University of Technology Sydney, Ultimo, Australia

There is an increasing interest in coupling the dynamic strain of surface acoustic waves (SAWs) to electronic excitations in 2D-material-based nanostructures to acoustically manipulate their optoelectronic properties. While optical phenomena in 2D nanostructures can be conveniently mapped by photoluminescence, local probing of mechanical properties remains challenging. This task can, nevertheless, be assisted by high-frequency (GHz) SAWs, which are particularly suitable for probing very thin objects due to their micron-size wavelengths and their confinement near the surface. Here, we use atomic force microscopy (AFM) to image SAWs propagating along a LiNbO3 acoustic resonator containing a multilayer hexagonal Boron Nitride (hBN) flake irradiated with Ar ions to create color centers. The high spatial resolution of AFM enables us to investigate the SAW strain transferred to the flake. We observe spatial inhomogeneities, revealing that the strain transferred to 2D materials can exhibit large spatial fluctuations. Possible mechanisms that affect the coupling will be discussed. Our method demonstrates a straight-forward way to characterize dynamic strain fields in hybrid SAW/2D-material systems.

HL 3.9 Mon 12:45 POT 151

Effect of helium ion implantation on nanomechanical resonators in 3C-SiC — •Nagesh Shamrao Jagtap[1,2], Yannick Klass[3], Felix David[3], Philipp Bredol[3], Eva Weig[3], Manfred Helm[1,2], Georgy Astakhov[1], and Artur Erbe[1,2] — [1]Helmholtz-Zentrum Dresden - Rossendorf, Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany — [2]Dresden University of Technology, 01062 Dresden, Germany — [3]Technical University of Munich, Chair of Nano and Quantum Sensors, 85748 Munich, Germany

Silicon carbide (SiC) is a suitable candidate for nanoelectromechanical systems due to its superior mechanical properties. It is also an interesting material platform to study the coupling of mechanical modes with localized spins associated with irradiation-induced defects. Such a spin-mechanical system can be used for quantum sensing applications [1]. The nanomechanical resonators in 3C-SiC are fabricated by standard semiconductor processing techniques such as electron beam lithography and reactive ion etching. They are characterized using Fabry-Pérot interferometer. In the preliminary experiments, we focus on the material modification by helium ion broad beam implantation on strained 3C-SiC resonators. The effect of varying fluence on resonance frequencies and quality factors is studied (see contribution of Philipp Bredol).

[1] A. V. Poshakinskiy and G. V. Astakhov, "Optically detected spin-mechanical resonance in silicon carbide membranes*, PhysRevB.100.094104 (2019)

HL 4: Perovskite and photovoltaics I (joint session HL/CPP)

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

HL 4.1 Mon 9:30 POT 251

Bandgap engineering of two-step processed perovskite top cells for application in perovskite-based tandem photovoltaics — •Ronja Pappenberger[1,2], Alexander Diercks[2], Ahmed Farag[1,2], Paul Fassl[1,2], and Ulrich W. Paetzold[1,2] — [1]Institut für Mikrostrukturtechnologie, KIT, Germany — [2]Lichttechnisches Institut, KIT, Germany

Tandem solar cells offer a promising concept of raising the efficiency of silicon solar cells above the theoretical limit of 29%. In this context, silicon is supplemented by a wide-bandgap perovskite top solar cell to make better use of the solar spectrum. Perovskite solar cells come into play given their favorable optoelectronic quality and tunable bandgap. Textured-front perovskite silicon tandem solar cells currently promise the highest energy yield for modules in the field. To avoid shunting, ensure high efficiency and economic production of the perovskite on the μm-sized pyramids, a conformal growth of the perovskite layer as well as a sufficient layer thickness are necessary. A two-step method - containing a separate deposition of the PbI_2 and the organic cations - enables high film quality, flexibility in choice of component/solution and the possibility of upscaling. Here, we investigate different strategies of increasing the bandgap of the perovskite. Thereby the location of the added bromine - cation solution and/or PbI_2 solution - is critical. With our approach, the device performance - PCE of 17.2%, FF of 76% and V_{oc} of 1.156 V ($E_g \approx 1.64$ eV) - and film quality can be maintained. Furthermore, the effect of an increasing bandgap in combination with planar/textured silicon bottom cells is studied.

HL 4.2 Mon 9:45 POT 251

Application of plasma enhanced atomic layer deposition process of alumina on perovskite film boosts efficiency of solar cells — •Małgorzata Kot[1], Mayank Kedia[2], Paul Plate[3], Ludwig Marth[3], Karsten Henkel[1], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg, Konrad-Zuse-Strasse 1, 03046 Cottbus, Germany — [2]Institut fuer Photovoltaik Universitaet Stuttgart, Pfaffenwaldring 47, 70569 Stuttgart, Germany — [3]SENTECH Instruments GmbH, Schwarzschildstraße 2, 12489 Berlin, Germany

It is assumed that plasma-enhanced atomic layer deposition (PEALD) cannot be used to prepare thin films on sensitive organic-inorganic perovskites because the plasma destroys the perovskite film and thus deteriorates its photophysical properties. Here, we prove that using an appropriate geometry of the ALD system (SENTECH SI PEALD system) and suitable process parameters it is possible to coat perovskites with alumina by PEALD. Spectromicroscopy followed by electrical characterisation reveal that as long as the PEALD process is not optimized (too long plasma pulses) one gets degradation of the perovskite as well as dissociation of the created iodine pentoxide (during PEALD) under light that causes a valence band maximum (VBM) shift to the Fermi level and thus significantly decreases the solar cell efficiency. However, once the PEALD process parameters are optimized, no VBM shift is observed. Moreover, the solar cell efficiency depends inversely on process temperature and layer thickness.

HL 4.3 Mon 10:00 POT 251

Tuning Crystallization for Highly Efficient Perovskite Silicon Tandem Solar Cells — •Mohamed Mahmoud[1,2], Oussama Er-Raji[1,2], Patricia Schulze[1], Anna Juliane Borchert[1,2], and Andreas W. Bett[1,2] — [1]Fraunhofer ISE — [2]University of Freiburg

Perovskite solar cells have the advantages of a strong absorption edge, defect tolerance, and potential cheap production due to easy production methods such as spin coating or slot-die coating as a highly scalable production method. In the industry, double-sided textured (micro-meter sized pyramid) silicon is commonly produced to decrease reflection losses and improve light trapping. Solution-based processing methods of perovskite on top of the textured Si showed low conformality, which resulted in shunts and non-working solar cells. To overcome this issue, the hybrid route was developed, in which inorganic precursors are co-evaporated using the thermal vapor deposition technique and then organic precursors are spin-coated followed by a thermal annealing. By doing that, high conformality of perovskite thin films on top of the textured silicon is achieved. However, the resulting perovskite grain size is rather low, which can lower the bulk quality. In this work, various additives were used to increase the grain size, and their working mechanisms were studied. In addition, we study the consequences of different grain sizes at the tandem level with respect to device efficiency as well as stability. Moreover, using the thermodynamics fundamentals of crystallization, we hypothesize for the first time a common general explanation for the working mechanism of all the different additives used.

HL 4.4 Mon 10:15 POT 251

Efficient Modeling Workflow for Accurate Electronic Structures of Hybrid Perovskites — Julian Gebhardt[1,2], •Wei Wei[1,2], and Christian Elsässer[1,2,3] — [1]Fraunhofer IWM, 79108 Freiburg — [2]Cluster of Excellence livMatS, University of Freiburg — [3]Freiburg Materials Research Center, University of Freiburg

Hybrid organic-inorganic halide perovskites are the most promising photovoltaic absorber materials to substitute or complement silicon in high-efficiency solar cells. These hybrid materials are often constrained by their low stability and critical elements like lead. Computational high-throughput screening studies, based on solid-state electronic-structure theory, are useful to identify promising substitute materials with targeted properties. In this work, we present an efficient computational approach based on density-functional theory, which is suitable to predict band gaps for arbitrary compounds reliably and in good quantitative agreement with experimental band gap data for known compounds. This approach is described and demonstrated for the building blocks of one of the most promising hybrid perovskites, namely, $(HC(NH_2)_2)_xCs_{1-x}Pb(I_yBr_{1-y})_3$, with x and y varied between zero and one.

J. G. et al. *J. Phys. Chem. C* **2021** 125, 18597.

HL 4.5 Mon 10:30 POT 251

Photon Management for Ultrathin Solar Cells: Enabling Waveguide Modes by Structured Back Contact — •Merve Demir, Thomas Schneider, Torsten Hölscher, Heiko Kempa, and Roland Scheer — Martin-Luther-Universität Halle-Wittenberg, Germany

The recent research based on Cu(In,Ga)Se2 (CIGSe) solar cells is focused on thinning down the absorber layer to enable less material consumption and cost effective large scale production. However, having ultra-thin CIGSe solar cells with absorber layer thickness in sub-micron level brings the cost of limited absorption of solar spectra and hence leads to lower energy conversion efficiencies. This problem can be overcome by the cell architecture including functional back contact elements for the enhancement of optical absorption. In this contribution, ultrathin CIGSe solar cells with 500 nm thick absorber layer were combined with nano-textured SiO2 back contacts together with aluminum back mirror. With this cell design, it is aimed to have increased power conversion efficiency for ultra-thin CIGSe solar cells due to enhanced absorption of long wavelength region photons. The solar cell parameters were extracted and compared with the conventional CIGSe back contact, flat molybdenum, to reveal the effects of functional back contact. The experimental findings on quantum efficiency measurements prove the positive effects of having highly reflective and textured back contact. Furthermore, the growth of CIGSe on textured substrates was examined throughout cross section cuts by scanning electron microscopy and energy dispersive X-ray diffraction.

30 min. break

HL 4.6 Mon 11:15 POT 251

Employing three-dimension structure analysis: digital twin for studying grain boundary effects in thin film solar cells — •Chang-Yun Song[1], Matthias Maiberg[1], Heiko Kempa[1], Ali Gholinia[2], Wolfram Witte[3], Dimitrios Hariskos[3], Daniel Abou-ras[4], and Roland Scheer[1] — [1]Martin-Luther-University Halle-Wittenberg, Halle, D — [2]University of Manchester, Manchester, UK — [3]Zentrum für Sonnenenergie- und Wasserstoff-Forschung, Stuttgart, D — [4]Helmholtz-Zentrum Berlin, Berlin, D

Grain boundaries (GBs) in polycrystalline Cu(In,Ga)Se2 (CIGSe), are believed to be one of the performance limiting factors of current record efficiency CIGSe solar cells. Numerous simulation studies have been conducted to unveil their effects. Most simulations, however, have

been done within two-dimensions (2D), thereby presumably using the simplified GBs shapes. In this study, we thus present a realistic three-dimensional (3D) GB model for a high-efficiency CIGSe layer. To this end, a combination of electron backscatter diffraction and focused ion beam was applied to obtain 3D data of the CIGSe layer, which then allowed the reconstruction of the 3D grain structure into a computer model. By using the computer model as input for 3D opto-electronic simulations, we study the electronic effects of GBs on the high-efficiency solar cell under investigation bulk parameter values for the simulations were obtained through a combination of simulation and experiments, such that the solar cell is consistently described. As an outcome, the 3D simulations confirm that the effect of GB was indeed underestimated in earlier conventional 2D simulations.

HL 4.7 Mon 11:30 POT 251

Interface Engineering to reduce non-radiative recombination losses at the perovskite/C60 interface in monolithic perovskite silicon tandem solar cells — •Johanna Modes, Patricia S. C. Schulze, Kaitlyn Mc Mullin, Maryamsadat Heydarian, Christoph Messmer, Juliane Borchert, and Andreas Bett — Fraunhofer ISE

Metal halide perovskites have emerged in recent years as a promising absorber material for solar cells with the potential to combine high power conversion efficiency with low production costs. However, significant non-radiative charge carrier recombination occurs at the perovskite interface to the contacts, thus preventing the full potential of the solar cell from being exploited. Photoluminescence quantum yield measurements clearly show that the Quasi-Fermi level splitting is reduced by evaporation of the electron contact C60 onto perovskites, leading to limited open-circuit voltage in devices. In recent literature, as well as in our investigations, different passivation layers are deposited between perovskite and the electron contact to reduce non-radiative recombination and to improve the open-circuit voltage. This is on the one hand pursued by increasing the selectivity at the contacts through field effects and band alignment and secondly by reducing defects at the interface through chemical passivation.

HL 4.8 Mon 11:45 POT 251

Spontaneous Polarization in $NaNbO_3$ — •Kisung Kang[1], Saud Bin Anooz[2], Jutta Schwarzkopf[2], Matthias Scheffler[1], and Christian Carbogno[1] — [1]The NOMAD Laboratory at the FHI of the Max-Planck-Gesellschaft and IRIS-Adlershof of the Humboldt-Universität zu Berlin — [2]Leibniz-Institut fur Kristallzüchtung (IKZ)

The perovskite $NaNbO_3$ is regarded as a promising lead-free piezoelectric material, also because its polarization properties can be further tailored via strain engineering. [1] In thin films, lattice strain can be incorporated by the heteroepitaxial growth on lattice mismatch. By tuning the epitaxial strain in the films, different polymorphs with distinctively different polarization strength and orientation can be realized [2, 3]. We investigate this question by using density-functional theory at the semi-local level of theory, which we carefully validate with hybrid-functional calculations. By this means, we compute the spontaneous polarization for ten phases of $NaNbO_3$ as a function of stress and strain. In line with experiments, we confirm that the monoclinic *Pm* phase features a non-vanishing in-plane polarization, the orientation of which is independent of the strain. Conversely, the polarization direction of the orthorhombic $Pmc2_1$ phase depends on the applied tensile strain. We analyze the underlying electronic and atomistic mechanism and discuss how the relevant properties are influenced by phase transformations.

[1] N. Bein, *et al.*, *Phys. Rev. Mater.* **6**, 084404 (2022).
[2] J. Schwarzkopf, *et al.*, *J. Appl. Cryst.* **45**, 1015 (2012).
[3] S. B. Anooz, *et al.*, *Appl. Phys. Lett.* **120**, 202901 (2022).

HL 4.9 Mon 12:00 POT 251

Peculiar bond length dependence and its impact on the band gap bowing in (Ag,Cu)(In,Ga)Se_2 thin film alloys — •Hans H. Falk[1], Stefanie Eckner[1], Konrad Ritter[1], Sergiu Levcenko[1], Timo Pfeiffelmann[1], Edmund Welter[2], Jes Larsen[3], William N. Shafarman[4], and Claudia S. Schnohr[1] — [1]Felix Bloch Institute for Solid State Physics, Leipzig University, Germany — [2]Deutsches Elektronen-Synchrotron DESY, Germany — [3]Department of Materials Science and Engineering, Uppsala University, Sweden — [4]Department of Materials Science and Engineering, University of Delaware, USA

Incorporation of Ag into Cu(In,Ga)Se_2 thin film solar cells improves several of their properties. However, with increasing Ag content, the band gap of (Ag,Cu)$GaSe_2$ increases even though the lattice expands and the Ga-Se bond length is predicted to decrease. This is counter-intuitive, since in other chalcopyrite alloys all bond lengths increase and the band gap decreases as the lattice expands. Therefore, we studied the element-specific average bond lengths of (Ag,Cu)$GaSe_2$, (Ag,Cu)$InSe_2$ and Ag(In,Ga)Se_2 using X-ray absorption spectroscopy for thin films grown on Mo-coated soda lime glass by a single stage co-evaporation process. As predicted, the Ga-Se bond length decreases with increasing Ag content in (Ag,Cu)$GaSe_2$. While the In-Se bond length of (Ag,Cu)$InSe_2$ shows the same behavior, Ag(In,Ga)Se_2 exhibits a dependence similar to that of Cu(In,Ga)Se_2, demonstrating that the peculiar behavior is related to mixing the group-I lattice site. Using the bond lengths we model the anion positions and estimate their effect on the band gap bowing.

HL 4.10 Mon 12:15 POT 251

Fast diffusion of spin polarized excitons in bulk lead halide perovskites — •Sergiu Anghel[1], Dmitri R. Yakovlev[1], Dmitry N. Dirin[2], Maksym V. Kovalenko[2], Manfred Bayer[1], and Markus Betz[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, Otto-Hahn-Straße 4a, D-44227 Dortmund, Germany — [2]Laboratory of Inorganic Chemistry, Department of Chemistry and Applied Biosciences, ETH Zürich, Zürich CH-8093, Switzerland

We investigate the spin diffusion of the free "hot" excitons in FA0.9Cs0.1PbI2.8Br0.2 bulk lead halide perovskite crystal at cryogenic temperatures by employing ultrafast time- and spatial-resolved magneto-optical Kerr microscopy. We measure the spin diffusion coefficient (D_s) of the free excitons of D_s~50 cm^2/s , which is a very surprising outcome, especially in the light of the recent results obtained on bulk or two-dimensional perovskites [1,2], where D_s is at least two orders of magnitude lower. D_s shows a roughly linear dependence on pump energy whereas the dependence on pump power is much more intricate - after a certain pump power threshold we observe an anomalous, nonlinear spatial dependence of D_s. We discuss our findings in view of efficient exciton-phonon coupling and Auger processes.

[1] A. Baldwin, G. Delport, K. Leng, R. Chahbazian, K. Galkowski, K. P. Loh, and S. D. Stranks, J. Phys. Chem. Lett. 12, 4003 (2021).
[2] S. D. Stranks, G. E. Eperon, G. Grancini, C. Menelaou, M. J. P. Alcocer, T. Leijtens, L. M. Herz, A. Petrozza, and H. J. Snaith, Science 342, 341 (2013).

HL 5: Heterostructures, interfaces and surfaces

Time: Monday 10:00–11:15 Location: POT 112

HL 5.1 Mon 10:00 POT 112

Time-resolved analysis of propagating exciton-polariton condensates in photonic potential landscapes. — •Christian G. Mayer, Philipp Gagel, Simon Betzold, Tristan H. Harder, Monika Emmerling, Adriana Wolf, Fauzia Jabeen, Sven Höfling, and Sebastian Klembt — Technische Physik, RCCM and Würzburg-Dresden Cluster of Excellence ct.qmat, University of Würzburg, Germany

Confining photons in a Fabry-Perot microcavity and coupling them strongly to excitons leads to the formation of hybrid matter-light particles named exciton-polaritons (polaritons). Owing to their bosonic statistics, they undergo a phase transition above a critical density to a dynamic condensate via stimulated scattering. Polaritons have quite long diffusion length compared to excitons because of their lower effective mass inherited by their photonic fraction. Propagation effects of a polariton condensate take place on a time scale of a few picoseconds and are caused by the repulsive potential facilitated by the matter fraction due to polariton-exciton and polariton-polariton interactions. By varying the light-matter composition of the polariton condensate, we investigate changes in the propagation properties such as velocity and length.
Using electron beam lithography, we spatially confine propagating polaritons in waveguides, as well as in resonator lattices supporting quantum valley Hall modes. Using a streak camera, the propagation of the polariton condensate is measured in a variety of confined structures and systems.

HL 5.2 Mon 10:15 POT 112

Tackling the band ordering problem for transport calculations in strained semiconductors: A $\mathbf{k} \times \mathbf{p}$ perspective — •Daniel Fritsch[1], Costanza L. Manganelli[2], Christian Merdon[1], and Patricio Farrell[1] — [1]Weierstrass Institute for Applied Analysis and Stochastics, Mohrenstr. 39, 10117 Berlin, Germany — [2]IHP Leibniz-Institute for High Performance Microelectronics, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

A reliable determination of band energies in strained semiconductor heterostructures is indispensable for subsequent transport calculations. However, one crucial problem is presently hidden within the change in valence band ordering due to intrinsically occurring strain in semiconductor heterostructures, nanowires, or quantum dots.

In order to tackle this problem, we present a numerical algorithm based on the Bir-Pikus $\mathbf{k} \times \mathbf{p}$ Hamiltonian, that takes into account additional wavevector dependent properties, e.g. the effective mass tensor, to identify the nature of the valence bands. It provides the necessary connection between arbitrary strain profiles for semiconductor nanostructures calculated by means of a finite element method [1] and transport calculations employing a drift diffusion model [2].

The new algorithm is applied to example strain profiles, e.g. biaxial and uniaxial strain, and results are compared to earlier theoretical and experimental findings.
[1] GradientRobustMultiPhysics.jl (10.5281/zenodo.7217591).
[2] ChargeTransport.jl (10.5281/zenodo.7124161).

HL 5.3 Mon 10:30 POT 112

Improved growth of unstrained HgTe quantum well on InAs — •Mahitosh Biswas[1,2], Hartmut Buhmann[1,2], and Laurens W. Molenkamp[1,2] — [1]Institute for Topological Insulators, Universität Würzburg, 97074 Würzburg, Germany — [2]Physikalisches Institut (EP3), Universität Würzburg, 97074 Würzburg, Germany

HgTe turned out to be a prototype material for investigations of transport properties in topological insulator materials. The material system also demonstrated its versatility when compressive strain is applied, resulting in Weyl and Kane semimetal states. It has been shown that the strain can be controlled sufficiently by the period of a CdZnTe/CdTe superlattices grown on a doped GaAs substrate. However, these strained and/ or strained layers exhibit a rather high surface roughness which makes them unsuitable for sub-micrometer device fabrication or local probe measurement techniques. Here we show that CdZnTe/CdTe superlattices grown on doped InAs improve the situation significantly. Surface roughness is about three times lower compared with GaAs. These observations are confirmed by TEM measurements which monitor dislocations originating at the III-V/II-VI semiconductor interface. Magneto-transport measurements reveal that the doped substrate can be used as a highly efficient back gate. Carrier variations between $2 \times 10^{11} cm^{-2}$ (electron) and $-2 \times 10^{11} cm^{-2}$ (hole) are observed for a medium ± 10 V gate range. These results manifest a (big) step forward toward the fabrication of functional top and back gated devices on topological materials.

HL 5.4 Mon 10:45 POT 112

Band alignment of thin strontium germanate layer on silicon from *ab initio* — •Tomáš Rauch[1,2], Pavel Marton[3,4], Silvana Botti[1,2], and Jiří Hlinka[3] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Germany — [2]European Theoretical Spectroscopy Facility — [3]Institute of Physics of the Czech Academy of Sciences, Praha, Czech Republic — [4]Institute of Mechatronics and Computer Engineering, Technical University of Liberec, Czech Republic

Silicon is one of the most used materials for optoelectronic applications. In photo-catalytic cells for hydrogen evolution reaction, Si must be capped by a protective layer, additionally allowing the photo-excited electrons to travel to the device surface. It has been demonstrated, that $SrTiO_3$ (STO) can fulfill these two functions [1].

In this work, we studied $SrGeO_3$ (SGO) as an alternative to STO, using density-functional theory. We calculated the structural properties of a chosen prototypical SGO/Si(001) interface and studied its electronic structure, focusing on the band offsets between Si and SGO. We found a metallic type-III interface with occupied conduction bands of SGO and a charge transfer from Si to SGO. Aligning the local band edges of the thin SGO layer with the redox potentials allows us to conclude that the SGO/Si interface should be suitable for water reduction.

We acknowledge funding by the Czech Science Foundation (project no. 21-20110K) and by the Volkswagen Foundation (project "dandelion").

[1] Li Ji et al., Nat. Nanotechnol. **10**, 84 (2015)

HL 5.5 Mon 11:00 POT 112

Evolution of vacancy like defects in heavily doped GaAs — •Maciej Oskar Liedke[1], Slawomir Prucnal[2], Maik Butterling[1], Juanmei Duan[2], Eric Hirschmann[1], Mao Wang[2], Manfred Helm[2], Shengqiang Zhou[2], and Andreas Wagner[1] — [1]Institute for Radiation Physics, Helmholtz-Zentrum Dresden - Rossendorf, Dresden, Germany — [2]Institute for Ion Beam Physics, Helmholtz-Zentrum Dresden - Rossendorf, Dresden, Germany

The effect of intense pulsed laser melting and flash lamp annealing on defects distribution and activation efficiency in chalcogenide-implanted GaAs was investigated by means of positron annihilation spectroscopy and transport measurements. Using positrons as a sensitive probe of open volumes and dedicated DFT calculations, we will highlight the capability of nanosecond pulsed laser melting to control the type and density of defect complexes, e.g. S or Te substituting As atoms associated to Ga vacancy, playing a crucial role for donor deactivation. The distribution of defects and carriers will be discussed regarding the depth distribution of implanted elements and the solidification velocity during recrystallization.

HL 6: Focus Session: Frontiers of Electronic-Structure Theory III (joint session O/HL)

Electronic-structure calculations, based on density-functional theory (DFT) and methodology beyond, are getting increasingly involved as they face the following challenges: First, investigations of modern materials typically require large unit cells, owing to complex crystal structures, mixed compositions, internal interfaces, etc. Second, at the same time, they often require advanced methods, including hybrid functionals of DFT, Green-function techniques from many-body perturbation theory (MBPT), high-level wavefunction-based methods like coupled-cluster (CC) theory, or quantum Monte-Carlo simulations. All these methods should ideally be implemented in scientific software that is running efficiently on modern supercomputers. With both methodology and computer architectures exhibiting increasing complexity, collaborative development and shared tools, including ready-to-use libraries and codes, are becoming indispensable. This interdisciplinary symposium covers recent progress in the broad area of electron-structure methods and highly-sophisticated tools that enable the entire community to explore most exciting materials from different perspectives to either predict peculiar features or get insight into measured counterparts.

Organizers: Claudia Draxl (HU Berlin), Dorothea Golze (TU Dresden), Xavier Gonze (U Louvain), and Andris Gulans (U Latvia)

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

HL 6.1 Mon 10:30 TRE Ma

Testing the hell out of DFT codes with virtual oxides — Emanuele Bosoni[1], •Stefaan Cottenier[2], and Giovanni Pizzi[3] — [1]ICMAB-CSIC, Spain — [2]Ghent University, Belgium — [3]EPFL, Switzerland

If you use DFT to predict a property of a crystal, how confident can you be that the prediction is computed in a bug-free way? And if your DFT-code uses pseudopotentials, can you trust that the pseudopotential does not modify your predictions? Answering such questions has been the goal of a study a few years ago, in which 71 unary crystals were examined in exactly the same way by 40 different DFT methods and codes [DOI 10.1126/science.aad3000]. In a next step, a consortium of 41 scientists (*) has done a similar exercise for a much larger pool of crystals: all elements of the periodic table up to Z=96, each in 10 different crystal structures, 6 of them being (virtual) oxides that sample a range of chemical bond types and 4 being unary crystals that sample low to high coordination environments. In this presentation, we will discuss the reasons to choose these crystals, the different quality criteria by which results can be compared, we will demonstrate how this exercise leads to more precise and more trustworthy pseudopotential libraries, and we will show how this data set is shared with the community in order to foster better-tested codes and pseudopotentials for all.

(*) Unfortunately the size of this abstract does not allow to mention them all.

HL 6.2 Mon 10:45 TRE Ma

High-throughput absorption spectra obtained by beyond-DFT workflows — •Fabian Peschel, Alexander Buccheri, and Claudia Draxl — Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

Fully converging *ab initio* calculations can be a challenging task, in particular when it comes to excited states, which require multiple ground-state calculations for different physical quantities. In this work, we aim at computing highly precise absorption spectra by employing the Bethe-Salpeter equation of many-body perturbation theory, as implemented in the all-electron full-potential package `exciting` [1,2]. To obtain benchmark data for a wide range of material classes, we have developed workflows where Python tools automatically create input files, start calculations, and evaluate results. For each material, all relevant input parameters, such as the number of k-points for the Brillouin-zone sampling, basis-set basis cutoff and the number of unoccupied states, are varied until the targeted convergence criteria are reached. With the help of a workflow manager, the calculations can be executed in a high-throughput fashion on a high-performance computing cluster. We demonstrate our approach with core-level spectra of elemental and binary solids, and provide an in-depth analysis of the obtained data. This work is carried out in the framework of the NOMAD Center of Excellence [3] and the CRC FONDA [4].

[1] A. Gulans et al., J. Phys. Condens. Matter **26**, 363202 (2014). [2] C. Vorwerk, B. Aurich, C. Cocchi, and C. Draxl, Electron. Struct. **1**, 037001 (2019). [3] https://nomad-coe.eu [4] https://fonda.hu-berlin.de

Topical Talk HL 6.3 Mon 11:00 TRE Ma

Large-scale machine-learning assisted discovery and characterization of materials — •Miguel Alexandre Lopes Marques — Institut für Physik Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany

In this talk we discuss our recent attempts to discover, characterize, and understand inorganic compounds using ab initio approaches accelerated by machine learning. We start by motivating why the search for new materials is nowadays one of the most pressing technological problems. Then we summarize our recent work in using crystal-graph attention neural networks for the prediction of materials properties. To train these networks, we curated a dataset of over 2 million density-functional calculations with consistent calculation parameters. Combining the data and the newly developed networks we have already scanned more than two thousand prototypes spanning a space of more than one billion materials and identified tens of thousands of theoretically stable compounds. We then discuss how simple, interpretable machine learning approaches can be used to understand complex material properties, such as the transition temperature of superconductors. Finally, we speculate which role machine learning will have in the future of materials science.

15 min. break

HL 6.4 Mon 11:45 TRE Ma

Predicting the electronic structure at any length scale with machine learning — •Attila Cangi — Helmholtz-Zentrum Dresden-Rossendorf, Görlitz, Germany

The properties of electrons in matter are of fundamental importance. They give rise to virtually all molecular and material properties and determine the physics at play in objects ranging from semiconductor devices to the interior of giant gas planets. Calculations rely primarily on density functional theory (DFT), which has become the principal method for predicting the electronic structure of matter. While DFT calculations have proven to be very useful, their computational scaling limits them to small systems. We have developed a scalable machine learning framework for predicting the electronic structure on any length scale [1,2,3]. It shows up to three orders of magnitude speedup on systems where DFT is tractable and, more importantly, enables predictions on scales where DFT calculations are infeasible. Our work demonstrates how machine learning circumvents a long-standing computational bottleneck and advances science to frontiers intractable with any current solutions.

[1] J. A. Ellis, L. Fiedler, G. A. Popoola, N. A. Modine, J. A. Stephens, A. P. Thompson, A. Cangi, S. Rajamanickam, Phys. Rev. B 104, 035120 (2021). [2] L. Fiedler, N. Hoffmann, P. Mohammed, G. A. Popoola, T. Yovell, V. Oles, J. A. Ellis, S. Rajamanickam, A. Cangi, Mach. Learn.: Sci. Technol. 3 045008 (2022). [3] L. Fiedler, N. A. Modine, S. Schmerler, D. J. Vogel, G. A. Popoola, A. P. Thompson, S. Rajamanickam, A. Cangi, arXiv:2210.11343 (2022).

HL 6.5 Mon 12:00 TRE Ma

Demonstrating temperature transferability of neural network models replacing modern density functional theory — •Lenz Fiedler and Attila Cangi — Helmholtz-Zentrum Dresden-Rossendorf / CASUS

Due to its balance between accuracy and computational cost, Density Functional Theory (DFT) is one of the most important computational methods within materials science and chemistry. However, current research efforts such as the modeling of matter under extreme conditions demand the application of DFT to larger length scales as well as higher temperatures. Such investigations are currently prohibited due to the computational scaling of DFT.

We have recently introduced a machine-learning workflow that replaces modern DFT calculations [1,2,3]. This workflow uses neural networks to predict the electronic structure locally. We show that by employing such an approach, models can be trained to predict the electronic structure of matter across temperature ranges. This paves the way for large-scale simulations of thermodynamically sampled observables relevant to modeling technologically important phenomena such as radiation damage in fusion reactor walls.

[1] J. A. Ellis *et. al*, Phys. Rev. B **104**, 035120
[2] L. Fiedler *et. al*, Mach. Learn.: Sci. Technol., **3** 045008
[3] L. Fiedler *et. al*, arXiv:2210.11343

HL 6.6 Mon 12:15 TRE Ma

Pure non-local machine-learned density functional theory for electron correlation — •Johannes T. Margraf — Fritz-Haber-Institut der MPG, Berlin, Germany

Density-functional theory (DFT) is a rigorous and (in principle) exact framework for the description of the ground state properties of atoms, molecules and solids based on their electron density. While computationally efficient density-functional approximations (DFAs) have become essential tools in computational chemistry, their (semi-)local treatment of electron correlation has a number of well-known pathologies, e.g. related to electron self-interaction. Here, we present a type of machine-learning (ML) based DFA (termed Kernel Density Functional Approximation, KDFA) that is pure, non-local and transferable, and can be efficiently trained with fully quantitative reference methods. The functionals retain the mean-field computational cost of common DFAs and are shown to be applicable to non-covalent, ionic and covalent interactions, as well as across different system sizes.

HL 6.7 Mon 12:30 TRE Ma

Predicting the response of the electron density to electric field using machine learning — •Alan Lewis and Mariana Rossi — MPI for Structure and Dynamics of Materials, Hamburg, Germany

The response of the electron density of a molecule or material to a homogeneous electric field defines its dielectric constant, along with its Raman and sum-frequency spectrum. We present a local and transferable machine learning approach capable of predicting the density response of molecules and periodic system on the same footing. This uses a very similar framework to that of the SALTED method recently introduced by these authors,[1,2] requiring only a small modification to the $\lambda-$SOAP descriptors used to represent the atomic environments. This allows us to predict the density response of liquid water to a field applied in each Cartesian direction from a single machine learning model. The tensorial dielectric constant can then be derived from this predicted density response, dramatically reducing the computational cost of calculating these properties relative to the standard approach of using density functional perturbation theory. We discuss the transferability of the model to different phases, and demonstrate the extrapolative power of this approach.

[1] Lewis, Grisafi, Ceriotti, Rossi, JCTC 17, 11, 7203 (2021)
[2] Grisafi, Lewis, Rossi, Ceriotti, accepted JCTC (2022)

HL 6.8 Mon 12:45 TRE Ma

Analysis of Batching Methods in Graph Neural Network Models for Materials Science — •Daniel Speckhard, Tim Bechtel, Jonathan Godwin, and Claudia Draxl — Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, Berlin, Germany

Graph neural network (GNN) based models have shown promising results for materials science [1]. These models often contain millions of parameters, and like other big-data based models, require only a portion of the entire training dataset to be fed as a mini-batch to update model parameters. The effect of batching on the computational requirements of training and model performance has been thoroughly explored for neural networks [2] but not yet for GNNs. We explore two different types of mini-batching methods for graph based models, static batching and dynamic batching. We use the Jraph library built on JAX to perform our experiments where we compare the two batching processes for two data-sets, the QM9 dataset of small molecules and the AFLOW materials database [3]. We show that dynamic batching offers significant improvements in terms of computational requirements for training. We also present results on the effect of the batch size and batching method on model performance.

[1] T. Xie *et al.*, Physical Review Letters, 120, 14 (2018).
[2] M. Li *et al.*, Proceedings of the 20th ACM SIGKDD (2014).
[3] S. Curtarolo *et al.*, Comp. Mat. Science, 58, 227-235 (2012).

HL 7: Poster I

Topics:
- Functional semiconductors for renewable energy solutions
- Heterostructures, interfaces and surfaces
- Optical properties
- Organic semiconductors
- Perovskite and photovoltaics
- Quantum dots and wires

Time: Monday 13:00–15:00 Location: P2/EG

HL 7.1 Mon 13:00 P2/EG

Investigation of the P-line in indium doped silicon with low temperature photoluminescence by applying an illumination and annealing cycle — •Dominik Bratek, Katharina Peh, Kevin Lauer, Dirk Schulze, Stefan Krischok, Aaron Flötotto, and Robin Müller — Institut für Physik, Technische Universität Ilmenau, Weimarer Str. 32, 98693 Ilmenau, Germany

In recent years a photoluminescent feature called P-line is of rising interest for the current research [1,2,3] and, in combination with the so called ASiSii-defect model, may lead to an explanation of the infamous light induced degradation (LID) process in indium doped silicon [2,3]. In this contribution we show studies of indium implanted silicon by using low temperature photoluminescence (LTPL) spectroscopy. We investigate the LID cycle and it*s influence on the P-line and show a possibility to explained the observed behavior by the proposed energy diagram of the ASiSii-defect. In addition we present activation energies, determined during these investigations, which can be associated to ASiSii-defect transitions. [1] K. Terashima und T. Matsuda, Japanese Journal of Applied Physics 41 Part 1, No. 3A (2002). [2] K. Lauer, C. Möller, D. Schulze, and C. Ahrens, AIP Advances 5, 017101 (2015). [3] K. Lauer, C. Möller, C. Teßmann, D. Schulze and N. V. Abrosimov, physica status solidi, c 14.5 (2017).

HL 7.2 Mon 13:00 P2/EG

Investigation of the influence of light-induced degradation on boron-doped silicon — •Robin Lars Benedikt Müller, Katharina Peh, Kevin Lauer, Dirk Schulze, Stefan Krischok, Dominik Bratek, and Aaron Flötotto — TU Ilmenau

For Si-based devices like solar cells or radiation detectors, the light-induced-degradation (LID) in doped Czochralski Si is a profound issue.

A reasonable explanation for the appearing LID process is the so-called ASi-Sii defect model [1,2], whose possible defect configuration manifests itself in indium-doped silicon by the appearance of the so-called P-line in the spectrum of low-temperature photoluminescence (LTPL) [3]. Comparatively, boron-doped Si does not exhibit a equivalent line, instead showing near the associated energy only the well-known electron-hole liquid (EHL) luminescence [4]. Therefore we investigate the influence of various treatments such as illumination, annealing or quenching on the LTPL spectrum of different boron-doped Si samples with emphasis on the behavior of the EHL. Additionally we present EPR studies on the impact of these treatments. [1]: Möller, C. et.al, (2013), Light-induced degradation in indium-doped silicon. Phys. Status Solidi RRL, 7: 461-464 [2]: Möller, C. et.al. , ASi-Sii-defect Model of Light-induced Degradation in Silicon, Energy Procedia, Volume 55, 2014, Pages 559-563 [3]: Lauer, K. et.al., "Identification of photoluminescence P line in indium doped silicon as InSi-Sii defect", AIP Advances 5, 017101 (2015) [4]: Peh, K. et.al., Low-Temperature Photoluminescence Investigation of Light-Induced Degradation in Boron-Doped CZ Silicon. Phys. Status Solidi A, 219: 2200180.

HL 7.3 Mon 13:00 P2/EG

Atomic layer deposition of iron titanate for use as a photoanode — •Nina Miller[1,2], Ryan Kisslinger[1,2], and Ian Sharp[1,2] — [1]Walter Schottky Institut Technical University of Munich — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Garching, Germany

TiO_2 is of significant importance in the field of energy research. However, to develop it for artificial photosynthesis, the band gap of TiO_2, which is 3.2 eV and consequently absorbs only ultraviolet light, must be paired with a material capable of absorbing visible light. Here, we experimentally explore the effect of depositing thin films of hematite (α - Fe_2O_3) on nanostructured TiO_2 using atomic layer deposition, with a further high-temperature annealing step to produce visible-light absorbing iron titanate (Fe_2TiO_5). Iron titanate may allow enhance charge transfer at the photoanode surface, and serve as a visible light absorbing layer. Furthermore, the TiO_2 nanotube arrays used as the substrate during atomic layer deposition can orthogonalize light absorption with respect to charge separation, leading to enhanced photocatalytic conversion during solar water splitting.

HL 7.4 Mon 13:00 P2/EG

Polaron Transport in $BiVO_4$ — •Sven Doll, Tim Rieth, David Vogl, Viktoria F. Kunzelmann, Ian D. Sharp, and Martin S. Brandt — Walter Schottky Institut and School of Natural Sciences, Technische Universität München, 85748 Garching

Bismuth vanadate ($BiVO_4$) is a promising photoelectrode material for solar-to-fuel conversion. This semiconductor is particularly interesting considering its strong visible light absorption, efficient charge carrier separation, and favorable quasi-Fermi-level alignment with relevant redox potentials. However, temperature-dependent photoconductivity measurements indicate thermally-activated hopping transport of small polarons, with transport barriers of several hundred meV. To gain further insight into charge carrier transport and the nature of these polaronic states, we explore whether the hopping of the small polarons in $BiVO_4$ is spin-dependent using electrically detected magnetic resonance. Since such spin-dependent signals are known (e.g., from similar experiments on doped crystalline silicon) to critically depend on the charge carrier density, we evaluate the possibility to use the persistent photoconductivity of $BiVO_4$ to tune the polaron density. This technique may provide valuable insights into the microscopic transport processes in modern photoelectrodes used for energy conversion. This work was supported by the DFG under Germany's Excellence Strategy - EXC 2089/1 - 390776260.

HL 7.5 Mon 13:00 P2/EG

In silico tuning the properties of inorganic-organic hybrid systems — •Mohammed El Amine Miloudi and Oliver Kühn — Institute of Physics, Rostock University, Albert-Einstein-Str. 23-24 18059 Rostock

Two-dimensional (2D) materials are expanding the range of processes that can be studied in two dimensions as well as in van der Waals (vdW) heterostructures. Integrating organic molecules into these systems has enormous potential because nature offers a finite number of 2D materials. Still, an almost unlimited range of molecules can be tailored and synthesized with predictable properties. Organic compounds are widely known for their high absorption with low mobility and charge stability, whereas inorganic compounds have comparatively low absorption with excellent charge transport properties. Thus, the formation of vdW heterostructures that combines an inorganic compound with organic molecules potentially offers the advantages of both. Molybdenum disulfide (MoS2), one of the transition-metal dichalcogenides (TMDs), is one of the most exciting 2D semiconductors holding promises for potential applications in transistors, optoelectronics, and catalysis. Perylenes are widely used dyes whose optical properties can be tuned by chemical modification of the perylene core. Here we report on a systematic study of the structural, electronic, and optical properties of MoS2/perylene hybrid systems by means of density functional theory. Using different perylenes (perylene orange, perylene diimide, and perylene red) highlights the extent to which property tuning can be achieved in the hybrid system.

HL 7.6 Mon 13:00 P2/EG

Epitaxial growth of GaN buffer layers on Si(111) by reactive magnetron sputtering — •Ralf Borgmann, Florian Hörich, Jürgen Bläsing, Anja Dempewolf, Frank Bertram, Jürgen Christen, Gordon Schmidt, Peter Veit, André Strittmatter, and Armin Dadgar — Otto-von-Guericke-Universität Magdeburg, FNW-IfP, Universitätsplatz 2, 39106 Magdeburg

GaN is a key material typically grown by MOVPE for high-voltage electronic devices. Reactive sputter epitaxy is an alternative to MOVPE, potentially offering much lower growth cost. Recently, we achieved high quality AlN layers on Si(111) [1] on which (Al,Ga)N layers can be grown. We present study on the effects of ammonia flow and growth temperature on GaN layer quality using MOVPE-grown GaN templates, high purity gases and targets. At Tgrowth ~705 °C and an ammonia flow of ~20 sccm, GaN shows a smooth surface and XRD (0002) ω-FWHMs around 340 arcsec. AlGaN layers can be grown in a large composition range by Al- and Ga- co-sputtering resulting in very smooth surfaces. A sputtered 1.4 mum thick AlN/AlGaN/GaN layer stack on Si(111) shows high resistivity and a vertical breakdown field strength >2.5 MV/cm, ideal as buffer for transistor devices. [1] F. Hörich et al., Journal of Crystal Growth 571, 126250 (2021)

HL 7.7 Mon 13:00 P2/EG

Molybdenum disulfide/diselenide deposition by radio frequency sputtering towards facile integration as heterojunction — •Oscar Alberto Lopez Galan[1,2], Manuel Ramos[3], and Torben Boll[1] — [1]Institute of Applied Materials (IAM-WK), Karlsruhe Institute of Technology (KIT), Eggenstein-Leopolshafen, Germany — [2]Institute of Nanotechnology (INT), Karlsruhe Institute of Technology (KIT), Eggenstein-Leopolshafen, Germany — [3]Instituto de Ingenieria y Tecnologia, Universidad Autonoma de Ciudad Juarez (UACJ), Ciudad Juarez, Mexico

The fabrication of heterojunctions using transition metal dichalcogenides remains a fundamental challenge in solid-state technology. In this work, we studied vertical MoS2/MoSe2 heterojunctions deposited by radio frequency sputtering at 3 thicknesses, 300 nm, 500 nm, and 600 nm. We found a dependency between thickness and crystal structure; the sample with a total thickness of 500 nm presents a crystal size of 64 nm while the thinner and thicker samples appear amorphous. Scanning electron microscopy and Raman spectroscopy reveal the presence of MoS2 and MoSe2 distinctly. Measurements by atom probe tomography indicate that MoS2 and MoSe2 are not having a sharp interface. This may influence the electrical performance of the device since dangling bonds and lattice mismatch between MoS2 and MoSe2 limit the charge carriers flow. Density functional calculations reveal a type-I heterojunction, with a reduced band gap of ~1.0 eV and a potential alignment of 0.5 eV.

HL 7.8 Mon 13:00 P2/EG

Atomic structure of As-modified Si(100) surfaces prepared in CVD ambience — Manali Nandy[1], Agnieszka Paszuk[1], Oleksandr Romanyuk[2], •Chris Yannic Bohlemann[1], Aaron Flötotto[3], Aaron Giess[1], Peter Kleinschmidt[1], Ivan Gordeev[2], Jana Houdkova[2], Erich Runge[3], and Thomas Hannappel[1] — [1]Fundamentals of Energy Materials, Institute of Physics, Ilmenau University of Technology, Ilmenau, Germany — [2]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic — [3]Theoretical Physics 1, Institute of Physics, Ilmenau University of Technology, Ilmenau, Germany

For highly efficient III-V-on-Si devices, a low-defect III-V nucleation and a sharp interface are prerequisites. Stabilization of Si surfaces by arsenic is a promising technological step allowing to grow As-based III-V epitaxial layers in consecutive process steps. Here, we study the

atomic structure of Si(100) surfaces prepared in As-rich ambiance utilizing MOCVD. Arsenic was supplied either directly via the precursor (TBAs) or indirectly as background As_4. The Si(100):As surfaces were analysed with a multitude of techniques such as STM, LEED, AR-XPS and FTIR after contamination-free transfer to ultra-high vacuum. The experimental results are supported by *ab initio* density functional theory (DFT) calculations. STM scans provide atomic-scale details of As-stabilized Si(100) surface structure consisting of rows of predominately asymmetric dimers. DFT simulations revealed a new stable structure with asymmetric As-Si-H dimers. The presence of hydrogen on the surface was confirmed by FTIR.

HL 7.9 Mon 13:00 P2/EG

Preparation of P- and III-rich GaInP (100) with subsequential water & oxygen exposure — •David Ostheimer, Mohammad Amin Zare Pour, Sahar Shekerabi, Agnieszka Paszuk, and Thomas Hannappel — Technische Universität Ilmenau, Ilmenau, Deutschland

III/V semiconductor multi-junction photoelectrochemical cells enable, either direct or indirect solar-to-fuel conversion with highest efficiencies to date, as their tunable bandgap enables optimal use of the solar spectrum. In tandem devices, GaInP has an appropriate bandgap for a top photoabsorber or a transparent, charge selective contact (window layer). A detailed understanding of the reactions at the semiconductor/electrolyte heterointerface is crucial to tailor the semiconductor surface appropriately to avoid trapping of the photogenerated charge carriers and reduce corrosion. Here, we study interaction of oxygen and water with the mixed-dimer, group-III-rich and phosphorus-rich GaInP (100) surface by combining in situ optical spectroscopy and in system photoelectron spectroscopy. The GaInP(100) surfaces were prepared by metal-organic chemical vapor deposition. The surface reconstruction of the as-prepared samples and after exposure was investigated by low energy electron diffraction. We find that the surface reconstruction of the GaInP(100) significantly affects its interaction with water. P-rich GaInP(100) surface shows much higher stability compared to the group-III-rich.

HL 7.10 Mon 13:00 P2/EG

Band energy diagrams of n-GaInP/n-AlInP(100) surfaces and heterointerfaces — •Mohammad Amin Zare Pour[1], Oleksandr Romanyuk[2], Dominik C. Moritz[3], Agnieszka Paszuk[1], Clément Maheu[3], Sahar Shekarabi[1], Kai Daniel Hanke[1], David Ostheimer[1], Thomas Mayer[3], Jan P. Hofmann[3], Wolfram Jaegermann[3], and Thomas Hannappel[1] — [1]Technische Universität Ilmenau, Ilmenau, Germany — [2]Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic — [3]Technical University of Darmstadt, Darmstadt, Germany

n-AlInP(100) charge selective contacts are commonly grown on n-p GaInP(100) top absorbers in high-efficiency III-V multijunction solar or photoelectrochemical cells. Understanding the atomic and electronic properties of the GaInP/AlInP heterointerface is crucial for the reduction of photocurrent losses in multijunction devices. We investigated chemical composition and electronic properties of n-GaInP/n-AlInP heterostructures by X-ray photoelectron spectroscopy (XPS). 1-50 nm thick n-AlInP(100) epitaxial layers were grown on n-GaInP(100) buffer layer on n-GaAs(100) substrates by metal organic vapor phase epitaxy. We observed (2x2)/c(4x2) low-energy electron diffraction patterns on both AlInP(100) and GaInP(100) as-prepared surfaces. An upward surface band bending probably caused by localized mid-gap electronic states was observed. Pinning of the Fermi level by localized electronic states remained in n-GaInP/n-AlInP heterostructures. A valence band offset of +0.2 eV was derived by XPS and band diagram models for the n-n junctions were suggested.

HL 7.11 Mon 13:00 P2/EG

GaAs/PEDOT:PSS Hybrid Solar Cell Improvement by the Incorporation of Ternary Quantum Dots — •Alexander Ehm[1], Oleksandr Selyshchev[1], Serhiy Kondratenko[2], and Dietrich R. T. Zahn[1] — [1]Semiconductor Physics, TU Chemnitz, Chemnitz D-09107, Germany — [2]Taras Shevchenko National University of Kyiv, 01601 Kyiv, Ukraine

Colloidal quantum dots (QD) have gained much interest over recent years due to their absorption and photoluminescence properties, which can be tuned by varying the particle size. Among these, ternary In-based chalcogenide QDs possess the advantage of low toxicity, making them more environmentally friendly candidates for the application in solar harvesting devices for green energy production.

As a prove of concept, colloidal AgInS and CuInS QDs [1] are deposited on n-GaAs(100) substrates in order to incorporate them in hybrid GaAs/PEDOT:PSS solar cells. The deposition is verified and analysed by X-ray photoemission and optical spectroscopy methods as well as atomic force microscopy. A significantly enhanced power conversion efficiency of such solar cells modified by colloidal QDs compared to the devices without QDs is shown by current density-voltage measurements under AM1.5 equivalent illumination.

[1] A. Raevskaya et al., J. Phys. Chem. C 2017, 121, 9032

HL 7.12 Mon 13:00 P2/EG

One-dimensional topological interface states: a novel approach for optical pressure sensors — •Jakob Lindenthal[1,2], Anton Widulla[1], Johannes Benduhn[1], and Karl Leo[1,2] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials, Technische Universität Dresden — [2]ct.qmat - Würzburg-Dresden Cluster of Excellence

The research field of nano-optics in connection with topological photonics has quickly evolved over the past decade. Topological considerations in the design of photonic systems open a wide range of possibilities for disorder protection and electric field alignment optimisation. Different material systems and topological setups are discussed in the context of pressure-sensitive nano-optical resonators, demonstrating a novel, highly versatile pressure sensor concept. The demonstrated system combines a compressible optical microcavity with an organic absorber material, which allows highly sensitive pressure-dependent tuning of the mode intensity. The contribution features modelling and characterisation results for systems with different topologies, showing pathways to significant topology-induced sensitivity enhancement. The use of coupled cavities is shown to provide additional sensing information with potential for industrial implementation.

HL 7.13 Mon 13:00 P2/EG

Electric-field-induced second harmonic generation in amorphous materials for hybrid photonic structures — •Laurids Wardenberg, Benito Bunk, and Jörg Schilling — Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany

We investigate electric-field-induced second harmonic generation (EFISH) on different amorphous materials, e.g a-Si and As_2S_3 films. These materials have sizeable $\chi^{(3)}$ values but a vanishing $\chi^{(2)}$ due to their amorphous structure. Applying a dc-voltage we gain the ability to create a quasi-$\chi^{(2)}$ and perform second order nonlinear optical processes. The possibility to manipulate value and polarity of the created quasi-$\chi^{(2)}$ allows an unprecedented control over these second order wavelength conversion processes. Introducing a way to electrically modulate and switch this nonlinearity, is of high practical interest for the realization of nonlinear active hybrid photonic structures.

Since EFISH is strongly associated with the $\chi^{(3)}$, we use the z-scan technique to determine the real and the imaginary parts of the $\chi^{(3)}$ of the investigated films. Subsequently chromium contacts were deposited on the films and electric fields up to 10^5 V/m were applied. Our voltage and intensity dependent SHG measurements show a quadratic dependence on input intensity and applied DC field, which is a clear indicator for EFISH. The nonlinear optical measurements are mainly performed at a wavelength of 1030 nm using a femtosecond laser system supplying 200 fs pulses at a repetition rate of 1 kHz. Additional measurements at wavelengths above 1200 nm, which are of interest for silicon photonics, will be demonstrated as well.

HL 7.14 Mon 13:00 P2/EG

Excitons in lithium niobate and their impact on non-linear optical properties — •Agnieszka Kozub, Wolf Gero Schmidt, and Uwe Gerstmann — Universität Paderborn, Department Physik, 33095 Paderborn, Germany

The influence of self-trapped and vacancy-trapped excitons on the lithium niobate ($LiNbO_3$, LN) dielectric function and nonlinear susceptibility is calculated based on density-functional theory. The PBE0 hybrid functional is used for the description of electron exchange and correlation. The dielectric function it obtained by solving the Bethe-Salpeter equation. This yields an absorption peak at 2.6 eV, in perfect agreement with experiment [1]. The second- and third order- nonlinear susceptibility tensors are obtained from a Berry-phase formulation of the dynamical polarization. A strong enhancement of the susceptibilities for photon energies in the band gap region is noted to arise from localized excitons.

[1] L.E. HALLIBURTON, K.L. SWEENEY and C.Y. CHEN, Nuclear Instruments and Methods in Physics Research Bl 344-347 (1984)

HL 7.15 Mon 13:00 P2/EG

Structured Gradient Index Silicon (Oxy)Nitride Layers for Antireflection in Silicon Solar Cells — •Florian Damerau[1], Maria Gaudig[1], Ralf Wehrspohn[1], Prerak Dhawan[2], Carsten Rockstuhl[2], and Alexander Sprafke[1] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, Heinrich-Damerow-Str. 4, 06120 Halle (Saale), Germany — [2]Institute of Theoretical Solid State Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

The frontside of crystalline silicon (c-Si) solar cells oftentimes is micro- or nanotextured to increase light in-coupling, and thus conversion efficiency. Current state-of-the-art textures comprise micron sized pyramidal structures, whereas future ultrathin c-Si solar cells demand new approaches such as submicron nanophotonic structures. However, directly nanotexturing the Si surface degrades its electronic properties strongly, such that a possible gain in absorption does not necessarily translate into an increased conversion efficiency. In this work, we aim to maintain the electronic properties of a planar c-Si interface by leaving it intact but place a nanophotonic structure on top. This structure consists of a nanstructured SiOxNy layer. Moreover, changing the stoichiometry (x,y) during deposition enables us to smoothly vary its refractive index between $n \approx 1.5 - 3.0$. Inspired by transformation optics, we aim to mimic the optical properties of strongly non-planar textures such as black silicon by a planar layer of smoothly varying spatial-dependant refractive index. In this contribution we will present experimental results on the microstructure as well as on the optical properties of our fabricated structures.

HL 7.16 Mon 13:00 P2/EG

Exciton-polariton emission in copper halides — •E. Krüger[1], S. Merker[2], S. Blaurock[2], R. Hildebrandt[1], A.L. Pereira[1], L. Käferstein[1], H. Krautscheid[2], M. Grundmann[1], and C. Sturm[1] — [1]Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Germany — [2]Universität Leipzig, Institut für Anorganische Chemie, Germany

Copper halides (CuI, CuBr, and CuCl) have recently attracted research interest since they combine intrinsic p-type conductivity with large bandgaps (3.1 eV - 3.4 eV) and high exciton binding energies (62 meV - 190 meV), making them promising candidates for applications in transparent optoelectronics [1].

Here, we present an overview of the optical properties of solution grown Cu-halide bulk single crystals, focusing especially on spectral- and time-resolved measurements of the near-band-edge luminescence for temperatures between 10 K and room temperature. The line shape of the emission lines at low temperatures is interpreted in terms of exciton-polaritons and their dispersion relation [2]. The different decay characteristics of free and localized states are explained by their coupled interaction. In addition to observation of an anomalous temperature-dependent bandgap shift to higher energies with increasing temperature we present in detail the temperature-dependent decay characteristics of the polariton emission and discuss the corresponding relaxation mechanisms.

[1] M. Grundmann et al., pss (a) **210**, 1671 (2013)
[2] E. Krüger et al., APL Mater. **9**, 121102 (2021)

HL 7.17 Mon 13:00 P2/EG

Persistent spectral holeburning of the donor-bound exciton transition in ultra-pure ^{28}Si:P — •Nico Eggeling[1], Michael Oestreich[1], Eduard Sauter[1], Jens Huebner[1], and N. V. Abrosimov[2] — [1]Leibniz Universität Hannover, Germany — [2]IKZ Berlin, Germany

We utilize persistent spectral hole burning to determine the origin of dynamic and static spectral broadening of the donor-bound exciton transition in ultra-pure ^{28}Si:P with 99.995% isotopic enrichment [1]. From time-dependent measurements of the spectral hole width and frequency shift we try to determine the impact of donor-acceptor interaction on the spectral transition broadening. The donor-acceptor pair recombination is on the order of seconds in the investigated sample with a donor concentration of $1.2 \times 10^{15}\mathrm{cm}^{-3}$ and an acceptor concentration of estimately $4.6(10) \times 10^{13}\mathrm{cm}^{-3}$. We expect to observe an impact of the recombination dynamics on the measured frequency and width of spectral holes. These results could lead to a better understanding of spin initialization for donors in ^{28}Si:P, which are a promising candidate for quantum computation [2].

[1] Sauter, E., Abrosimov, N. V., Hübner, J., & Oestreich, M., Phys. Rev. Lett. **126(13)**, 137402 (2021).
[2] Morello, A. et al., Adv. Quant. Tech. **3(11)**, 2000005 (2020).

HL 7.18 Mon 13:00 P2/EG

Manipulating the luminescence of a rare-earth doped spacer — •Sören Lerner[1], Francesco Vitale[1], Thomas Siefke[2], Uwe Zeitner[2,3], and Carsten Ronning[1] — [1]Institute of Solid State Physics, Friedrich-Schiller Universität, Helmholtzweg 3, 07743 Jena, Germany — [2]Institute of Applied Physics, Friedrich Schiller Universität, Albert-Einstein-Straße 15, 07745 Jena, Germany — [3]Fraunhofer Institute for Applied Optics and Precision Engineering IOF, Albert-Einstein-Straße 7, 07745 Jena, Germany

The coupling of rare-earth elements with surface plasmon polaritons can lead to a change of their emission properties. We implant rare-earth elements in a nanometric silica spacer on top of an aluminum layer by ion beam implantation. The luminescence properties of such systems were examined by photo- and cathodoluminescence measurements. Placing zinc oxide nanowires on top of this two-layer system allows for additional coupling with surface plasmon polaritons, which generate a high electric field density in the spacer layer. The respective effects and the possibilities of tailoring the emission will be discussed.

HL 7.19 Mon 13:00 P2/EG

Coupling of Excitons and Plasmons with Phonons in Raman scattering for CuI — •R. Hildebrandt[1], S. Blaurock[2], H. Krautscheid[2], M. Grundmann[1], and C. Sturm[1] — [1]Universität Leipzig, Felix Bloch Institute for Solid State Physics, Germany — [2]Universität Leipzig, Institute of Inorganic Chemistry, Germany

CuI is an intrinsic p-type with potential for opto-electronic applications. Via resonance effects, various of its fundamental properties may be accessed. For CuI we investigate phonon-exciton- and phonon-plasmon-interactions by Raman spectroscopy.

We present Raman spectra with excitation wavelength of 532 nm, 355 nm and 325 nm for single crystals and thin films. Each excitation wavelength indicates different fundamental Raman scattering processes. With 532 nm fundamental modes as well as second order Raman singals are observed and analyzed [1]. For doped samples with $p = 10^{18}\,\mathrm{cm}^{-3}$, phonon-plasmon coupling is observed which is compared with Hall measurements. By 355 nm excitation, slightly above the bandgap, a phonon damped-plasmon mode coupling modifies the Raman spectra [2]. Finally with a 325 nm a transition close to $\mathrm{E_g}+\Delta_0$, indicates a cascade exciton scattering process. This is dominated by the Fröhlich interaction and n-LO overtones up to $n = 7$ are observed [3]. For each excitation wavelength, an overview of possible applications and possible limits for CuI is shown.

[1] J. Birman, J., Phys. Rev., **131**, 1489, 1963.
[2] A. Mlayah *et al.*, J. Appl. Phys., **69**, 4064, 1991.
[3] Y. Zhang, J. Semicond., **40**, 091102, 2019.

HL 7.20 Mon 13:00 P2/EG

Raman spectra of CuI alloys with Ag and Br — •A.L. Pereira[1], R. Hildebrandt[1], J. Bredow[1], C. Dethloff[1], V. Gottschalch[2], S. Vogt[1], H. Krautscheid[2], M. Grundmann[1], and C. Sturm[1] — [1]Universität Leipzig, Felix Bloch Institute for Solid State Physics, 04103 Leipzig, Germany — [2]Universität Leipzig, Institute of Inorganic Chemistry, 04103 Leipzig, Germany

CuI is a p-type semiconductor with a wide band gap of 3.1 eV that has potential for (opto-) electronic applications [1]. By alloying CuI with isoelectronic Ag or Br its properties such as e.g. the charge carrier concentration, lattice constant or band gap can be tuned.

We present our investigations on CuI alloys and their phonon properties with Raman spectroscopy. $\mathrm{Ag}_x\mathrm{Cu}_{1-x}\mathrm{I}$ and $\mathrm{CuBr}_x\mathrm{I}_{1-x}$ (both $0 \leq x \leq 1$) thin films were produced with various deposition techniques such as solid-state reaction, close distance sublimation, sputter deposition and pulsed laser deposition. Raman spectroscopy measurements were conducted at low temperatures and the phonon modes were analyzed regarding their energetic position, broadening and intensity. This was supported by an oscillator strength model [2]. The Cu(Br,I) alloy revealed a nonlinear dependence of the Raman shift on the composition. In the (Ag,Cu)I alloy an apparent three-mode behavior due to a defect mode was observed and characterized.

[1] E. Krüger, *et al.*, Appl. Phys. Lett. 113, 172102, 2018.
[2] G. Livescu, *et al.*, J. Phys. C: Solid State Phys. 19 2663, 1986.

HL 7.21 Mon 13:00 P2/EG

Excited-state properties of PbWO4 from ab initio calculations — •Ather Ahmad and Kai-Thomas Brinkmann — II. Phys. Inst. Gießen

Fast response, high density and radiation hardness make lead tungstate

(PbWO4 or PWO) a well suited scintillator for an electromagnetic calorimeter. Lead tungstate crystals are already used as working material in various experiments, e.g. the CMS at the LHC in CERN. New generation crystals (PWO-II) with improved properties were developed for the PANDA experiment at FAIR in Darmstadt. To reduce absorption of the scintillation light within the crystals, the lead tungstate is doped with Lanthanum and Yttrium. This results in a change of the electronic and optical properties.
In order to assess the functionality of the calorimeter, we first need to analyse these electronic and optical properties of lead tungstate. In our work, we investigate these properties of lead tungstate containing different impurities and defects with ab initio calculations to derive its radiation hardness and scintillation mechanism.

This project is supported by HFHF and HGS-hire

HL 7.22 Mon 13:00 P2/EG

Multiphoton absorption induced photoluminescence in CuI — •Andreas Müller[1], Sebastian Henn[1], Evgeny Krüger[1], Steffen Blaurock[2], Harald Krautscheid[2], Marius Grundmann[1], and Chris Sturm[1] — [1]Felix-Bloch-Institut für Festkörperphysik, Universität Leipzig, Linnéstr. 5, 04103 Leipzig, Germany — [2]Institut für Anorganische Chemie, Universität Leipzig, Johannisallee 29, 04103 Leipzig, Germany

Two- and three-photon absorption induced photoluminescence (2PAPL, 3PAPL) are nonlinear optical processes useful for energy upconversion or, in contrast to near-to-the-surface single-photon absorption, excitation within the bulk material.

In this work, we report on low temperature (30 K) 2PAPL and 3PAPL in transparent conducting CuI crystals ($E_g = 3.1$ eV), analyzed employing excitation energy and density-dependent, steady-state, and time-resolved photoluminescence. Using an excitation energy that corresponds to half of the bandgap energy, the observed intensity dependence on the excitation power shows an almost parabolic behavior. By a further reduction of the photon energy, the cubic contribution of the excitation power on the intensity increases, and for low excitation energies, an almost cubic behavior is obtained. We describe the experimental findings, taking into account the sum of the two- and three-photon transition rates and including the Gaussian spectral intensity distribution of the laser. Through this analysis, the ratio of the cross-sections for the two- and three-photon absorption is estimated to be 10^{-5} cm^2/s.

HL 7.23 Mon 13:00 P2/EG

Optical properties of the organic semiconductor Dimethylanthradithiophene (DMADT) — •Anncharlott Kusber and Martin Knupfer — IFW Dresden, Helmholtz Straße 20, D-01069 Dresden, Germany

This work presents an analysis of the optical properties of anti- and syn-dimethylanthradithiophene. We have produced 120 nm thick thin films by physical vapour deposition. Using optical spectroscopy, we were able to characterize the films in the visible range. Davydov splitting, due to the existence of two molecules in the unit cell, was observed. Besides that, we measured the exciton dispersion by using electron energy-loss spectroscopy. There we found a positive dispersion of the lowest lying excitation. Comparing the measured values and the calculated coupling strengths, we came to the conclusion that both materials are very weak J-aggregates and that charge transfer exciton coupling is the dominant process and determines the delocalization of the lowest lying excitations.

HL 7.24 Mon 13:00 P2/EG

Highly dipolar molecule on single crystals: Impact of chemical affinity on the interface formation — •Baris Öcal and Selina Olthof — Department of Chemistry, University of Cologne, Greinstraße 4-6, 50939 Cologne, Germany

Merocyanines are functional dyes with interesting electronic properties due to their resonant structure between charged and uncharged states. Their bandgap can be widely tuned via the donor and acceptor strength, which makes them interesting as active material in organic-based solar cells, especially since they show very strong absorption. Their physical properties can be further improved by ordering them. The ordering of the molecules is closely related to initial growth on the substrate underneath and interaction between this substrate and molecule. In my work, I investigate the effect of substrate/molecule and molecule/molecule interactions on the electronic structure by photoelectron spectroscopy methods. Highly dipolar HB238 merocyanine has been chosen to observe the chemical interaction and its effect of the charge states of the molecule easier. Surfaces such as SiC/graphene, Au(100), Ag(100) and Cu(100) are used as templating substrates due to their different chemical affinity and ordered structure. Thickness dependent X-ray Photoelectron spectroscopy (XPS) measurements helps us to understand the chemical effect of substrate on the charge states, while Ultraviolet Photoelectron Spectroscopy (UPS) measurement gives information on the molecular phase changes such as dimerization, orientation change. We find that chemical interaction of the substrate significantly affects molecule/molecule interaction.

HL 7.25 Mon 13:00 P2/EG

Spontaneous orientation polarization in phosphine oxides and how to control it — •Albin Cakaj, Markus Schmid, Alexander Hofmann, and Wolfgang Brütting — Institut für Physik, Universität Augsburg, Germany

The orientation of small organic molecules in amorphous thin films prepared by vapor-deposition is an important aspect in further improvement of organic semiconductor devices. This feature can influence the optical and electrical properties of organic light emitting diodes (OLEDs) drastically. Due to their asymmetric molecular structure, microscopic properties like the permanent dipole moment (PDM) can show preferential alignment and lead to a macroscopic film polarization in the organic layer. This so-called spontaneous orientation polarization (SOP) affects the charge injection and accumulation behaviour in a device. In our studies, we investigated the electrical and optical orientation of a group of organic molecules, characterized by P=O double bonds, and how to control it by their design and the film-growth conditions. Many of these phosphine oxides have a large PDM, due to a strong electronegative oxygen. However, the magnitude of their SOP is often affected by the presence of multiple molecular conformers. Thus, using less polar species with only one P=O bond yields superior performance with record-high SOP of up to 160mV/nm, even though optical measurements hint to almost no preferred orientation on average.

HL 7.26 Mon 13:00 P2/EG

Impact of solution processing on the photophysical properties of TADF emitters — •Konstantin Rausch, Rishabh Saxena, and Anna Köhler — Soft matter Optoelectronics, University of Bayreuth, Germany

Continuous innovation of thermally activated delayed fluorescence (TADF) compounds has led to the rapid development of these materials as emitters in efficient vacuum-deposited organic light emitting diodes (OLEDs). However, the cost of device fabrication, inefficient use of materials and limitation on pixel size are some detracting features of vacuum-deposition. An alternative cost- and materials-efficient fabrication technique is solution processing. In this regard, it is important to understand the impact of different processing conditions, such as varying solvents and host materials, on the photophysical properties of TADF emitters. In general, a donor-acceptor (D-A) strategy is adopted for the chemical design of TADF emitters. Recent studies suggest that conformational flexibility associated with the D-A dihedral angle leads to a distribution of reverse intersystem crossing rates (k_RISC); a parameter that determines the efficiency of the TADF process. In this study, we perform inverse Laplace transform fitting of emission decay, obtained using time-resolved photoluminescence measurements, to extract this distribution. Furthermore, we investigate the impact of different film-preparation methods (spin-coating and evaporation), matrix polarity and conformational rigidity of TADF emitter on the RISC rate distribution with an aim to optimize the performance of solution-processed TADF OLEDs.

HL 7.27 Mon 13:00 P2/EG

single molecule spectroscopy of emitters in hexagonal boron nitride(hBN) — •osama farooqui and klas lindfors — department of chemistry, university of cologne

Efficient interaction of light with atoms or molecules has been found crucial in the study of materials that can be used in the development of high-speed communication devices [1]. The central goal of this project is to observe and investigate the light emission and absorption processes in heterostructures of two- and one-dimensional materials and single emitter molecules.

Previously, single terrylene diimide (TDI) molecules on glass substrate have been investigated using single molecule spectroscopy. In order to address the problem of stability of the molecules, hBN is used to encapsulate emitter molecules to avoid chemical reactions with

the ambient environment. The preliminary data of time traces of triisopropylsilyl pentacene (TIPS-pentacene) molecules encapsulated in hBN flakes shows that the molecules do not get photobleached over 1 hour at room temperature. However, fast photoblinking was observed in the time traces of the molecules. The cause of fast photoblinking could be the interaction of the molecules with close-by two-level systems, which appears to be related to hBN flakes.

Reference [1] Toninelli, C. et al. Single organic molecules for photonic quantum technologies. Nat. Mater. 1-14 (2021).

HL 7.28 Mon 13:00 P2/EG

Electronic and optical properties of p-type delafossite transparent conducting oxides: Density Functional Theory calculations — •Moufdi Hadjab[1,2] and Olga Guskova[2] — [1]Mohamed Boudiaf University of Msila, Msila, Algeria — [2]IPF Dresden, Germany

Transparent conducting oxides (TCO) possessing high optical transparency and electrical conductivity have been studied widely due to their applications in optoelectronics. Delafossite materials with chemical formula AIBIIIO2 are among the promising p-type TCOs. In this study, we have investigated physical properties of three novel semiconductors to address some problems related to the photovoltaic industry. The structural, electronic and optical properties of delafossite transparent conducting oxides CuMO2 have been studied using the Full-Potential Linearized Augmented Plan Wave method based on DFT as implemented in Wien2k computational code. The LDA and PBE generalized gradient approximation have been utilized as the exchange-correlation term for calculating the structural and electronic parameters. Moreover, Tran-Blaha modified Beck-Johnson potential has been used to achieve better degree of accuracy in calculations of the electronic and optical properties. The observations have been compared with published theoretical and experimental data. The ternary delafossite transparent conducting oxide compounds can be considered as an alternative material in photovoltaic applications.

HL 7.29 Mon 13:00 P2/EG

Simulating multi-component target ablation: A new pulsed laser deposition technique — •Arne Jörns, Holger von Wenckstern, and Marius Grundmann — University of Leipzig, Felix Bloch Institute for Solid State Physics, Semiconductor Physics Group

Laterally and radially segmented targets allow the fabrication of functional thin films with lateral and vertical composition spreads, respectively [1]. The latter also enables the creation of material libraries consisting of homogeneous thin films with discrete material composition. However, fabrication of such targets is technically demanding with respect to powder blending, insufficient hardening or thermic decomposition due to deviating sintering temperatures of the source powders for the respective segments.

In this work we present a new target design and deposition technique for pulsed laser deposition in order to create vertical composition spreads as well as discrete composition material libraries but bypassing the above mentioned drawbacks. Simulations for the expected material contents will be presented. Then, experimentally determined elemental distributions and growth rates are compared to calculated values. Electrical and optical properties of samples obtained by such techniques will be reported.

[1] H. von Wenckstern et al.,Phys. Status Solidi 2020, 257, 1900626

HL 7.30 Mon 13:00 P2/EG

Wide bandgap aeromaterials and prospects for their applications — •Vladimir Ciobanu, Tudor Braniste, Eduard Monaico, and Ion Tiginyanu — National Center for Materials Study and Testing, Technical University of Moldova, Chisinau, Moldova

We report on the fabrication of aeromaterials based on GaN, Ga2O3, TiO2 and Zn2TiO4 using hydride vapor phase epitaxy (HVPE) or Atomic Layer Deposition (ALD) approaches. The fabrication process is based on growth of the preferred material on sacrificial templates consisting of interconnected ZnO microtetrapods. During the epitaxial growth of GaN at high temperatures and corrosive environment, the ZnO is etched away and, consequently, hollow microtetrapods with the wall thickness of the tubes in the range of 20 - 100 nm are obtained. Further, GaN can be transformed into Ga2O3 through an annealing process at temperature as high as 800 °C. Alternatively, ALD approach is used to fabricate aero-TiO2 or aero-Zn2TiO4 materials using sacrificial ZnO templates.

The fabricated materials demonstrated new interesting properties: aero-GaN exhibits good electromagnetic shielding in X-band and THz region, on the other hand aero-Ga2O3 is completely transparent at GHz and THz frequencies, up to 3 THz. We also established that aero-GaN is characterized by dual hydrophilic-hydrophobic behavior. This phenomenon enabled one to demonstrate novel liquid marbles. Due to high active surface area of developed aero-Ga2O3 decorated with noble metal nanodots, aero-TiO2 and aero-Zn2TiO4, these materials are shown to be promising for photocatalytic applications.

HL 7.31 Mon 13:00 P2/EG

Graded $Zn_xMg_{1-x}O$ layers as building blocks for ultra-compact wavemeters — Philipp Firme, •Christoph Brunhuber, Lukas Trefflich, Peter Schlupp, Daniel Splith, Holger von Wenckstern, Chris Sturm, and Marius Grundmann — Universität Leipzig, Felix Bloch Institute for Solid State Physics, 04103 Leipzig, Germany

Recently, a new design for a monolithic, ultra-compact wavemeter was proposed, which can be used in a wide spectral range [1]. The building blocks of this wavemeter are two vertically stacked, photosensitive layers, separated by a transparent, insulating layer. In order to achieve a spectral sensitivity, the top layer must consist of a material with a vertical absorption gradient. Here, we discuss the suitability of vertically graded $Zn_xMg_{1-x}O$ layers as top layer of such an ultra-compact wavemeter with wurtzite photosensitive ZnO layer as backside. The layers were deposited by pulsed laser deposition, using a vertical continuous composition spread (VCCS-PLD) technique. In doing so, we were able to achieve out-of-plane composition gradients from $x = 1.0$ up to $x \approx 0.5$. XRD $2\theta - \omega$-scans do not indicate a phase separation, and confirm the wurtzite phase. The Mg incorporation was also confirmed by photoluminescence spectroscopy. The suitability of the films as building blocks for the wavemeter was tested by photocurrent measurements. By radiation with monochromatic light of different wavelengths, a response similar to the theoretically calculated one [1] is obtained.

[1] M. Grundmann. Phys. Stat. Sol. A **215**, 1800651 (2018)

HL 7.32 Mon 13:00 P2/EG

Synthesis of bismuth ferrite hollow spheres and their application in the photocatalytic degradation of dyes — •Valeria Sanchez[1], Thomas Cadenbach[2], Alexis Debut[3], Karla Vizuete[3], and Maria J. Benitez[1] — [1]Departamento de Física, Facultad de Ciencias, Escuela Politécnica Nacional, Ladrón de Guevara E11-253, Quito, Ecuador — [2]Colegio de Ciencias e Ingenierías, Universidad San Francisco de Quito, Diego de Robles y Vía Interoceánica, Quito, Ecuador — [3]Centro de Nanociencia y Nanotecnología, Universidad de las Fuerzas Armadas ESPE, Av. Gral. Rumiñahui s/n, Sangolquí, Ecuador

In this work, we show the synthesis and application of next generation semiconductor photocatalysts, i.e. GdxBi1-xFeO3 (x = 0, 0.05. 0.10, 0.15) hollow spheres which function as both, an advanced adsorption material and photocatalytic active semiconductor. The presented spheres were prepared by two distinct novel synthetic protocols, i.e. via a citric acid/urea/ethylene glycol assisted hydrothermal method and via an evaporation induced self-assembly strategy. In both cases, we study the mechanism of formation of phase pure GdxBi1-xFeO3 hollow spheres with a narrow size distribution by varying synthetic conditions such concentration, temperature and treatment time. The samples were characterized by X-ray powder diffraction, scanning electron microscopy and UV-vis diffuse reflectance spectroscopy. All synthesized materials were applied in the photocatalytic degradation of dyes under visible light irradiation. The photocatalysts show superior efficiencies which outperformed previously reported BiFeO3 materials.

HL 7.33 Mon 13:00 P2/EG

Monitoring Phase Transitions in (Hot-)Pressed $FAPbI_3$ Films by In-Situ Reflection Measurements — •Lorenz Kiel[1], Christina Witt[1], Konstantin Schötz[1], Nico Leupold[2], Ralf Moos[2], Anna Köhler[1], and Fabian Panzer[1] — [1]Soft Matter Optoelectronics, University of Bayreuth, Bayreuth 95440, Germany — [2]Department of Functional Materials, University of Bayreuth, Bayreuth 95440, Germany

In recent years, a remarkable increase in efficiencies of halide perovskite-based solar cells has been achieved. Record cells on laboratory scale, realized with the perovskite formamidinium lead iodide ($FAPbI_3$), are now competing with established silicon devices.[1] However, phase stability of $FAPbI_3$ is still challenging as the photoactive black α-phase is prone to degrade in the inactive yellow δ-phase or

intermediate orange and red phases.[2, 3] To address this issue, we evaluate the temperature and pressure dependence of occurring phase transitions using in-situ reflection measurements during (hot-)pressing δ-$FAPbI_3$ powder, and analyze associated strain in the resulting thick films. We show that for our powder based thick films the phase transitions occur at significantly lower pressure and temperature compared to literature reports. The correlation of these parameters with resulting film properties like film morphology suggests strain to be decisive for the phase transition and phase stability.

[1] Jeong et al. Nature 2021, 592.
[2] Cordero et al. Nanomaterials 2021, 11.
[3] Cordero et al. J. Phys. Chem. C 2020, 124.

HL 7.34 Mon 13:00 P2/EG

Phase diagram of two-dimensional ferroelectric large polarons — •Florian Kluibenschedl, Georgios Koutentakis, and Mikhail Lemeshko — Institute of Science and Technology Austria (ISTA), Am Campus 1, 3400 Klosterneuburg, Austria

We present a minimal, coarse-grained, two-dimensional model of charge transport in lead halide perovskites, which provides an intuitive explanation for the recently proposed formation of ferroelectric large polarons [1]. The phase-diagram analysis reveals the presence of three phases characterized by the distinct order of the molecular dipole moments which is strongly dependent on the tunneling anisotropy of the carriers. The most striking outcome is the formation of ferroelectric domains that amplify the anisotropy in the carrier tunneling dynamics which has been argued to lead to improved optoelectronic properties. These results provide the groundwork for realizing a top-down approach for understanding the complex carrier dynamics in hybrid organic-inorganic perovskites.

[1] F. Wang, Y. Fu, M. E. Ziffer, Y. Dai, S. F. Maehrlein, and X.-Y. Zhu. Journal of the American Chemical Society 2021 143 (1), 5-16. DOI: 10.1021/jacs.0c10943

HL 7.35 Mon 13:00 P2/EG

Optical spectroscopy on hBN-encapsulated perovskites — •Lisa Böhme, Eugen Klein, Rico Schwartz, Christian Klinke, and Tobias Korn — University of Rostock, Institute of Physics, 18059 Rostock, Germany

Perovskites shows promising optoelectronic properties that can be used in a wide range of technologies. For example, they play a central role in the development of more efficient and low-cost solar cells and are also used in LED or low-threshold lasers. However, they pose experimental challenges that need to be solved: perovskites degrade in contact with air and lose their attractive properties. A possibility to avoid this is encapsulation in hexagonal Boron Nitride (hBN). We have examined how lead-halogen perovskites with organic ligands can be encapsulated and whether they retain their stability. We use the Scotch-Tape method to exfoliate hBN crystals and deposit perovskite crystals on top using drop casting. To check the successful encapsulation of the perovskites, photoluminescence measurements were taken over different time periods and at different temperatures. Our measurements showed that the fully encapsulated perovskites remained stable for more than ten days.

HL 7.36 Mon 13:00 P2/EG

Reflection Electron Energy Loss Spectroscopy of Organic and Perovskite Semiconductors — •Seren Dilara Öz and Selina Olthof — Department of Chemistry, University of Cologne, Greinstraße 4-6, 50939 Cologne, Germany

The analysis of fundamental semiconductor properties, such as energy level positions and bandgaps, are important to enhance our understanding of these materials and to further improve their performance in applications. In this context, many spectroscopic tools such as ultraviolet photoelectron spectroscopy or UV-vis measurements are exploited. In this project, we explore the use of reflection electron energy loss spectroscopy (REELS) which is a rarely used technique in order to investigate the surface density of states (DOS) and bandgap of organic and perovskite based semiconductor materials.

This measurement technique records the energy loss due to inelastic electron scattering processes which excites electronic transitions. It presents an intriguing technique to gain insights on the joint valence and conduction band density of states over a wide energy range. Due to the extreme surface sensitivity, the band gap of ultra-thin layers can be accessed.

In this work, we try to understand the observed energy loss spectra in order to establish guidelines to investigate surface properties of semiconductor materials. For that reason, information gathered using REELS are compared to UPS, IPES, and UV-vis measurements. Our results show that the REELS technique can be used as an effective tool to explore surface properties of perovskite and organic semiconductors.

HL 7.37 Mon 13:00 P2/EG

Combinatorial synthesis of $BaZrS_3$ thin films: Influence of off-stoichiometry on optoelectronic and electronic properties — •Adriana Röttger, Marin Rusu, Hannes Hempel, Daniel Abou-Ras, Orestis Karalis, Ibrahim Simsek, and Thomas Unold — Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Deutschland

The chalcogenide perovskite $BaZrS_3$ is composed of earth-abundant elements and has potential applications for photovoltaic energy conversion. In this work, compositionally graded $BaZrS_3$ thin films are synthesized from oxide precursors deposited by pulsed laser deposition. The compositional gradient in a range of $0.8<[Ba]/[Zr]<1.3$ enables a high throughput characterization approach of structural, optical and optoelectronic properties. Sulfurization was performed in a tube furnace using H_2S in Ar gas at 1000°C. For all the examined compositions, $BaZrS_3$ forms as the main phase. Under Ba excess, Ruddlesden-Popper phases $Ba_3Zr_2S_7$ and $Ba_4Zr_3S_{10}$ emerge, while excess Zr forms ZrO_2 on the Zr-rich side. Optical absorption spectroscopy mapping shows that the band-gap energy exhibits a minimum at $1.0 < [Ba]/[Zr] < 1.1$ and ranges from 1.65 to 2.1 eV. Analysis of the optical constants n and k by ellipsometry mapping verified this trend. Low-temperature photoluminescence spectroscopy revealed deep defect states present for all compositions. Using time-resolved photoluminescence spectroscopy and optical -pump-terahertz probe spectroscopy, we found longer carrier lifetimes on the Ba-rich side, while the Zr-rich side features a higher mobility of charge carriers.

HL 7.38 Mon 13:00 P2/EG

Defect tolerance of halide perovskites solar absorbers via machine learning — •Anoop K. Chandran[1], Christoph Friedrich[1], Uwe Rau[2], Stefan Blügel[1], Thomas Kirchartz[2], and Irene Aguilera[3] — [1]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany — [2]IEK5-Photovoltaik, Forschungszentrum Jülich, Germany — [3]Institute of Physics, University of Amsterdam, The Netherlands

The deformation potential measures the changes in the bandgap of materials upon compression of the bonds, which helps to identify the bonding or anti-bonding nature of the valence and conduction bands. Previous works indicate that the bonding or anti-bonding nature impacts a material's tendency to exhibit shallow or deep intrinsic defect levels. Our high-throughput search is based on all-electron density functional theory calculations. Among 1173 studied halide perovskites, only 18% present a favourable anti-bonding valence band. We also establish the calculation of the deformation potential as an effective way to determine the bonding or anti-bonding nature near the band edges. However, subsequent supercell calculations reveal no explicit connection between the nature of the band edges and the defect tolerance. Deep learning neural networks require large datasets. To overcome this limitation, we devised a novel approach for the one-shot binary classification of the deformation potentials. Instead of learning to classify a single material, the network learns the similarity or the difference between two materials.

HL 7.39 Mon 13:00 P2/EG

Dressed-state analysis of two-color excitation schemes — •Thomas Bracht[1,2], Tim Seidelmann[3], Yusuf Karli[4], Florian Kappe[4], Vikas Remesh[4], Gregor Weihs[4], Vollrath Martin Axt[3], and Doris E. Reiter[2] — [1]Institut für Festkörpertheorie, WWU Münster, DE — [2]Condensed Matter Theory, TU Dortmund, DE — [3]Theoretische Physik III, Universität Bayreuth, DE — [4]Institut für Experimentalphysik, Universität Innsbruck, AT

For coherent control of a few-level quantum emitter, typically pulses with an energy resonant to the transition energy are used, which requires sophisticated filtering of the signal. However, two-color excitation protocols were recently employed to circumvent the necessity for filtering.

Here I present an analysis of two-color excitation schemes, using the laser dressed states of the system. It can be shown, that the two-color excitation approach can be understood as a driving of transitions between the dressed states. We investigate how these transitions depend on the pulse parameters and explain how the different combinations of laser energies can excite the system. In addition to the results for a simple two-level system (2LS), we consider a three-level exciton-biexciton

system (3LS) that is typically found in semiconductor quantum dots and often used to generate entangled photon pairs. While in the 2LS, we can give clear conditions for the applicability, in the 3LS, due to strong state mixing, the conditions are less obvious. Nonetheless, we can find regimes of parameters to drive the system into either the exciton or the biexciton in the 3LS.

HL 7.40 Mon 13:00 P2/EG

Controlling the dimensions of top-down GaN nanowire ensembles via self-assembled metal islands — •Rose Mary Jose, Jingxuan Kang, Miriam Oliva, Thomas Auzelle, Abbes Tahraoui, Oliver Brandt, and Lutz Geelhaar — Paul-Drude-Institut für Festkörperelektronik, 10117 Berlin, Germany

The large surface-to-volume ratio of semiconductor nanowires and their potential for enhanced light absorption are attractive for photoelectrochemical applications. In this context, large-scale nanowire arrays are needed. For top-down fabrication, a scalable and rapid way to form a nano-island mask is the dewetting of a metal film.

In this work, we study how Pt films evolve upon thermal treatment into nano-islands which serve as a shadow mask for the top-down etching of GaN nanowire ensembles. To gain control over the nano-island ensembles' dimensions, we explore variations of the annealing conditions, Pt film thickness, and the surface energy by investigating Pt dewetting on GaN, SiNx, and SiOx surfaces. The islands' size and density are determined by the initial Pt film thickness. However, nano-island diameter and spacing are coupled by a fixed ratio. Therefore, individually controlling the spacing between nano-islands and their diameter is challenging in this approach.

Nanowire arrays are fabricated using Pt dewetting masks by plasma etching followed by KOH wet etching. The resulting nanowires' dimensions are consistent with those of the original nano-islands. In our experiments, diameters in the range 30 nm-200 nm and lengths of 500-1000 nm are demonstrated.

HL 7.41 Mon 13:00 P2/EG

Investigation of SiNWs [100] and [111] applying DFT with doping — •Nedhal Al-Nuaimi, Hilser Florian, and Gemming Sibylle — Chemnitz University of Technology, Chemnitz (Germany)

We present an ab initio study of Silicon nanowires (SiNW) with p-type impurities (doping) of Boron (B) and n-type impurities of Phosphorus (P) using Abinit and VESTA Software. We compare total energy and band dispersion in the [100] and [111] directions with that of pure bulk (semiconductor) silicon. The resulting band structure shows metallic behaviour due to additional states within the band gap. Furthermore dangling bonds lead to localized surface states without dispersion. Saturating these states can cause shifts in the electrostatic potential and may be used to tune the sensing properties of SiNWs.

HL 7.42 Mon 13:00 P2/EG

Growth and characterisation of local droplet etched InAs quantum dots in an InGaAs matrix — •Nikolai Spitzer, Hans-Georg Babin, Andreas Wieck, and Arne Ludwig — Ruhr-Universität Bochum, Lehrstuhl für Angewandte Festkörperphysik, Universitätsstraße 150, 44801 Bochum

We present a new local droplet etching (LDE) method for selforganized InGaAs quantum dots (QDs). We use gallium droplets to etch on an InGaAs matrix layer and fill the nanoholes with InAs. The impact of the indium concentration in the InGaAs-layer and of the deposited InAs amount after etching is investigated by atomic force microscopy and photoluminescence spectroscopy.

HL 7.43 Mon 13:00 P2/EG

Enhancement of Quantum Dot Emission in the Telecom C-Band via Photonic Micro Cavities — •Raphael Joos, Christian Rupp, Sascha Kolatschek, Stephanie Bauer, Cornelius Nawrath, Robert Sittig, Ponraj Vijayan, Michael Jetter, Simone Luca Portalupi, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen (IHFG), Center for Integrated Quantum Science and Technology (IQST) and SCoPE, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

Potential quantum technology applications such as quantum communication rely on the availability of carrier of quantum information. For that matter single-photons can be utilized as „flying-qubits“ imprinting information in their polarization state. For these applications it is beneficial to operate at the telecom C-band which offers reduced dispersion and minimum loss in optical fibers. In the recent years InAs quantum dots (QDs) have shown to be capable of emission of single and entangled photons in the telecom C-band. However, as-grown QD structures have limited collection efficiency of the emitted light due to total internal reflection. To tackle this issue photonic cavity structures can be employed which can enhance the photon extraction efficiency and decrease the decay time due the underlying Purcell effect. While there are different approaches to photonic structures ranging from planar cavities to Gaussian micro lenses, this work mainly deals with circular Bragg grating structures. These offer high collection efficiency in a broadband manner as well as a cavity spectrum which potentially allows simultaneous Purcell enhancement of exciton and biexciton.

HL 7.44 Mon 13:00 P2/EG

Voronoi-Cell Analysis of Density Modulated InAs Quantum Dots — •Peter Zajac[1], Nikolai Bart[1,2], Christian Dangel[2], Kai Müller[3], Andreas D. Wieck[1], Jonathan Finley[2], and Arne Ludwig[1] — [1]Ruhr-Universität Bochum, Universitätsstraße 150, 44801 Bochum, Germany — [2]Walter Schottky Institut and Physik Department, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany — [3]Walter Schottky Institut and Department of Electrical and Computer Engineering, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany

InAs quantum dots (QDs) grown by molecular beam epitaxy exhibit a density modulation upon growth on top of a GaAs gradient layer [1]. The local variation of the nucleation probability is ascribed to the roughness of the underlying GaAs layer. It is of interest to study the QD formation on such a surface under the scope of the capture-zone model [2]. Here, the results of AFM data analysis with focus on correlations between Voronoi cell areas and QD size parameters such as height and volume are presented.

[1] Bart, N., Dangel, C. et al. Wafer-scale epitaxial modulation of quantum dot density. *Nat. Commun.* **13**, 1663 (2022).
[2] Löbl, Matthias C., et al. Correlations between optical properties and Voronoi-cell area of quantum dots. *Phys. Rev. B* **100**, 155402 (2019).

HL 7.45 Mon 13:00 P2/EG

Enhancing the extraction efficiency of photons from low intensity decay processes with solid immersion lenses — •Patricia Kallert[1], Björn Jonas[2], Eva Schöll[1], Tim Langer[1], Dirk Reuter[1], Artur Zrenner[1], and Klaus D. Jöns[1] — [1]hqpd lab, PhoQS Institute and Department of Physics, Paderborn University, Germany — [2]Photonic Quantum Engineering Group, Walter Schottky Institute, and Department for Electrical and Computer Engineering, Technical University of Munich, Germany

Single photons are basic building blocks for photon-based quantum technologies, such as quantum computation and communication concepts. A promising source offering high single-photon purity and indistinguishability are semiconductor quantum dots in photodiodes. A major drawback of this platform is the low extraction efficiency. Due to the refractive index mismatch of the semiconductor and the surrounding environment, total internal reflection occurs already for very small angles of incidence on the interface. In this study, the enhancement capability and the practical limits of using solid immersion lenses of hemispherical and Weierstrass geometry are investigated and compared. The hemispherical lens is insusceptible to misalignment but offers a mediocre enhancement in collection efficiency. In contrast, the Weierstrass geometry is sensitive to nonperfect alignment but improves the extraction by a factor of up to 2.9. Avoiding the need of the fabrication of complex structures as micropillars and other cavities, consequently, we can triple the detection of photons from low-intensity decay processes.

HL 7.46 Mon 13:00 P2/EG

Magnetic Field-Dependence of the Auger Recombination Rate in a Self-Assembled Quantum Dot — •Fabio Rimek[1], Hendrik Mannel[1], Marcel Zöllner[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

A quantum dot (QD) is an ideal system to study electron-electron interaction in a confined nanostructure [1]. The Auger recombination is a special case, where the recombination energy is transferred to a third charge carrier that leaves the dot [2] or is excited to a higher energy level. Therefore, the Auger effect destroys the radiative recombination of the charged exciton (trion) - an effect, which should be

minimized for future applications that use spin states as stationary qubits, which can be transferred to photons via the QD trion transition. In this work, we investigate how the Auger rate is affected by an external magnetic field, applied perpendicular to the plane of the dots. In the magnetic field, the trion transition of a QD is no longer spin degenerate and splits up. We use two-color, time-resolved resonance fluorescence to investigate the quenching of the trion recombination due to the Auger effect. Two color excitation allows us to excite two quantum dot transitions (both trions or one trion and one exciton) and neglect spin relaxation as well as spin-flip Raman scattering. This ensures that we can directly measure the Auger and the tunneling rate of an electron into the dot. [1] A. Kurzmann et al., Nano Lett. **16**, 3367-3372 (2016).
[2] P. Lochner et al., Nano Lett. **20**, 1631-1636 (2020).

HL 7.47 Mon 13:00 P2/EG

Towards solid-state quantum emitters strongly coupled to crossed nanobeam cavities — •Jan-Gabriel Hartel, Oscar Camacho Ibarra, and Klaus D. Jöns — hqpd lab, PhoQS Institute and Department of Physics, Paderborn University, Germany

The strong coupling regime of quantum electrodynamics, theoretically described via the Jaynes-Cummings model, offers insight into purely quantum mechanical effects in the interaction of a two-level system and a single mode light field. An extension of this model to the interaction of a two-level system with two resonant modes yields the possibility of free exchange of the excitation between the light modes as well as subsequent applications in quantum gates. While the fundamental case has been experimentally studied, the realization of this extension has proven to be elusive due to the technological challenges of fabricating a stable coupled cavity system.

In this work, we seek to approach this realization by exploring nanofabrication of on-chip crossed nanobeam cavity systems, realized via Bragg mirrors. We numerically explore heuristic extensions of existing design recipes for 1D nanobeam cavities, based on the creation of a localized defect mode. We emphasize the challenges of conserving high Q-factors at the specified resonance frequency while minimizing coupling between the crossed cavities, developing novel design ideas.

HL 7.48 Mon 13:00 P2/EG

Towards frequency-converted polarization-entangled photon pairs from semiconductor quantum dots — •Tim Strobel[1], Andre Bisquerra[1], Tobias Bauer[2], Nand Lal Sharma[3], Marlon Schäfer[2], Stefan Kazmaier[1], Cornelius Nawrath[1], Lukas Wagner[1], Ankita Choudhary[3], Michael Jetter[1], Caspar Hopfmann[3], Christoph Becher[2], Simone L. Portalupi[1], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Science and Technology (IQST) and SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]Fachrichtung Physik, Universität des Saarlandes, Campus E2.6, 66123 Saarbrücken, Germany — [3]Institute for Integrative Nanosciences, Leibniz IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany

Fiber-based distribution of entangled, single photon pairs is a key requirement for future developments of terrestrial quantum networks. Quantum repeater schemes at telecom wavelengths can overcome the restriction set by fiber transmission losses over long distances. In this context semiconductor quantum dots (QDs) are promising candidates as deterministic sources of on-demand polarization-entangled photon pairs. Here, we investigate photons emitted via the biexciton-exciton cascade of GaAs QDs grown via Al droplet etching and integrated into a GaP solid immersion lens. To be compatible with existing fiber network infrastructures, quantum frequency conversion is employed to convert the QD emission from 780nm to telecom wavelengths.

HL 7.49 Mon 13:00 P2/EG

Strongly driven germanium qubit — •Bashab Dey and John Schliemann — Institute for Theoretical Physics, University of Regensburg, Regensburg, Germany

Hole qubits in germanium heterostructures are promising candidates for coherent control and manipulation of the spin degree of freedom by electric dipole spin resonance. The suppression of contact hyperfine interaction due to p-type character of the holes, possibility of nuclear-spin free isotopes and absence of valley degeneracies in germanium are favourable for sustaining longer spin coherence and relaxation times in these qubits. We study the time dynamics of a germanium qubit confined laterally by a parabolic potential and strongly driven by coherent circularly polarized radiation in presence of p-cubic Rashba spin-orbit coupling and perpendicular magnetic field. We calculate the transition rates between the lowest (Zeeman-split) levels of the qubit using Floquet theory. We observe peculiar beating patterns in the Rabi oscillations which depend on the strength of the driving field. When the driving frequency is resonant with Zeeman gap, the maxima of the oscillations is a decreasing function of driving amplitude which is in contrast to that of a harmonically driven two-level system. Furthermore, the time period of oscillations, time interval between the beating nodes and the number of oscillations between the nodes also decrease with the radiation amplitude.

HL 7.50 Mon 13:00 P2/EG

Swing-Up Dynamics in Quantum Dot Cavity Systems — •Nils Heinisch, Nikolas Köcher, David Bauch, and Stefan Schumacher — Physics Department and CeOPP, Paderborn University, Germany

In this work, we further investigate the recently proposed [1] and experimentally demonstrated [2] SUPER-scheme (Swing-UP of the quantum EmitteR population). In the SUPER-scheme optical excitation of a quantum emitter is achieved using two off-resonant red-detuned Gaussian pulses. Here, we expand the studies to quantum dot cavity systems and aim for high quality photons, generated during the decay process following the excitation. After successful proof-of-principle studies with a two-level system, we present the successful single-photon and photon-pair generation using the SUPER-scheme for excitation of diamond-shaped exciton-biexciton quantum dot model systems. For a more realistic simulation we also take phonons into account. For all systems studied it can be concluded that a cavity neither hinders the swing-up process nor degrades the quality of the generated photons which is in contrast to excitation schemes using resonant Gaussian pulses. [1] T. K. Bracht et al., PRX Quantum 2, 040354 (2021). [2] Y. Karli et al., Nano Letters 22, 6567 (2022).

HL 7.51 Mon 13:00 P2/EG

Time-Resolved Wave-Function Mapping in Self-Assembled Quantum Qots — •Jens Kerski[1], Daniel Hecker[1], Nelson Creutzburg[1], Arne Ludwig[2], Andreas D. Wieck[2], Martin Geller[1], and Axel Lorke[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [2]Chair of Applied Solid State Physics, Ruhr-University Bochum, Germany

The static and dynamic properties of self-assembled quantum dots (QDs) are often modeled using the QD's single particle wavefunctions. Although this approximation is very successful, the influence of the electron-electron interaction on the few-particle wave-functions and their nonequilibrium dynamics has not yet been studied in detail.

We investigate an ensemble of InAs/GaAs QDs, embedded in a high electron mobility transistor. The QDs are tunnel-coupled to a two-dimensional electron gas (2DEG). By applying a voltage pulse to the gate, we induce charge carriers from the 2DEG to tunnel into targeted quantum dot states. We monitor the temporal evolution of the conductivity σ_{2D} of the 2DEG, which is sensitive to the transfer of charge into the QDs. A rate-equation-based evaluation of σ_{2D} allows us to separate tunneling processes into different equilibrium or non-equilibrium QD states. We use an in-plane magnetic field perpendicular to the tunneling direction for wave-function mapping [1, 2] of the quantum dot states. This allows us to study the shape and dynamics of the (excited) electron states.
[1] W. Lei et al., Phys. Rev. Lett. 105, 176804 (2010).
[2] D. Zhou et al. J. Appl. Phys. 134, 064401 (2022).

HL 7.52 Mon 13:00 P2/EG

Development and deterministic nanofabrication of quantum dot based single-photon sources with emission in the 780 nm-930 nm range — •Dinara Basharova[1], Stephan Reitzenstein[1], Sven Rodt[1], Caspar Hopfmann[2], Nand Lal Sharma[2], Normen Auler[3], and Dirk Reuter[3] — [1]Institute of Solid State Physics, Technische Universität Berlin, D-10623 Berlin, Germany — [2]Leibniz Institute for Solid State and Materials Research Dresden, 01069 Dresden, Germany — [3]Center of Optoelectronics and Photonics, Universität Paderborn, 33098 Paderborn, Germany

Important goals of quantum technology are to demonstrate the elementary building blocks of a quantum repeater and to integrate them into the infrastructure of a quantum network. A network of quantum repeaters allows the distribution of quantum entanglement, thereby enabling secure exchange of information between multiple parties. To implement such building blocks, we use semiconductor heterostructures (HS) with GaAs quantum dots (QDs) integrated into circular

Bragg gratings (CBG). GaAs QDs are excellent single-photon emitters with almost negligible multi-photon emission probability and photon extraction efficiencies exceeding 60%. For this purpose, we deterministically integrate QDs on structures with back-side distributed Bragg reflector and in hybrid approach with backside Au mirror for comparison. In-situ electron beam lithography (iEBL) is an ideal technique for deterministic fabrication of such QD-based quantum light sources. The fabricated QDs are characterized by microphotoluminescence and quantum optical spectroscopy.

HL 7.53 Mon 13:00 P2/EG

Fabrication of electrically controllable quantum dots in PIN diodes integrated within circular Bragg gratings — •Setthanat Wijitpatima[1], Normen Auler[2], Sven Rodt[1], Dirk Reuter[2], and Stephan Reitzenstein[1] — [1]Institute of Solid-State Physics, Technische Universität Berlin, D-10623 Berlin, Germany — [2]Center of Optoelectronics and Photonics, Universität Paderborn, 33098 Paderborn, Germany

A quantum repeater is one emerging device of the decade that has been promised to play a crucial role in quantum communication. To produce an ideal quantum light source with high single-photon purity, nanophotonic structures must be fabricated on self-organized semiconductor quantum dots, which pose challenges due to their random occurrences and requirements of exact spatial and spectral integration. In addition to nanophotonic enhancement, such devices can be designed to allow an electrical manipulation of the excitonic state of quantum dots. Here, we propose a design that allows electrical controls via a PIN diode integrated within circular Bragg gratings (CBGs). Numerical simulations are done to optimize the design to yield the photon extraction efficiency (PEE) of 0.69 at N.A.=0.8. The deterministic fabrication is done with the use of cathodoluminescence (CL) scans and electron beam epitaxy (EBL), and the fabricated devices are characterized by electric-field dependent micro-photoluminescence (μPL) measurements.

HL 7.54 Mon 13:00 P2/EG

Patterned growth of vertical zinc oxide nanowires on sputtered zinc oxide thin films — •Jan Böhmer, Lukas Jäger, Alexander Koch, and Carsten Ronning — Institute of Soild State Physics, Friedrich Schiller University Jena, Max-Wien-Platz 1, 07743 Jena

Because of the wide band of zinc oxide, ZnO nanowires have promising applications in short wavelength optoelectronics, like building photodetectors or laser emitters using nanowire arrays. ZnO nanowires can be easily grown by vapor transport techniques in a high temperature furnace on silicon substrates utilizing the vapor-solid-liquid (VLS) mechanism. However, the nanowires produced in this way typically show random orientations and often overlap each other. A pre-deposited thin film of aluminum doped zinc oxide (Al:ZnO or AZO) by RF sputtering on the substrate creates a polycrystalline ZnO surface with a preferred orientation, on which the nanowires can grow epitaxially. The ZnO nanowires grown this way are almost all orientated perpendicular to the substrate surface resulting in vertical/upstanding nanowires. By now pattering the pre-deposited AZO thin films, selective area growth (SAG) of nanowires is possible. In this contribution, we will discuss our growth results and our goal to control the exact position of nanowire growth to create ordered nanowire arrays.

HL 7.55 Mon 13:00 P2/EG

Energy transfer between Si quantum dots and protoporphyrin molecules as a function of distance, orientation and size — •Athanasios Koliogiorgos[1] and Tomas Polcar[2] — [1]Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic — [2]Department of Control Engineering, Faculty of Electrical Engineering, Czech Technical University in Prague, Czech Republic

Organic molecules such as protoporphyrin IX (PPIX) can be attached to bulk or nanostructured silicon to enhance its optical and electronic properties. In this study, the interaction between PPIX molecules (donor) and Si nanocrystals (acceptor) up to 2.5 nm for varying distances and orientations is studied by DFT, semi-empirical and TDDFT methods. Simulations show an effect on electronic structure, indicative of electron charge transfer in parallel orientation and very small distances and non-electron energy transfer for different orientations and larger distances. An absorption-emission spectral overlap is observed. We use the Transition Density Cube method to calculate the electronic couplings and energy transfer rates between donor and acceptor. The Si quantum dots with the smallest size yield larger couplings than the larger nanocrystals. The coupling is enhanced by adding a plasmon nanoparticle as a bridge between donor and acceptor. Results using Au nanoparticles show increased energy transfer rates up to four orders of magnitude and lower distance dependence.

HL 7.56 Mon 13:00 P2/EG

The internal photoeffect from a single solid-state quantum emitter: Excitation energy and band-structure dependence — •B. Maib[1], M. Zöllner[1], F. Rimek[1], P. Lochner[1], H. Mannel[1], A.D. Wieck[2], A. Ludwig[2], A. Lorke[1], and M. Geller[1] — [1]University of Duisburg-Essen and CENIDE, Germany — [2]Ruhr-University Bochum, Germany

The coherence time is one of the limiting factors for using single quantum emitters, like self-assembled quantum dots, in future applications of quantum information processing. Besides spin and charge noise [1] the physical limits are given by the Auger recombination [2] and an internal photoeffect [3] that is present even for resonant excitation.
We have studied in detail the photoeffect in a single self-assembled quantum dot for different energies of a non-resonant laser that excites a single electron from the bound quantum dot state into the continuum of the conduction band. These measurements are realized by time-resolved two-color resonance fluorescence (RF) excitation. The first resonant laser drives the exciton transition, while the second pulsed laser simultaneously excites the photoelectron to the final state in the conduction band, caused by the internal photoeffect.
The results can be used to reduce the internal photoeffect and therefore suppress the photoemission, which would increase the coherence time in such a single photon emitter even under resonant excitation.
[1] A. V. Kuhlmann, Nature Physics, **9**, 570-575 (2013).
[2] A. Kurzmann, Nano Letters **16**, 3367-3372 (2016).
[3] P. Lochner, Phys. Rev. B, **103**, 075426 (2021).

HL 7.57 Mon 13:00 P2/EG

Calibrating Photoluminescence Yield for Quantum emitters in Planar Photonic Heterostructures — •Timo Kruck, Hans-Georg Babin, Andreas D. Wieck, and Arne Ludwig — Ruhr-Universität-Bochum; Lehrstuhl für angewandte Festkörperphysik, Bochum, Deutschland

When performing photoluminescence (PL) measurements the spectral intensity of the emitted radiation strongly depends on the dielectric structure surrounding the quantum emitter. Here we show a method for calibrating PL measurements to obtain the unaltered spectrum of the optically active medium [1]. For this purpose, the spectral reflectivity and the wavelength dependent standing wave field are used. The reflectivity, which is determined by reflectometer measurements , and a simulation based on the transfer matrix method are used to compensate for the true layer thickness. This is then used to calculate the standing wave field, the outcoupling efficiency and the quantum yield. To validate the method, the calibrated spectra are compared with cleaved-edge PL measurements where the QDs are excited from the side and the light is also collected from the side.
[1] Babin et al.; Nanomaterials 2021, 11(10), 2703;

HL 7.58 Mon 13:00 P2/EG

Nanowire-based light absorber patterning for artificial photosynthesis — •Juliane Koch[1], Jiajia Qiu[2], Peter Kleinschmidt[1], Huaping Zhao[2], Yong Lei[2], and Thomas Hannappel[1] — [1]TU Ilmenau, Institute for Physics, Fundamentals of energy materials, Ilmenau, Germany — [2]TU Ilmenau, Institute for Physics, Applied nanophysics, Ilmenau, Germany

Due to the increased degrees of freedom in device structures and properties, III-V nanowires (NWs) have been predicted to outperform planar devices. In the context of energy conversion in solar cells and photoelectrochemical devices, the kinetics and transport behavior of different charge carriers in light absorbers are closely related to the selected materials and their shape. A key factor for commercially relevant development is the enhanced light absorption, in particular in an uniform NW array, combined with lower costs and material usage (e.g. of III-Vs) for nanowire-based light absorbers. This may ultimately require fabrication techniques with homogenous patterning over a large range. In this work we demonstrate the fabrication techniques for creation of a NW array and key requirements during MOVPE NW growth. By applying a surface patterning technique with anodic aluminum oxide (AAO) templates, arrays of gold droplets can be deposited on a surface, which acts as a catalyst for NW growth during metalorganic vapor phase epitaxy (MOVPE). Under defined process parameters ver-

tical III-V semiconductor NW can be achieved via vapor-liquid-solid (VLS) growth in a horizontal MOVPE system.

HL 7.59 Mon 13:00 P2/EG

Enhancing spatial resolution for terahertz waveform near-field microscopy — •Fabian Brütting, Moritz Heindl, and Georg Herink — Experimental Physics VIII, University of Bayreuth, Germany

The quantum confined Stark-effect induces field-driven modulations in the optical transitions of quantum emitters. Harnessing this ultrafast interaction in colloidal quantum dots enables us to image THz near-field waveforms with fluorescence microscopy in the visible spectrum [1]. The spatial resolution of fluorescence microscopy is principally not diffraction-limited and can be extended to the few-nanometer scale using super-resolution techniques such as stimulated emission depletion (STED) microscopy. The efficient depletion of quantum dot emission presents a key requirement [2]. In this contribution, we present our investigations on the STED process in the quantum dots employed as field-probes in the luminescence-based Quantum-probe field microscopy (QFIM) scheme.

[1] Heindl, M. B. et al., Ultrafast imaging of terahertz electric waveforms using quantum dots. Light Sci. Appl. 11, 5 (2022).

[2] Hanne, J. et al., STED nanoscopy with fluorescent quantum dots. Nat. Comm. 6, 7127 (2015).

HL 7.60 Mon 13:00 P2/EG

Investigation of the biexciton decay in semiconductor In(Ga)As/GaAs quantum dots — •Christopher Buchholz, Sebastian Krehs, and Artur Zrenner — Universität Paderborn, Paderborn, Deutschland

The biexciton-exciton cascade is a widely used promising emission mechanism in quantum dots for generating entangled photon pairs with high fidelity. An often overlooked critical parameter for the quality of the emitted photons is the different lifetimes of electron and hole. Since the lifetimes of excitonic states can be influenced via external electrical fields (quantum confined stark effect), we studied this parameter in Schottky-contacted GaAs heterostructures. We approached this challenge by placing the quantum dots at different distances to the n-contact, 40 nm and 80 nm, respectively. The quantum dots were first characterized by voltage-dependant photoluminescence (PLV) measurements under above-band excitation and further investigated by photocurrent spectroscopy (PC) under resonant excitation and PLV under two-photon excitation (TPE). From the resonances in the PC measurements, the electron lifetime was extracted, whereas the TPE measurements showed the occurrence of the biexciton and charged exciton states as a function of the voltage. The results suggest that an increased distance to the n-contact leads to a decreased tunneling rate of electrons into the quantum dot. At the same time, the tunneling from the quantum dot is not affected.

HL 7.61 Mon 13:00 P2/EG

Influence of the quantum dot geometry on higher excited states — •Jan Kaspari and Doris E. Reiter — Condensed Matter Theory, TU Dortmund, Otto-Hahn-Straße 4, 44227 Dortmund

The energetic structure and absorption spectra of semiconductor quantum dots are strongly dependent on the dot geometry. In particular the higher excited states, typically denoted as p- or d-shell, can become highly mixed and depend strongly on the specific dot. We derive a theoretical model to describe higher excited quantum dot states based on the envelope function approximation. The four-band Luttinger theory as well as the direct and short-range Coulomb interactions are treated within a configuration interaction approach. The quantum dot confinement is approximated by an anisotropic harmonic potential. We show that a variation of the size of a cylindrical symmetric quantum leads to energetic shifts of higher excited quantum dot states. Breaking this cylindrical symmetry significantly alters the absorption spectrum as further energy splittings in the energetic structure appear and state mixtures change which results in differences of oscillator strenghts of some peaks. Our results give insight into the quantum dot energy structure especially for higher excited states, which become relevant in radiative Auger processes or for ultrafast quantum logic operations.

HL 7.62 Mon 13:00 P2/EG

Towards remote on-chip two-photon interference in gallium arsenide based-photonic integrated circuits — •Ulrich Pfister[1], Moritz Speidel[1], Florian Hornung[1], Stephanie Bauer[1], Robert Sittig[1], Eric Reutter[2], Michael Jetter[1], Simone L. Portalupi[1], Jürgen Weis[2], and Peter Michler[1] — [1]Institut für Halbleiter und Funktionelle Grenzflächen (IHFG), Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Allmandring 3, Germany — [2]Max-Planck-Institut für Festkörperforschung (MPI), University of Stuttgart, Heisenbergstraße 1, Germany

InGaAs quantum dots (QDs) are a promising source of single and indistinguishable photons for the on-chip realization of two-photon interference (TPI) with remote QDs. One of the challenges is the inhomogeneously distributed emission frequency of the QDs, which makes frequency tuning necessary. We show that strain-induced emission frequency tuning is applicable for ridge waveguides and it can be considered a promising step towards remote on-chip TPI [1]. Additionally, a successful TPI with one single QD and an on-chip multimode interference beamsplitter as a part of a Mach*Zehnder interferometer has been realized and the feasibility of remote on-chip TPI with MOVPE-grown InGaAs QDs is discussed.

[1] Hepp, S. *et al.*, Appl. Phys. Lett. **117**, 254002 (2020)

HL 7.63 Mon 13:00 P2/EG

Quantum frequency conversion of entangled photon pair from GaAs Quantum dot to Sn-vacancy center in Diamond — •Ankita Choudhary, Tim Pokart, Nand lal Sharma, Moritz Langer, and Caspar Hopfmann — Institute for Integrative Nanosciences, Leibniz IFW Dresden, Helmholtzstraβe 20, 01069 Dresden, Germany

The distribution of entangled photons in future long-distance quantum networks requires both on-demand and high-fidelity entangled photon pair generation as well as their temporary storage in low dephasing quantum memory systems. While GaAs quantum dots have proven to be excellent entangled photon pair sources, this is system suffers from strong dephasing of its spin qubits. Diamond color centers on the other hand are excellent quantum memories, but not ideal entangled photon pair sources. In order to combine the complementary properties of both material system in a hybrid quantum network approach, the efficient conversion between the operating photon energies without the loss of quantum information using quantum frequency conversion is required. In this study we present quantum frequency conversion from of 780nm to 619nm, i.e. from GaAs quantum dot emission to the zero-phonon line of the diamond Sn vacancy center, using sum frequency generation in a periodically poled lithium niobate crystal and an infrared laser pump of about 3 *m wavelength. We find that a conversion efficiency of at least 25% can be achieved.

HL 7.64 Mon 13:00 P2/EG

Design of circular Bragg resonators in the telecom band for efficient emission of entangled and indistinguishable photons from semiconductor quantum dots — •Dustin Siebert, David Bauch, Klaus D. Jöns, Stefan Schumacher, and Jens Förstner — Electrical Engineering Department, Physics Department, CeOPP and PhoQS, Paderborn University, Germany

The generation of indistinguishable and entangled photons via the biexciton-exciton cascade in semiconductor quantum dots can be tailored by a photonic environment providing an increased emission rate through the Purcell effect and a cavity feedback [1,2].

Circular Bragg resonators exhibit exactly these properties and enable good collection efficiency over a large bandwidth. We developed an optimization strategy based on a two-step process. First, we use a batch of 2D electromagnetic simulations within Bayesian global optimization and finally polish the optimum through Nelder-Mead local optimization based on full 3D simulations.

The optical properties obtained are then used within a quantum mechanical simulation of the carrier dynamics in the semiconductor quantum dots including phonon interaction [3]. After optimization, we achieve a tremendous enhancement of the indistinguishability of the emitted photons even considering that real structures might suffer fabrication imperfections.

[1] E. Schöll, et al., Phys. Rev. Lett. 125, 233605 (2020) [2] F. Sbresny, et al., Phys. Rev. Lett. 128, 093603 (2022) [3] D. Bauch et al., Phys. Rev. B 104, 085308 (2021)

HL 7.65 Mon 13:00 P2/EG

Origin of Antibunching in Resonance Fluorescence — •Lukas Hanschke[1], Eva Schöll[1], Eduardo Zubizarreta Casalengua[2,3], Melina Peter[4], Ailton Garcia Jr.[4], Saimon F. Covre da Silva[4], Santanu Manna[4], Armando Rastelli[4], Kai Müller[5], Fabrice P. Laussy[3], Elena del Valle[2], and Klaus D. Jöns[1] —

[1]PhoQS, CeOPP, and Department of Physics, Paderborn University — [2]Departamento de Fisica Teorica de la Materia Condensada, Universidad Autonoma de Madrid — [3]Faculty of Science and Engineering, University of Wolverhampton — [4]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz — [5]Walter Schottky Institute, Technical University of Munich

Resonance fluorescence, the coherent emission of a quantum two-level system under weak resonant driving, exhibits sub-natural linewidth and inherits the coherence properties of the excitation laser. While previous experiments suggest that this emission also maintains antibunched, our results prove recent theoretical insights into the origin of the antibunching and the underlying interplay between the coherent and incoherent emission of the quantum system. This allows us to specifically manipulate the composition of the resonance fluorescence by frequency filtering and interference with the excitation laser field to enable single photons with sub-natural linewidth [PRL 123, 170402 (2020)].

HL 7.66 Mon 13:00 P2/EG

Near Fourier-Transform Limited Blinking Free Quantum Dots — •Eva Schöll[1], Lukas Hanschke[1], Melina Peter[2], Ailton Garcia Jr.[2], Patricia Kallert[1], Francesco Salusti[1], Saimon Filipe Covre da Silva[2], Santanu Manna[2], Armando Rastelli[2], and Klaus D. Jöns[1] — [1]PhoQS, CeOPP, and Department of Physics, Paderborn University, Warburger Straße 100, 33098 Paderborn, Germany — [2]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, 4040 Linz, Austria

Tailored quantum light sources are crucial building blocks for applications in quantum technologies. Al droplet etched GaAs Quantum Dots are promising candidates for such sources, as they show very good characteristics for example in terms of single-photon purity, indistinguishability on short time scales and entanglement fidelity. However, these QDs usually exhibit an unstable charge environment, which leads to reduced coherence on long time scales, broadened linewidths and blinking. Embedding the QDs into a p-i-n diode structure enables energy tuning via the Stark effect and stabilizes the charge environment. Here we demonstrate a solid-state single-photon source with no signs of blinking on up to ms time scales and near Fourier-transform limited linewidths. This opens up possibilities for experiments for a fundamentally deeper understanding of quantum level schemes and realization towards a quantum network, where quantum interference between separate sources is required.

HL 8: 2D Materials II (joint session HL/CPP)

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

HL 8.1 Mon 15:00 POT 81

Twist- and gate-tunable valley splitting in TMDC/CrI_3 heterostructures — •Klaus Zollner, Paulo E. Faria Junior, and Jaroslav Fabian — Institute of Theoretical Physics, University of Regensburg, 93053 Regensburg, Germany

Van der Waals heterostructures composed of twisted monolayers promise great tunability of electronic, optical, and magnetic properties. Twistronics has already demonstrated its potential in tuning proximity spin-orbit and exchange coupling in graphene-based heterostructures [1,2]. In this talk, we present the strong manipulation of the valley splitting upon twisting and gating in TMDC/CrI_3 heterostructures [3]. In particular, upon twisting from 0° to 30°, the proximity-induced TMDC valence band edge exchange splitting can be reversed (−2 to 2 meV), while the TMDC conduction band edge exchange splitting remains nearly constant (−3 meV). Further giant tunability (few meV) of the proximity exchange coupling is provided by a transverse electric field. Consequently, twisting and gating then allow to tailor the valley splitting of the first intralayer exciton peak in the range of 0 to 12 meV in WSe_2/CrI_3, which is equivalent to gigantic external magnetic fields of up to about 60 Tesla.

This work was supported by DFG SFB 1277, DFG SPP 2244, and the EU Horizon 2020 Research and Innovation Program (Graphene Flagship).

[1] K. Zollner and J. Fabian, Phys. Rev. Lett. 128, 106401 (2022).
[2] Lee *et al.*, Phys. Rev. B 106, 165420 (2022).
[3] K. Zollner, P. E. F. Junior, J. Fabian, arXiv:2210.13794 (2022).

HL 8.2 Mon 15:15 POT 81

Giant Enhancement of Interlayer Exciton Luminescence in $WSe_2/WSe_2/MoSe_2$ in Heterotrilayers. — •Chirag Palekar, Ching-Wen Shih, Imad Limame, Bárbara Rosa, and Stephan Reitzenstein — Institute of Solid State Physics, Technische Universität Berlin, D-10623 Berlin, Germany

TMDC heterolayers have gained lot on interest as a promising platform to study intricate many-body physics phenomena. Here we observe giant enhancement of interlayer exciton PL in a $WSe_2/WSe_2/MoSe_2$ heterotrilayers (HTL) system prepared by employing exfoliation and dry transfer method. The IX exciton forming at the heterojuction in the HTL region exhibits 10-fold increase in PL yield when compared to HBL region on the same sample. Such an enhancement can be attributed to the close to 0^0 twist angle between stacked WSe_2 homobilayers providing smaller interlayer separation and hybridization in the WSe_2 band structure, which in turn results in an efficient charge transfer. Further, PLE and reflection contrast reveal the twist angle dependence of the enhancement factor in such type II HTL systems as the large twist angel between WSe_2 homobilayers (57^0) results in only up to 10% percent enhancement of IX PL in the HTL region when compared with the HBL. This fundamental study of excitons in the HTL system deepens the current understanding of physics of twisted TMDC heterostructures and paves the way for future experiments and theoretical work.

HL 8.3 Mon 15:30 POT 81

Photoluminescence tuning in hybrid devices of monolayer transition metal dichalcogenides and rylene dyes — •Theresa Kuechle[1], Gergely Knorr[2], Kalina Peneva[2], and Giancarlo Soavi[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany — [2]Institute of Organic Chemistry and Macromolecular Chemistry, Friedrich Schiller University Jena, Lessingstraße 8, 07743 Jena, Germany

Monolayer transition metal dichalcogenides (TMDs) are direct gap semiconductors that hold great promise for applications in nanoscale photonics and optoelectronic devices. A viable path for the development of devices with advanced functionalities and tunable properties is the integration with other nanoscale systems such as nanowires [1] and molecules [2]. Here, we realize hybrid devices based on TMDs and rylene dyes and study their optical properties via steady state photoluminescence. Preliminary results show that the PL emission in hybrid structures of WS_2/CN_4PMI can be quenched by a factor of 3, in the case of WSe_2/CN_4PMI by 300. We tentatively assign this variation to a different band alignment in the two heterostructures and to the interplay between charge transfer (in type II) and energy transfer (in type I). Future experiments including ultrafast pump-probe spectroscopy of pristine and hybrid systems as well as hybridization of different (tunable) molecules will further elucidate the role of band alignment in the ultrafast charge and energy transfer processes at the nanoscale.

[1] Kim *et al.*, *ACS Nano* **14**, 9, 4323 (2020)
[2] Park *et al.*, *Adv. Mat. Interfaces* **8**, 12, 2100215 (2021)

HL 8.4 Mon 15:45 POT 81

Coherence of interlayer exciton ensembles in $MoSe_2/WSe_2$ heterobilayers — •Christos Paspalides[1], Mirco Troue[1], Johannes Figueiredo[1], Lukas Sigl[1], Manuel Katzer[2], Malte Selig[2], Andreas Knorr[2], Ursula Wurstbauer[3], and Alexander Holleitner[1] — [1]TU Munich — [2]Technische Universität Berlin — [3]University of Münster

Transition metal dichalcogenides exhibit strong light-matter interactions, which suggests them to be ideal candidates for novel 2D optoelectronic applications. Corresponding van der Waals heterostacks allow the excitation and formation of long-lived interlayer excitons [1]. We present coherence measurements of the ground state in such interlayer exciton ensembles by performing Michelson-Morley interferometry over a wide range of exciton density and temperature [2]. Moreover, we discuss the expansion dynamics of the interlayer excitons presumably driven by dipole-dipole interactions. The presented work paves the way towards a detailed understanding of excitonic many-body quan-

tum phenomena in two-dimensional materials [3].

[1] B. Miller et al., Nano Letters 17, 5229 (2017).
[2] M. Troue and J. Figueiredo, et al (2023).
[3] L. Sigl et al., Signatures of a degenerate many-body state of interlayer excitons in a van der Waals heterostack, Phys. Rev. Res. 2, 042044 (2020).

15 min. break

HL 8.5 Mon 16:15 POT 81

Theoretical description of interlayer excitons in TMD homobilayers — •Ruven Hübner[1], Alexander Steinhoff[1], and Matthias Florian[2] — [1]Institut für Theoretische Physik, Universität Bremen, Bremen, Germany — [2]University of Michigan, Dept. of Electrical Engineering and Computer Science, Ann Arbor, MI, USA

In recent years, interlayer excitons in bilayers of transition metal dichalcogenides (TMDs) have received a rapid increase in attention. On the one hand, they feature the main characteristics of conventional excitons in the corresponding monolayers, namely an absorption spectrum in the optical regime combined with a high binding energy. On the other hand, they differ to such intralayer excitons by a massively increased life time, a non-zero dipole moment in the out-of-plane direction and a strong sensitivity to material combination as well as stacking arrangement of adjacent monolayers. In this talk we focus on special excitonic properties inside TMD homobilayers that are particularly demanding from a theoretical point of view. In this context we discuss moiré excitons in twisted bilayers as well as high-lying excitons and trions at around twice the band gap energy arising within a highly non-parabolic band dispersion.

HL 8.6 Mon 16:30 POT 81

Raman signature of interlayer coupling and lattice dynamics in 2D TMDCs — •Yang Pan[1,2] and Dietrich R. T. Zahn[1,2] — [1]Semiconductor Physics, Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]Center for Materials, Architectures, and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, Chemnitz, Germany

Vertical stacking of two-dimensional (2D) homo- and heterostructures are intriguing research objects, as they are essential for fundamental studies and a key towards 2D device applications. It is paramount to understand the interlayer coupling in 2D materials and to find a fast yet precise characteristic signature. In this work, we report on a Raman fingerprint of interlayer coupling in 2D transition metal dichalcogenides (TMDCs). We observed that the out-of-plane B_{2g} vibrational mode is absent when two monolayers form a vertical stack yet remain uncoupled but emerges after strong coupling. Using systematic Raman, photoluminescence (PL), and atomic force microscopy (AFM) studies of WSe_2/WSe_2 homo-bilayers and $MoSe_2/WSe_2$ hetero-bilayers, we conclude that the B_{2g} vibrational mode is a distinct Raman fingerprint of interlayer coupling in 2D TMDCs. Our further investigations confirmed its applicability on twisted 2D homo- and hetero-bilayers. Our results propose an easy, fast, precise, and reliable measure to evaluate the interlayer coupling and twisting angles in 2D TMDCs.

HL 8.7 Mon 16:45 POT 81

Correlated states of moiré interlayer excitons in twisted transition metal dichalcogenide heterostructures — •Nils-Erik Schütte[1], Niclas Götting[1,2], Frederik Lohof[1,2], and Christopher Gies[1,2] — [1]Institute for Theoretical Physics, University of Bremen, Bremen — [2]Bremen Center for Computational Material Science, University of Bremen, Bremen

Stacking two transition metal dichalcogenide (TMD) monolayers on top of each other with a small relative twist yields a moiré pattern with a long lattice period. Quasiparticles perceive the resulting bandstructure modulation as a potential landscape, making it possible to consider moiré heterostructures as a realization of a Bose-Hubbard model in a semiconductor material.

We address the question in how far correlated states of moiré excitons can emerge and study their phase transition behavior in relation to the twist angle between both monolayers. Expanding on previous results [1], we discuss the effect of nearest-neighbor interaction that gives rise to a variety of different phases, such as inhomogeneous insulating and supersolid phases. Special attention is paid to the possibility of local atomic reconstructions that are now known to occur at small twist angles.

[1] Götting et al., Phys. Rev. B 105, 165419 (2022)

HL 8.8 Mon 17:00 POT 81

Electronic structures of twisted bilayer graphene and tungsten diselenide investigated by transferable tight-binding-models — •Xiaoyu Liu, Stefan Blügel, and Hyun-Jung Kim — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Since the discovery of intrinsic unconventional superconductivity in the Moiré superlattice from bilayer graphene stacked with a small twist angle, a new venue so-called twistronics has opened. Beyond graphene, transition metal dichalcogenides as a class of two-dimensional (2D) materials have attracted much attention due to their interesting optical properties. With the growing interest in 2D layered materials, accurate models describing the band structure and electronic properties of twisted bilayer graphene and tungsten diselenide are highly desirable. Here, we provide sets of parameters for the transferable tight-binding (TB) model, based on the Slater-Koster (SK) scheme with the exponential scaling law for the interlayer and overlap integral parameters. The workflow, to obtain transferable TB model parameters, is automatized by introducing global optimization methods such as particle swarm optimization (PSO) and conformational space annealing (CSA) methods. The fitness of the parameter set is assessed not only by comparing with ab-initio band energies, but also with its orbital similarity. Accurately produced electronic structures of twisted bilayers graphene and tungsten diselenide provide a chance to research their unique electronic and optical attributes.

Hyun-Jung Kim acknowledges support by the AvH Foundation.

15 min. break

Invited Talk HL 8.9 Mon 17:30 POT 81

Time-resolved optical spectroscopy of 3R-stacked MoS_2 — •Swarup Deb, Michael Kempf, Rico Schwartz, and Tobias Korn — Institute of Physics, Rostock University

Manipulation of in-plane rotational and out-of-plane stacking symmetry in engineered two-dimensional (2D) crystals has provided means to realize a variety of exotic phases in extremely thin structures. The emergence of out-of-plane ferroelectricity in rhombohedrally-stacked 2D materials, such as boron nitride and transition metal dichalcogenides (TMDs), is a recent addition to this, but so far, most research on rhombohedrally stacked (3R) TMDs focussed on bilayer units.

Here, we present a systematic study of low-temperature absorption, differential reflectivity, and Kerr rotation in 3R-stacked MoS_2 as a function of thickness, aiming to probe the effects of ferroelectricity and interlayer charge transfer on ground-state exciton properties, valley and photocarrier dynamics. We observe clear signatures of an energetic splitting of the A exciton, as well as valley and energy relaxation dynamics on a few-ps timescale.

HL 8.10 Mon 18:00 POT 81

Constructing minimal tight-binding models for twisted TMDC bilayers — •Michael Winter, Dominik Benner, and Tim Wehling — I. Institute of Theoretical Physics, Universität Hamburg, Notkestraße 9-11, 22607 Hamburg, Germany

Transition metal dichalcogenides bilayers attract considerable attention within the last years due to the wide range of observable correlation effects, e.g. superconductivity, exciton condensation and therelike. One possible parameter to tune these phenomena is the twist angle between the two layers.

We study the electronic structure of twisted transition metal dichalcogenides from ab initio DFT calculations and subsequent Wannier construction on untwisted snapshots of commensurate structures. By choosing a subspace of only three Wannier orbitals per transition metal, we construct a minimal model for the description of twisted bilayers.

HL 9: Focus Session: Graphene quantum dots (joint session HL/TT)

Quantum dots have emerged as one of the contenders for a future quantum information processor. Bilayer graphene is now established as a material that allows high quality bi-polar Coulomb blockade measurement, time-dependent transport measurements and first relaxation time measurements. In contrast to the more conventional GaAs and Si-based systems, several exiting and unexpected observations in graphene have been explained by the peculiar graphene bandstructure, which is gate- tunable, the additional valley degree of freedom, and spin-valley coupling.

Organized by Klaus Ensslin

Time: Monday 15:00–17:45 Location: POT 361

Invited Talk HL 9.1 Mon 15:00 POT 361
Spin and valley lifetime in graphene quantum dots — •Guido Burkard — University of Konstanz, Germany

Graphene with its low nuclear spin density and weak spin-orbit coupling allows for long electron spin relaxation and coherence times. The spin and valley degrees of freedom of localized electrons can therefore be seen as potential embodiments of classical or quantum bits for computation. However, the formation of localized states in quantum dots requires some form of badgap engineering, and the mechanisms for spin and valley relaxation have not been completely understood so far. Bilayer graphene has an electrically controllable bandgap that allows for the formation of quantum dots. We present general theoretical considerations regarding the formation of quantum dots in graphene and report on recent progress in understanding the relevant physical mechanisms of spin and valley relaxation in electrostatically gated bilayer graphene quantum dots.

Invited Talk HL 9.2 Mon 15:30 POT 361
Microscopic modelling of electrostatically induced bilayer graphene quantum dots — •Angelika Knothe — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany

Quantum nanostructures, e.g., quantum wires and quantum dots, are needed for applications in quantum information processing devices, such as transistors or qubits. In gapped bilayer graphene, one can confine charge carriers purely electrostatically, inducing smooth confinement potentials and thereby limiting edge-induced perturbances while allowing gate-defined control of the confined structure. In this talk, I will give an overview of our recent contributions toward the theoretical modelling of gate-defined bilayer graphene quantum dots, taking into account microscopic details of the material properties and the confinement. As an outlook, I will point towards current and future challenges in describing coupled bilayer graphene nanostructures, e.g., setups with multiple bilayer graphene quantum dots.

HL 9.3 Mon 16:00 POT 361
Valley relaxation in a single-electron bilayer graphene quantum dot — •Lin Wang and Guido Burkard — Department of Physics, University of Konstanz, D-78457, Germany

Bernal-stacked bilayer graphene (BLG) has a tunable gap controlled by an out-of-plane electric field. This makes BLG a possible candidate to form quantum dots (QDs) via quantum confinement. Spin-based qubits in BLG QDs have received great attention due to outstanding spin-coherence properties. Very recently, long spin relaxation times of a single-electron state in BLG QDs was reported [1,2]. In addition to spin, valley pseudospin is another degree of freedom in BLG. The two valleys experience opposite Berry curvatures and associated magnetic moments via an out-of-plane electric field. This provides a promising way to control valleys and further establish valley qubits. To assess the potential of valley qubits, the valley relaxation time is a crucial parameter since it directly limits the lifetime of encoded information. Here, we investigate the valley relaxation in a single-electron BLG QD due to intervalley coupling assisted by (i) 1/f charge noise and (ii) electron-phonon couplings arising from the deformation potential and bond-length change. Our calculation shows that valley relaxation time decreases with a power law dependence as a function of magnetic field, which is in a good agreement with very recent experiment.

References: [1]L. Banszerus, K. Hecker, S. Möller, E. Icking, K. Watanabe, T. Taniguchi, C. Volk and C. Stampfer, Nat. Commun. 13, 3637 (2022). [2] Lisa Maria Gächter et al., PRX Quantum 3, 020343 (2022).

30 min. break

Invited Talk HL 9.4 Mon 16:45 POT 361
Single-shot spin and valley Pauli blockade read-out in bilayer graphene quantum dots — •Chuyao Tong[1], Rebekka Garreis[1], Wister Wei Huang[1], Annika Kurzmann[1,2], Jocelyn Terle[1], Samuel Jele[1], Kenji Watanabe[3], Takashi Taniguchi[3], Thomas Ihn[1], and Klaus Ensslin[1] — [1]ETH Zurich, CH-8093 Zurich, Switzerland — [2]RWTH Aachen University, Aachen, 52074, Germany — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

In bilayer graphene quantum dots, apart from spins up and down, the additional valley degree of freedom K- and K+ gives rise to an unconventional single-dot two-carrier ground state: spin-triplet valley-singlet, altering the canonical even-odd double dot Pauli spin blockade picture. This ground state can be switched to a spin-singlet valley-triplet by a perpendicular magnetic field, allowing us to switch between valley-blockade at low, and spin-blockade at higher magnetic field for the two-carrier Pauli blockade (1,1) to (0,2). We employ charge sensing technology and perform single-shot Pauli blockade read-out at the two field regimes, probing characteristic relaxation times T1 between spin or valley -triplet and -singlet. The spin-T1 is measured to be up to 60ms, drastically decreasing with increasing inter-dot tunnel coupling and corroborating with recent experiments performed with single-dot Elzerman read-out. Moreover, we observe exceedingly long valley T1 longer than 500ms, robust with inter-dot tunnel coupling. These promisingly long spin- and valley T1 herald for long-living spin and valley bilayer graphene quantum dot qubits.

Invited Talk HL 9.5 Mon 17:15 POT 361
Particle-hole symmetry protects spin-valley blockade in graphene quantum dots — •Christian Volk[1,2], Luca Banszerus[1,2], Samuel Möller[1,2], Katrin Hecker[1,2], Eike Icking[1,2], Kenji Watanabe[3], Takashi Taniguchi[4], Fabian Hassler[5], and Christoph Stampfer[1,2] — [1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich — [3]Research Center for Functional Materials, NIMS, Tsukuba, Japan — [4]International Center for Materials Nanoarchitectonics, NIMS, Tsukuba, Japan — [5]JARA-Institute for Quantum Information, RWTH Aachen University

Particle-hole symmetry plays an important role for the characterization of topological phases in solid-state systems. Graphene is a prime example of a gapless particle-hole symmetric system. The intrinsic Kane-Mele spin-orbit coupling in graphene leads to a lifting of the spin-valley degeneracy and renders graphene a topological insulator in a quantum spin-Hall phase while preserving particle-hole symmetry.

Here, we show that the Kane-Mele spin-orbit gap leads to a lifting of the spin-valley degeneracy in bilayer graphene quantum dots, resulting in Kramer's doublets with different ordering for electron and hole states preserving particle-hole symmetry. We observe the creation of single electron-hole pairs with opposite quantum numbers and use the electron-hole symmetry to achieve a protected spin-valley blockade in electron-hole double quantum dots. The latter will allow spin-to-charge and valley-to-charge conversion, which is essential for the operation of spin and valley qubits.

HL 10: Focus Session: Progress in Hybrid Phononic Quantum Technologies II

Time: Monday 15:00–18:30 Location: POT 151

Invited Talk HL 10.1 Mon 15:00 POT 151

Surface Acoustic Wave Cavity Optomechanics with 2D Materials — •Galan Moody — University of California, Santa Barbara, CA, USA

Surface acoustic waves (SAWs) are a versatile tool for coherently interfacing with a variety of solid-state quantum systems spanning microwave to optical frequencies, including superconducting qubits, spins, and quantum emitters. In this presentation, I will discuss our progress on integrating 2D material quantum emitters with planar lithium niobate SAW resonators driven by superconducting electronics. Using steady-state photoluminescence spectroscopy and time-resolved single-photon counting, we map the temporal dynamics of modulated 2D emitters under coupling to different SAW cavity modes, showing energy-level splitting consistent with strong deformation potential coupling. We leverage the large anisotropic strain from the SAW to modulate the exciton and biexciton fine-structure splitting of 2D semiconductors, which may find applications for on-demand entangled photon-pair generation from 2D materials. I will conclude with a discussion on the prospects and outlook for SAW cavity optomechanics with 2D quantum emitters for high-speed single-photon modulators, efficient transducers, compact sensors, and exploring quantum electro-optomechanics with 2D materials.

Invited Talk HL 10.2 Mon 15:30 POT 151

Phononic Microresonators Coupled by Surface Acoustic Waves — •Sarah Benchabane, Maciej Baranski, Feng Gao, Olivier Gaiffe, Valérie Soumann, Roland Salut, and Abdelkrim Khelif — FEMTO-ST, CNRS, Université Bourgogne-Franche-Comté, Besancon, France.

The implementation of scalable phononic circuits has become an appealing prospect in view of increasing the versatility of electro-acoustic devices for radio-frequency signal processing. Recent demonstrations have made convincing steps towards this objective by proposing phononic architectures inspired by photonic integrated circuits or combining the rich dynamics of micro- and nano-electromechanical (M/NEMS) resonators with propagating elastic waves. In this work, we propose to exploit the interaction between surface acoustic waves (SAW) and locally-resonant, micron-scale mechanical resonators in order to achieve coherent driving of the resonator motion with SAW and, reciprocally, to control the elastic energy distribution at a deep subwavelength scale. Optical measurements by laser scanning interferometry allows retrieving both the resonator frequency response and mode shape, hence enabling direct observation of the vectorial nature of the interaction. We investigate the proposed physical system both in the linear and non-linear regimes and reveal that the elastic field behavior can be further controlled through resonator-to-resonator coupling, leading to a variety of interaction schemes. The proposed devices illustrate the potential of SAW-based architectures for the implementation of high-frequency phononic-NEMS circuits.

HL 10.3 Mon 16:00 POT 151

On-chip generation and dynamic piezo-optomechanical rotation of single photons — •Matthias Weiss[1,2], Dominik D. Bühler[3], Antonio Crespo-Poveda[4], Emeline D. S. Nysten[1,2], Jonathan J. Finley[5], Kai Müller[5,6], Paulo V. Santos[4], Mauricio M. de Lima Jr.[3], and Hubert J. Krenner[1,2] — [1]Physikalisches Institut, WWU Münster, Germany — [2]Institut für Physik, Universität Augsburg — [3]Materials Science Institute, University of Valencia, Spain — [4]Paul-Drude Institute for Solid State Electronics, Berlin, Germany — [5]Walter Schottky Institut, TU München, Germany — [6]Department of Electrical and Computer Engineering, TU München, Germany

Integrated photonic circuits are key components for photonic quantum technologies and for the implementation of chip-based quantum devices. Future applications demand flexible architectures to overcome common limitations of many current devices, for instance the lack of tuneability or built-in quantum light sources.

Here, we report on a dynamically reconfigurable integrated photonic circuit comprising integrated quantum dots (QDs), a Mach-Zehnder interferometer (MZI) and surface acoustic wave (SAW) transducers directly fabricated on a monolithic semiconductor platform. We demonstrate on-chip single photon generation by the QD and its sub-nanosecond dynamic on-chip control, enabling dynamic single photon routing with frequencies exceeding one gigahertz.

Bühler, D.D., Weiß, M., Crespo-Poveda, A. et al. Nat Commun 13, 6998 (2022)

HL 10.4 Mon 16:15 POT 151

Towards room temperature polaromechanics — •Ismael dP. Embid, Alexander S. Kuznetsov, Klaus Biermann, and Paulo V. Santos — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany

Microcavity exciton-polaritons have emerged as a promising platform for novel solid-state devices ranging from low threshold lasers to quantum and classical simulators. The transition to a polariton condensate at high particle densities with long (ns) temporal coherence and enhanced sensitivity to vibrations has opened the way for polariton-based optomechanics in the GHz frequency domain [1]. Such highly coherent states have, however, so far been observed only at low temperatures (10K). Here, we show that long coherences can be maintained by confining the polariton condensates within μm-sized intracavity traps in (Al,Ga)As microcavities. In particular, we demonstrate temporal coherences in the GHz range up to temperatures exceeding 77K. Furthermore, we show that these condensates can be non-adiabatically modulated at these temperatures by electrically injected GHz phonons, leading to the formation of several phonon side bands. These results enable the generation of GHz optical frequency combs tunable by the electrical power, a relevant feature for the precise control of quantum states.

1. Kuznetsov et al., arXiv:2210.14331v1

30 min. break

HL 10.5 Mon 17:00 POT 151

Readout of phonon statistics via resonance fluorescence of a single photon emitter — •Daniel Groll[1], Thilo Hahn[1], Ortwin Hess[2], Paweł Machnikowski[3], Tilmann Kuhn[1], and Daniel Wigger[2] — [1]Institute of Solid State Theory, University of Münster, Germany — [2]School of Physics, Trinity College Dublin, Ireland — [3]Department of Theoretical Physics, Wrocław University of Science and Technology, Poland

Single photon emitters in a solid state environment are inevitably coupled to phonon modes of the host material. On the one hand, decoherence induced by this coupling is often detrimental for harnessing the full potential of such emitters. On the other hand, this interaction in principle allows for control of the emitter not only optically, but also acoustically. Hybrid systems, comprised of optical, acoustic and excitonic components thus offer a high degree of flexibility by making use of all available interaction channels.

We consider here a single photon emitter located inside a phononic resonator and driven by an external laser. We derive analytical expressions for the resonance fluorescence (RF) spectrum, depending explicitly on the quantum statistics of the resonator mode. We show that, in principle, the statistics of the phonon mode can be determined from a given RF spectrum using our analytical model. We thus establish a simple and direct connection between the optical and acoustic components of such a hybrid system, paving the way for using single photon emitters as quantum transducers between the optical and acoustic domain.

HL 10.6 Mon 17:15 POT 151

Dry processing of high Q 3C-silicon carbide nanostring resonators — •Felix David, Philipp Bredol, Eva Weig, and Yannick Klass — Technical University of Munich, Chair of Nano and Quantum Sensors, 85748 Munich, Germany

We fabricate string resonators from strongly stressed 3C-silicon carbide (SiC) grown on a silicon substrate. In the conventional fabrication process, we do electron-beam lithography with PMMA to define a metallic hard mask for the subsequent dry-etching step via a liftoff process. This requires some wet-chemical process steps, which can destroy our samples. Here we describe an alternative process, which avoids all wet-chemical process steps to enable superior quality. It involves the use of a negative electron-beam resist as an etch mask, as well as the completely reactive-ion etching-based release of the nanos-

trings. The dry-processed nanostrings can be fabricated with a high yield and exhibit high mechanical quality factors at room temperature.

HL 10.7 Mon 17:30 POT 151

Acousto-optoelectric spectroscopy on transition metal dichalcogenide monolayers with surface acoustic waves — Matthias Weiss[1,2], Benjamin Mayer[1], Tobias Petzak[2], Clemens Strobl[1], •Emeline Nysten[1,2], Ursula Wurstbauer[1], and Hubert Krenner[1,2] — [1]Physikalisches Institut, WWU Münster, Germany — [2]Lehrstuhl für Experimentalphysik 1, Universität Augsburg, Germany

Surface acoustic waves have proven to be a useful tool for the control of semiconductor nanostructures optical properties and the dynamical transport of charge carriers [1,2,3]. For instance, SAW spectroscopy was already used to probe the electrical transport inside CVD-grown MoS_2 on $LiNbO_3$ in a contact-free manner [1]. In this work, we integrated transition metal dichalcogenide monolayer flakes into $LiNbO_3$ surface acoustic wave devices through a classical exfoliation process. The impact of the SAW on the photoluminescence of the monolayer was systematically studied. The results show a clear increase in the photoluminescence intensity of the monolayer as well a SAW-periodic modulation which can be linked to the SAW-controlled diffusion of the excitons inside the monolayer. [1] Nature Communications 6:8593 (2015) [2] Nano Letters 19:8701-8707 (2019) [3] IEEE Transactions on Quantum Engineering 3:1-17 (2022)

HL 10.8 Mon 17:45 POT 151

Strongly Stressed 3C-SiC Nanostring Resonators With High Quality Factors — •Philipp Bredol[1], Yannick Klass[1], Felix David[1], Eva Weig[1], Nagesh S. Japtap[2,3], Manfred Helm[2,3], Georgy Astakhov[2], and Artur Erbe[2,3] — [1]Technical University of Munich, Chair of Nano and Quantum Sensors, 85748 Munich, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany — [3]Dresden University of Technology, 01062 Dresden, Germany

Strongly stressed SiC nanostring resonators are a promising platform for sensing applications. SiC is mechanically, chemically, and thermally robust and process compatible with many Si technologies. Mechanical quality factors in the 10^5 range are achieved at room temperature with devices of $\approx 70 \times 1\,\mu m^2$ footprint.

Because the mechanical quality factor often determines sensitivity and resolution of nanomechanical sensors, the understanding of mechanical loss mechanisms is important for possible applications. In this contribution we show how to separate intrinsic material losses and dissipation dilution effects by analyzing mechanical response spectra. We apply these methods to analyze how He^+ irradiation damage affects the mechanical properties of SiC nanostring resonators (see contribution of Nagesh S. Jagtap).

HL 10.9 Mon 18:00 POT 151

Coupling single electrons and photons at photonic-chip based microresonators — •Armin Feist[1,2], Guanhao Huang[3,4], Germaine Arend[1,2], Yujia Yang[3,4], Jan-Wilke Henke[1,2], Arslan Sajid Raja[3,4], F. Jasmin Kappert[1,2], Rui Ning Wang[3,4], Hugo Lourenço-Martins[1,2], Qiu Zheru[3,4], Junqiu Liu[1,2], Ofer Kfir[3,4], Tobias J. Kippenberg[3,4], and Claus Ropers[1,2] — [1]MPI for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Germany — [3]Institute of Physics, Swiss Federal Institute of Technology Lausanne, Switzerland — [4]Center for Quantum Science and Engineering, Swiss Federal Institute of Technology Lausanne, Switzerland

Integrated photonics facilitates control over fundamental light-matter interactions in manifold quantum systems. Extending these capabilities to electron beams [1] fosters free-electron quantum optics.

Here, we show the coupling of single electrons and photons at a high-Q integrated photonic microresonator [2]. Spontaneous scattering at empty resonator modes creates electron-photon pair states [3], enabling single-particle heralding schemes and noise-supressed mode imaging. This provides a pathway toward novel hybrid quantum technology with entangled electrons and photons, as well as the capability for quantum-enhanced electron imaging and Fock-state photon sources.

[1] J.-W. Henke *et al.*, Nature **600**, 653 (2021).
[2] A. Feist *et al.*, Science. **377**, 777 (2022).
[3] X. Bendaña *et al.*, Nano Lett. **11**, 5099 (2011).

HL 10.10 Mon 18:15 POT 151

Brillouin scattering selection rules in polarization-sensitive photonic resonators — Anne Rodriguez[1], Priya Priya[1], Edson Cardozo[1], Abdelmounaim Harouri[1], Isabelle Sagnes[1], Florian Pastier[2], Martina Morassi[1], Aristide Lemaître[1], Loic Lanco[1], •Martin Esmann[1,3], and Daniel Lanzillotti-Kimura[1] — [1]Université Paris-Saclay, CNRS, Centre de Nanosciences et de Nanotechnologies, Palaiseau, France — [2]Quandela SAS, Palaiseau, France — [3]Institut für Physik, Universität Oldenburg, Germany

Spontaneous Brillouin scattering in bulk crystalline solids is governed by intrinsic selection rules which lock the relative polarization of excitation laser and Brillouin signal. In this work, we independently manipulate the polarization states of the two, using polarization-sensitive optical resonances in elliptical micropillars [1,2].

The induced wavelength-dependent polarization rotation [3] enables a polarization-based filtering technique [4]. We employ it to experimentally detect acoustic phonon resonances with frequencies in the range of 20-100 GHz, difficult to access with both standard Brillouin and Raman spectroscopy techniques. The strong modification of selection rules extends to any optical system with polarization-sensitive modes: plasmonic resonators, photonic crystals, birefringent micro- and nanostructures. It is thus relevant for applications in optomechanical, optoelectronic, and quantum optics devices [1,2].

[1] H. Wang et al. Nat. Phot. 13, 770 (2019). [2] S. Gerhard et al. PRB 100, 115305 (2019). [3] B. Gayral et al. APL 72, 1421 (1998). [4] A. Rodriguez et al. arXiv:2209.12659 (2022).

HL 11: Quantum transport and quantum Hall effects I (joint session HL/TT)

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

HL 11.1 Mon 15:00 POT 251

Local Chern patches and networks of chiral modes in quantum Hall phases with spatial magnetic field profiles. — •Suraj Hegde and Tobias Meng — Institute of Theoretical Physics and Wurzburg-Dresden Cluster of Excellence ct.qmat, Technische Universitat Dresden, 01069 Dresden, Germany.

Transport experiments on curved Hall bars show a variety of non-trivial transport signatures. Motivated by these experiments, we develop a model that accounts for various features in multi-terminal Hall bar measurements and perform numerical simulations using KWANT. We model the effect of curvature of the sample through spatial variation of the magnetic field profile and find that it results in patches of quantum Hall phases characterised by different local Chern markers. We find that most of the transverse and longitudinal transport can be understood in terms of local Chern patches and an intricate interplay of chiral modes at the interface of different patches. We also show that the spatial magnetic field textures could provide a novel platform to engineer lattices formed by networks of chiral modes.

HL 11.2 Mon 15:15 POT 251

Effect of the external fields in high Chern number quantum anomalous Hall insulators — •Yuriko Baba[1,2], Francisco Domínguez-Adame[1], and Rafael A. Molina-Ferández[2] — [1]GISC, Departamento de Física de Materiales, Universidad Complutense, E–28040 Madrid, Spain — [2]Instituto de Estructura de la Materia, IEM-CSIC, E–28006 Madrid, Spain

Multilayer structures consisting of alternating magnetic and undoped topological insulator layers have been proved so far to be a convenient platform for creating a quantum Anomalous Hall state with a high Chern number [1]. However, in previous proposals, the Chern number can only be tuned by varying the doping concentration or the width of the magnetic topological insulator TI layers. This restricts the applications of the dissipationless chiral edge currents in electronics, since the number of conducting channels remains fixed. In this work, we propose a way of varying the Chern number at will by means of an external electric field applied along the stacking direction. The electric field generates the hybridization of the inverted bands, generating

new topological channels. In this way, the number of Chern states can be tuned externally in the sample, without the need of modifying the number and width of the layers or the doping level. We showed that this effect can be uncovered by the variation of the transverse conductance as a function of the electric field at constant injection energy at the Fermi level. [2]

[1] Zhao, Y. F. et al., Nature, 588 (2020) 419
[2] arXiv:2208.03585

HL 11.3 Mon 15:30 POT 251

Novel thermo-electric transport channel in the conformal limit of tilted Weyl semimetals — Thorvald Ballestad[1], Alberto Cortijo[2], Maria Vozmediano[3], and •Alireza Qaiumzadeh[1] — [1]Center for Quantum Spintronics, Norwegian University of Science and Technology, Trondheim, Norway — [2]Universidad Autonoma de Madrid, Madrid, Spain — [3]Instituto de Ciencia de Materiales de Madrid, CSIC, Madrid, Spain

Recently, a new contribution to the Nernst current was proposed in 3D Dirac and Weyl semimetals, originated from quantum conformal anomaly [1,2]. In the present study, we analyze the effect of the tilt on the transverse thermo-electric coefficient of Weyl semimetals in the conformal limit, i.e., zero temperature and zero chemical potential. Using the Kubo formalism, we find a non-monotonic behavior of the thermoelectric conductivity as a function of the tilt perpendicular to the magnetic field, and a linear behavior when the tilt is aligned to the magnetic field. An "axial Nernst" current is generated in inversion symmetric materials when the tilt vector has a projection in the direction of the magnetic field. This analysis will help in the design and interpretation of thermo-electric transport experiments in recently discovered topological quantum materials [3].

[1] M. N. Chernodub et al, Phys. Rev. Lett. 120, 206601 (2018). [2] V. Arjona et al, Phys. Rev. B 99, 235123 (2019). [3] T. M Ballestad, A. Cortijo, M. A. H. Vozmediano, A. Qaiumzadeh, arXiv:2209.14331 (2022).

HL 11.4 Mon 15:45 POT 251

Selective scattering between counter-propagating edge states in a topological insulator — •Meng Hao[1,2], Li-Xian Wang[1,2], Fabian Schmitt[1,2], Hartmut Buhmann[1,2], and Laurens W. Molenkamp[1,2] — [1]Institute for Topological Insulators, Würzburg, Germany — [2]Physikalisches Institut (EP III) Würzburg University, Würzburg, Germany

The quantum Hall state, known by its dissipationless nature, comprises chiral edge states in a two-dimensional electron gas (2DEG). In the ordinary quantum Hall effect, all edge states propagate in the same direction, populated equally. Thus, they are immune to inter-edge-state scattering. In contrast, counter-propagating edge states, populated unequally, are naturally sensitive to the scattering process. However, a realization of this scenario so far was only possible by stacked layers of high-mobility 2DEGs, e.g., quantum wells or graphene. Here we realize the counter-propagating edge states in a three-dimensional topological insulator controlled by top and bottom gates. Surprisingly, the counter-propagating edge states prove to scatter into each other selectively. Our first attempt shows that this inter-edge-state scattering occurs exclusively between Landau levels with the same Landau index. We further propose a cross bar equipped with split-gates to determine the selection rule of scattering and scattering parameters unambiguously. Following this proposal, we will show some preliminary results and report our experimental advances.

30 min. break

HL 11.5 Mon 16:30 POT 251

Edge modes, Hall conductivity and topological features of a dice lattice: Fate of flat bands under strain — •Sayan Mondal and Saurabh Basu — Indian Institute of Technology Guwahati

We study the topological properties of a dice lattice, which has three atoms per unit cell (A, B, and C). In addition, the bands are systematically deformed via the introduction of anisotropy among the nearest neighbour (NN) hoppings in two distinct ways. In the first case, we apply the uniaxial strain, which alters the NN hoppings (between the sublattices A-B and B-C) along the direction of applied strain. While in the second case, we selectively tune the NN hopping between A and B sublattices which may be achieved by a controlled chemical pressure. The first case yields the Chern insulating lobes in the phase diagram with $C = \pm 2$ till a certain critical anisotropy, where the spectral gap vanishes. The quantized plateau in the anomalous Hall conductivity and the pair of chiral edge modes at each edge of a ribbon support the obtained values of the Chern numbers. Whereas, the second case (selective strain) shows distorted flat band in the dispersion spectrum, which alters the gap-closing condition as compared to the case of uniaxial strain. Also, the Chern insulating lobes in the phase diagram and the Hall conductivity have distinct features compared to the case above. However, in both cases, topological phase transitions take place which is demonstrated via the Chern number changing discontinuously from ± 2 to zero across the gap-closing transitions.

HL 11.6 Mon 16:45 POT 251

Structure-imposed electronic topology in graphene nanoribbons — •Florian Arnold[1], Tsai-Jung Liu[1], Agnieszka Kuc[2], and Thomas Heine[1,2,3] — [1]Technische Universität Dresden, Dresden, Germany — [2]HZDR, Leipzig, Germany — [3]Yonsei University, Seoul, Republic of Korea

Zigzag graphene nanoribbons (ZGNR) can be transformed into new structure types by removing terminal carbon atoms in a regular pattern. When a single atom is removed on each zigzag edge so-called cove-edged ZGNR (ZGNR-C) are created, while removing multiple atoms results in gulf-edged ZGNR (ZGNR-G). In our seminal work, we demonstrated the direct structure-electronic structure relation based on the structural parameters that unambiguously characterize ZGNR-C. This allowed to create a scheme that classifies their electronic state, i.e., if they are metallic, topological insulators or trivial semiconductors, and to find an empirical formula for the band gap of the semiconducting ribbons. Since then, we were able to expand this description to ZGNR-G systems where the chemical space of possible structures increases further due to the variable size of the gulf edges. With this, we give guidance to realize new graphene nanoribbon heterojunctions hosting topological states and investigate the transport properties of exemplary systems.

HL 11.7 Mon 17:00 POT 251

Massive and topological surface states in strained HgTe and evidence for parity anomaly — •Wouter Beugeling[1,2], Lixian Wang[1,2], David M. Mahler[1,2], Valentin L. Müller[1,2], Ewelina M. Hankiewicz[3], Hartmut Buhmann[1,2], and Laurens W. Molenkamp[1,2] — [1]Institute for Topological Insulators, Würzburg, Germany — [2]Physikalisches Institut (EP III), Würzburg University, Würzburg, Germany — [3]Institute for Theoretical Physics and Astrophysics (TP IV), Würzburg University, Würzburg, Germany

The idea that band inversion in a narrow-gap material can lead to Dirac-type surface states was noted by Volkov and Pankratov in the 1980's. Only about two decades later, it was realized that the surface states of topological insulators are the gapless Dirac states predicted by them. The massive Volkov-Pankratov states received much less attention. They are pulled from the bulk in a sufficiently large electric field and are topologically trivial. Until recently, direct evidence in the form of transport measurements was elusive.

From our magneto-transport experiments on a three-dimensional topological insulator heterostructure (strained HgTe), we demonstrate the coexistence of massless and massive Volkov-Pankratov states. The well-developed Hall quantization in the n- and the p-type regime is due to the topological surface state and the massive Volkov-Pankratov states, respectively, as confirmed by k·p theory. In a second series of experiments, we find a remarkable re-entrant quantum Hall effect in the p-type regime, which we can trace to spectral asymmetry, a salient manifestation of parity anomaly in a solid-state system.

HL 12: Semiconductor lasers I

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

HL 12.1 Mon 15:00 POT 112

Adjustment of the active region on an InGaAsP VECSEL around 760nm for red pumping — •Rebecca Rühle, Marius Grossmann, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, Universität Stuttgart, Allmandring3, 70569 Stuttgart, Germany

The quantum defect between the emission and the pump wavelength of vertical external-cavity surface-emitting lasers (VECSEL) has a huge impact on the performance of the structure. Especially to improve the thermal behavior, a longer wavelength pump laser is favorable. For the InGaAsP quantum well (QW) VECSEL with an emission wavelength at around 760nm, a pump laser at 675nm is preferable to one at 532nm. But the QWs are embedded in GaInP-barriers, thus are transparent for the pump light and the pump efficiency is rather small. To overcome this the composition of the GaInP can be changed so that the barrier again can absorb the pump light. The effects of adjusting the barrier in the active region and the performance of the VECSELs have now been investigated in detail. Photoluminescence and laser output power measurements were performed to compare the behavior of the different structures. A further study was carried out to evaluate the effect of the different gallium to indium ratio in the crystal structure on the surface roughness of the device.

HL 12.2 Mon 15:15 POT 112

Cavity effects in hybrid resonators embedding InGaAs quantum dots — •Kartik Gaur, Sarthak Tripathi, Imad Limame, Ching-Wen Shih, Chirag Palekar, Sven Rodt, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, Germany

InGaAs quantum dots (QDs) embedded in microcavities based on highly reflective distributed Bragg reflectors (DBRs) allow for the development of high Q-factor, low mode volume micropillar cavities which feature high light-matter interaction. This makes them almost ideal candidates for quantum light sources and high-β microlasers. However, epitaxially grown GaAs/AlAs DBRs suffer from relatively low refractive index contrast, and often high absorption of the optical pumping laser. Here, we propose replacing the upper III-V DBR with dielectric DBR based on $\lambda/4$-thick layers of SiO_2 and Si_3N_4 deposited using plasma-enhanced chemical vapor deposition. Numerical simulations are carried out to optimize the fabrication parameters and subsequently validate the optical properties. The MOCVD-grown InGaAs QD active region is integrated in the central one-λ GaAs cavity on top of the bottom DBR with 33 $Al_{0.2}Ga_{0.8}As/Al_{0.9}Ga_{0.1}As$ mirror pairs, followed by electron beam lithography processing step to define photonic defects for lateral mode confinement. Such defects in the form of microlenses are created using a SiO_2 hard mask and wet chemical etching. We then deposit dielectric top DBR consisting of 15 $\lambda/4$-thick SiO_2 and Si_3N_4 mirror pairs. The final structure is investigated via low-temperature micro-photoluminescence.

HL 12.3 Mon 15:30 POT 112

Latest developments on membrane external-cavity surface-emitting lasers (MECSELs) — •Hermann Kahle[1,2], Patrik Rajala[2], Philipp Tatar-Mathes[2], and Mircea Guina[2] — [1]Institute for Photonic Quantum Systems (PhoQS), Department of Physics, Paderborn University, Warburger Straße 100, 33098 Paderborn, Germany — [2]Optoelectronics Research Centre (ORC), Physics Unit / Photonics, Tampere University, Korkeakoulunkatu 3, 33720 Tampere, Finland

MECSELs have experienced a rapid progress in recent years. Based on the membrane geometry of MECSELs, an intrinsically excellent beam quality is one important benefit of this new vertically emitting kind of lasers. The most important recent progress, like continuous wave broadband tuning ($\Delta\lambda_{FWHM} \approx 70\,nm$ around $\lambda_0 = 985\,nm$) and anti-resonant gain membrane design will be discussed.

HL 12.4 Mon 15:45 POT 112

Membrane saturable absorber mirror (MESAM) in a red-emitting VECSEL for the generation of stable ultrashort pulses — •Ana Ćutuk, Marius Grossmann, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, Universität Stuttgart, Allmandring 3, 70569 Stuttgart

Optically-pumped semiconductor disk lasers, also known as vertical external-cavity surface-emitting lasers (VECSELs), provide several advantageous properties like near-diffraction-limited beam profile and the flexibility to add optical components inside the laser cavity and thereby modify the laser characteristics. One example is the semiconductor saturable absorber mirror (SESAM), a monolithic semiconductor structure consisting of a saturable absorber region on top of a distributed Bragg reflector (DBR). However, the epitaxial growth of SESAMs can be limited by the DBR design, making it difficult to fabricate pulsed lasers with wavelengths within spectral gaps. We demonstrate a membrane saturable absorber mirror (MESAM) which overcomes the growth restrictions of the DBR. A membrane containing the active region only is combined with a dielectric mirror and thus simulates a SESAM with an increased flexibility in design. We compare the dynamic properties of a SESAM- and MESAM-mode-locked VECSEL. With both devices we obtain fundamental mode locking with pulse durations in the ps-range.

30 min. break

HL 12.5 Mon 16:30 POT 112

AlGaInP-based VECSELs with grating waveguide structures — •Peter Gierss[1], Ana Ćutuk[1], Maxim Leyzner[2], Uwe Brauch[2], Marwan Abdou Ahmed[2], Michael Jetter[1], Thomas Graf[2], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, Universität Stuttgart, Allmandring 3, 70569 Stuttgart — [2]Institut für Strahlwerkzeuge, Universität Stuttgart, Pfaffenwaldring 43, 70569 Stuttgart

Vertical external-cavity surface-emitting lasers (VECSELs) provide several superior properties like a near-diffraction beam profile and the flexibility to add optical components inside the cavity for further tailoring of the laser parameters. However, the heat generated by the pump laser within the active region proves to be a limiting factor for achieving higher output powers. This is mainly due to the poor thermal conductivity of the thick distributed Bragg reflector (DBR), which could be overcome by placing a heatspreader right next to the active region.

In this contribution, we present our recent progress in the development of an AlGaInP-VECSEL based on a grating waveguide structure (GWS). Excluding the DBR and adding a heatspreader instead improves the heat removal from the gain region while the guided-mode resonances from the GWS should provide good coupling of the pump and laser field and a high reflectivity to replace the function of the DBR. Our current research focuses on the fabrication and characterization of the high-contrast grating on top of a gain membrane.

HL 12.6 Mon 16:45 POT 112

Manipulating the emission characteristics of VCSEL in the red spectral range with polymer microlenses and etched surface reliefs — Farnaz Khamseh, •Lena Engel, Michael Zimmer, Sergej Vollmer, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technol- ogy (IQST) and SCoPE, Universität Stuttgart, Allmandring 3, 70569 Stuttgart

Vertical-cavity surface-emitting lasers (VCSELs) are promising candidates for various applications like sensing, printing and data transfer due to their low power consumption and the possibility of arranging them in arrays. Especially in the red spectral range around 660nm VCSEL are interesting for example in biomedical applications. However, their implementation is often hampered as light is emitted under an angle of divergence of 10° for single mode operation and higher order transverse modes are emitted especially for higher output power operation, further increasing the divergence and limiting the fiber coupling efficiency. Thus, the aim of this work is to improve the emission characteristics of red emitting VCSELs. Therefore, polymer microlenses for beam collimation are integrated directly on the VCSEL surface. Their ideal geometry and the tolerances for the alignment relative to the oxide aperture are thoroughly investigated utilizing ray-optics sim-

ulations. Additionally, etched surface reliefs are used to suppress the emission of higher order modes via a spatial modulation of the top mirror loss.

HL 12.7 Mon 17:00 POT 112

Multifold lasing threshold reduction of optically pumped micropillar lasers with low-absorbing $Al_{0.2}Ga_{0.8}As/Al_{0.9}Ga_{0.1}As$ distributed Bragg reflectors — •Ching-Wen Shih[1], Imad Limame[1], Chirag Palekar[1], Sebastian Krüger[1], Aris Koulas-Simos[1], Daniel Brunner[2], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Berlin, Germany — [2]Département d'Optique P. M. Duffieux, Institut FEMTO-ST, Université Bourgogne-Franche-Comté CNRS UMR 6174, Besançon, France

Micropillar photonic devices, where the active layers are in an optical cavity sandwiched between epitaxially grown dielectric Bragg mirrors (DBRs), are one of the fundamental elements to study cavity quantum electrodynamics and to enable devices for quantum technology applications. Here, we report on the experimental realization of multifold lasing threshold reduction of optically pumped micropillar lasers by simply replacing the commonly used $GaAs/Al_{0.9}Ga_{0.1}As$ DBRs with low-absorbing $Al_{0.2}Ga_{0.8}As/Al_{0.9}Ga_{0.1}As$ DBRs, which minimizes the DBRs absorption of the optical pump power. In pump-wavelength-dependent I/O measurements, we demonstrate that the incorporation of 20% Al content in the DBRs opens an optical pumping window from the absorption edge of $Al_{0.2}Ga_{0.8}As$ at 700 nm to the one of GaAs at 820 nm, where the excitation laser light can effectively reach the GaAs cavity above its bandgap while remaining transparent to the DBRs, resulting in high power conversion efficiency, low lasing threshold, and high thermal stability.

HL 13: Focus Session: Frontiers of Electronic-Structure Theory II (joint session O/HL)

Time: Monday 15:00–17:15 Location: TRE Ma

Topical Talk HL 13.1 Mon 15:00 TRE Ma

Coupled-cluster theory for complex solids made ready — •Andreas Grüneis — TU Wien, Institute for Theoretical Physics, Wiedner Hauptstraße 8-10/136, 1040 Vienna, Austria

This talk will review recent progress in applying periodic coupled-cluster theory, which has the potential to achieve a systematically improvable level of accuracy, to solids and surfaces. We will discuss novel techniques that reduce the computational cost by accelerating the convergence of calculated properties towards the complete basis set as well as the thermodynamic limit. The newly developed techniques have been implemented in the free and open source simulation software Cc4s that is interfaced to a growing number of widely-used electronic structure theory codes. These developments have enabled an increasing number of ab initio studies and allowed for assessing the level of accuracy of coupled-cluster theory by comparing to experimental findings as well as quantum Monte Carlo results. The presented applications will cover a wide range of materials science problems including the study of phase diagrams, molecule-surface interactions and properties of defects.

HL 13.2 Mon 15:30 TRE Ma

Speedup of structural optimisations using hybrid functionals: Case studies for energy materials — •Daniel Fritsch — Weierstrass Institute for Applied Analysis and Stochastics, Mohrenstr. 39, 10117 Berlin, Germany — Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, Berlin, 14109, Germany

First-principles calculations based on density functional theory have been established as de facto standard for computational materials investigations. Depending on the size of the unit cell, for every material of interest a suitable choice for the unknown exchange and correlation functional has to be made; taking not only into account the desired accuracy, but also the available computational resources.

In recent years, a promising combination of two approaches emerged, starting from a structural relaxation based on a simpler (semi)local functional, supplemented by a single shot hybrid functional calculation. Here, we propose a new method for combining different levels of exchange and correlation functional for structural relaxations.

In a first benchmarking step, this new method will be applied to various sets of promising energy materials, where full hybrid functional calculations are available, with a main focus on the performance of this new approach on the structural properties and the required computational resources. In a second step, this new approach will be applied to materials, which up-to-now have not been accessible to hybrid functional calculations due to the required computational resources. All the presented results on the structural, electronic, and optical properties will be critically discussed alongside experimental findings.

HL 13.3 Mon 15:45 TRE Ma

All-Electron Large-Scale Hybrid Density Functional Simulations — Florian Merz[1], Andreas Marek[2], •Sebastian Kokott[3], Christian Carbogno[3], Yi Yao[3], Mariana Rossi[4], Markus Rampp[2], Matthias Scheffler[3], and Volker Blum[5] — [1]Lenovo HPC Innovation Center, Stuttgart — [2]Max Planck Computing and Data Facility, Garching — [3]The NOMAD Laboratory at the FHI-MPG and IRIS-Adlershof HU, Berlin — [4]MPI for the Structure and Dynamics of Matter, Hamburg — [5]Duke University, North Carolina, USA

The localized resolution-of-identity approach [1] enables $O(N)$ hybrid density functional simulations and, thus, the computation of accurate electronic properties of large scale atomistic models in the range of ten thousands of atoms in *FHI-aims* [2]. In this range, parallelization and memory requirements of the exact exchange part, and the evaluation of the Hartree potential remain challenging. The solution of the generalized eigenvalue problem with direct eigensolvers like ELPA [3] naturally becomes a bottleneck due to $O(N^3)$ scaling. In this work, we present recent algorithmic advances for the exact exchange part and the evaluation of the Hartree potential, as well as optimizations of the ELPA library. We systematically perform benchmark tests on CPU and GPU-accelerated architectures covering inorganic solids, large molecules, and organic crystals with up to 50,000 atoms.

[1] Ihrig *et al.*, *New J. Phys.* **17**, (2015).
[2] Levchenko *et al.*, *Comp. Phys. Commun.* **192**, (2015).
[3] Marek *et al.*, *J. Phys. Condens. Matter* **26**, (2014).

15 min. break

HL 13.4 Mon 16:15 TRE Ma

A Koopman's compliant exchange correlation potential for semiconductors — •Michael Lorke[1], Peter Deak[2], and Thomas Frauenheim[2] — [1]Institute for Theoretical Physics, University of Bremen, Otto-Hahn-Allee 1, Bremen, 28359, Germany — [2]BCCMS, University of Bremen, Germany

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. We propose a novel exchange correlation potential[1] for semiconductor materials, that is based on physical properties of the underlying microscopic screening. We demonstrate that it reprocuduces the low temperature band gap of several materials. Moreover it respects the required linearity condition of the total energy with the fractional occupation number, as expressed by the generalized Koopman*s theorem. We also show that this novel functional can be used as a kernel in linear response TDDFT to reproduce excitonic effects in optical spectra [1] Physical Review B 102 (23), 235168 (2020)

HL 13.5 Mon 16:30 TRE Ma

Accurate and efficient treatment of spin-orbit coupling via second variation employing local orbital basis functions — •Hannah Kleine[1], Andris Gulans[2], Sven Lubeck[1], Cecilia Vona[1], and Claudia Draxl[1] — [1]Institut für Physik and IRIS Adler-

shof, Humboldt-Universität zu Berlin — [2]Department of Physics, University of Latvia

Spin-orbit-coupling (SOC) effects can significantly change the properties of materials containing heavy elements, mostly by introducing shifts and splittings in the band structure. Including SOC effects in density-functional-theory (DFT) calculations can be challenging. In the linearized augmented planewaves plus local orbitals (LAPW+LO) method, SOC is treated as a perturbation and solved by a second variational (SV) scheme where eigenvectors of the scalar-relativistic Kohn-Sham Hamiltonian are used as basis functions for the SO-coupled problem. For certain materials, especially those with strong SOC effects, many SV basis functions are required which leads to high computational costs. By adding LOs to the SV basis, we are able to drastically reduce the basis-set size and thus the computational cost. We implement this approach in the all-electron full-potential computer package exciting [1] and combine it with the use of relativistic LOs to achieve high accuracy results for a variety of different materials.

[1] A. Gulans et al., J. Phys. Condens. Matter 26, 363202 (2014).

HL 13.6 Mon 16:45 TRE Ma

Exact sum-rule approach to polarizability and asymptotic van der Waals functionals – derivation of exact benchmarks — •Alberto Ambrosetti[1], John Dobson[2], Matteo Ricci[1], and Pier Luigi Silvestrelli[1] — [1]Dipartimento di Fisica e Astronomia, Università degli Studi di Padova, via Marzolo 8, 35131, Padova, Italy — [2]Nanoscale Science and Technology Centre, Griffith University, Nathan, Queensland 4111, Australia

Using a sum-rule approach we develop an exact theoretical framework for polarizability and asymptotic van der Waals correlation energy functionals of isolated objects[1]. The functionals require only monomer groundstate properties as input. Functional evaluation proceeds via solution of a single position-space differential equation, without the usual summations over excited states or frequency integrations. Explicit functional forms are reported for reference physical systems, including atomic hydrogen and single electrons subject to harmonic confinement, and immersed in a spherical-well potential. Direct comparison with the popular Vydrov-van Voorhis density functional shows that this performs best when density decay occurs at atomic scales. The adopted sum-rule approach implies general validity of our theory, enabling exact benchmarking of van der Waals density functionals, and direct inspection of the subtle long-range correlation effects that constitute a major challenge for approximate (semi-)local density functionals.

[1] M Ricci, PL Silvestrelli, JF Dobson, A Ambrosetti J. Phys. Chem. Lett. 13, 8298-8304

HL 13.7 Mon 17:00 TRE Ma

Interacting electrons and bosons in the doubly screened $G\widetilde{W}$ approximation — •Yaroslav Pavlyukh — Department of Theoretical Physics, Wroclaw University of Science and Technology

In Ref. [1] we built on the Generalized Kadanoff-Baym Ansatz for electrons and bosons to map a broad class of nonequilibrium Green's function theories onto a coupled system of ordinary differential equations with linear time-scaling. Available methods to treat *e*-*e* correlations include GW [2], T-matrix and Faddeev, while *e*-*b* correlations are described by Ehrenfest and second-order diagrams in the *e*-*b* coupling [3].

In this work we present a substantial advance in the treatment of correlations, requiring no extra computational cost and preserving all conserving properties. Specifically, we include the effects of dynamical screening due to *both* *e*-*e* and *e*-*b* interactions ($G\widetilde{W}$ approximation). The $G\widetilde{W}$ extension opens the door to a wealth of phenomena ranging from carrier relaxation and exciton recombination to molecular charge migration and transfer in optical or plasmonic cavities.

[1] Y. Pavlyukh, E. Perfetto, D. Karlsson, R. van Leeuwen, and G. Stefanucci, Phys. Rev. B **105**, 125134 (2022).

[2] E. Perfetto, Y. Pavlyukh, and G. Stefanucci, Phys. Rev. Lett. **128**, 016801 (2022).

[3] D. Karlsson, R. van Leeuwen, Y. Pavlyukh, E. Perfetto, and G. Stefanucci, Phys. Rev. Lett. **127**, 036402 (2021).

HL 14: 2D Materials III (joint session HL/CPP)

Time: Tuesday 9:30–12:15 Location: POT 81

HL 14.1 Tue 9:30 POT 81

Sub-THz detection in two dimensional systems and CVD graphene heterostructures — Franziska Linss[1], Vincent Strenzke[1], Pai Zhao[1], Chithra S. Sharma[1], Lars Tiemann[1], •Qin Hua[2], and Robert H. Blick[1] — [1]Center for Hybrid Nanostructures, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany — [2]Suzhou Institute of Nanotech and Nanobionics (SINANO) of the Chinese Academy of Sciences (CAS), China

Electromagnetic radiation in the THz range can induce surface plasmons, i.e., a collective motion of electrons, in graphene-based devices. We fabricated a field-effect-transistor with asymmetric dual-grating gates (ADGG) to detect sub-THz radiation using large-scale graphene that was synthesized by chemical vapor deposition (CVD). The CVD graphene sheet is encapsulated between two flakes of hBN and placed on a highly doped Si wafer that acts as a back gate. The ADGG was structured on the top hBN flake. The control of the carrier concentration via electrostatic gates is crucial to match the resonance condition of the plasmons. The sample was characterized by sweeping the top gate voltage from -1 V to 2 V and the charge neutrality point was reached at a top gate voltage of 0.87 V at 4.2 Kelvin. Furthermore, we used a high electron mobility transistor (HEMT) to detect THz radiation, where the detection mechanism is based on a mixing with a reference radiation in a nonlinear medium. In this device, we can demonstrate sub-THz radiation at room temperature.

HL 14.2 Tue 9:45 POT 81

Theory of non-local Andreev reflection through Andreev molecular states in graphene Josephson junctions — •Andor Kormányos[1], Eduárd Zsurka[1], Noel Plaszkó[1], and Péter Rakyta[1,2] — [1]Department of Physics of Complex Systems, Eotvos Lorand University, Budapest, Hungary — [2]Wigner Research Center for Physics, 29-33 Konkoly-Thege Miklos Str., H-1121 Budapest, Hungary

We propose that a device composed of two vertically stacked monolayer graphene Josephson junctions can be used for Cooper pair splitting. The hybridization of the Andreev bound states of the two Josephson junction can facilitate non-local transport in this normal-superconductor hybrid structure, which we study by calculating the non-local differential conductance. Assuming that one of the graphene layers is electron and the other is hole doped, we find that the non-local Andreev reflection can dominate the differential conductance of the system. Our setup does not require the precise control of junction length, doping, or superconducting phase difference, which could be an important advantage for experimental realization.

HL 14.3 Tue 10:00 POT 81

Quantum Hall measurements near electric field controlled Lifshitz transitions in trigonally warped bilayer graphene — •Martin Statz, Anna Seiler, Jonas Pöhls, Moritz Knaak, Francesca Farlorsi, and Thomas Weitz — 1st Physical Institute, Faculty of Physics, University of Göttingen, Friedrich-Hund-Platz 1, Göttingen 37077, Germany

Various spontaneous symmetry broken phases such as Stoner ferromagnetism, spin-polarized superconductivity, a quantum anomalous Hall octet and a topologically non-trivial Wigner-Hall crystal phase have recently been reported in bilayer graphene (BLG) [1]. Since these interaction-driven phenomena are dictated by the ratio of the Coulomb and kinetic energy of carriers, they can be promoted by the formation of flat bands and a divergent density of states (DoS) near Lifshitz transitions (LT). Trigonally warped BLG at low vertical displacement fields (D-field) and carrier densities ($\sim 10^{11}$ cm^{-2}) displays one centre and three off-centre Dirac cones in each valley, and therefore offers a rich playground for correlated phases (CP) and changes in the Fermi surface topology by inducing charge density and D-field driven LT. Here, we report on quantum Hall measurements near charge density and D-field driven LT in trigonally warped BLG encapsulated in hexagonal boron-nitride in a dual-gated architecture with graphite contacts and graphite gates at 10 mK. We further outline our status

on the temperature dependence of several CP in the aforementioned regimes.

[1] Seiler, A.M. et al. Nature 608, 298-302 (2022)

HL 14.4 Tue 10:15 POT 81

Tuning electronic properties of graphene with a transferred ultrathin Ga_2O_3 encapsulation — Matthew Gebert[1], •Semonti Bhattacharyya[2], Christopher Bounds[1], Nitu Syed[3,4], Torben Daeneke[4], and Michael S. Fuhrer[1] — [1]School of Physics and Astronomy, Monash University, Melbourne — [2]Leiden Institute of Physics, Leiden University, Leiden — [3]School of Physics, The University of Melbourne, Parkville, Melbourne — [4]School of Engineering, RMIT University, Melbourne

Although graphene holds immense potential for future electronics and spintronics, it is tricky to find a suitable large-area encapsulation layer for graphene that enhances its properties. In this talk, I will demonstrate a large-area passivation layer for graphene by mechanical transfer of ultrathin Ga_2O_3 synthesized on the surface of liquid Ga metal.[1]

Electrical measurements of millimetre-scale passivated and bare CVD graphene on SiO_2 substrate indicate that the passivated graphene maintains its high field effect mobility, desirable for applications. Surprisingly, the temperature-dependent resistivity is reduced in our passivated graphene over a range of temperatures below 230 K, due to the interplay of screening of the remote optical phonon modes of the SiO_2 by the high dielectric constant of Ga_2O_3, and the relatively high characteristic phonon frequencies of Ga_2O_3. Raman spectroscopy and electrical measurements indicate that Ga_2O_3 passivation also protects graphene from further processing such as plasma-enhanced atomic layer deposition of Al_2O_3.

1. Gebert, Bhattacharyya et al, Nano Lett, https://doi.org/10.1021/acs.nanolett.2c03492

HL 14.5 Tue 10:30 POT 81

Hopping transport in ultraclean dual graphite gated bilayer graphene — •David Alexander Darek Emmerich[1], Eike Thomas Icking[1,2], Philipp Schmidt[1,2], Frank Volmer[1,3], Kenji Watanabe[4], Takashi Taniguchi[5], Bernd Beschoten[1], and Christoph Stampfer[1,2] — [1]RWTH Aachen University, Germany — [2]Forschungszentrum Jülich, Germany — [3]AMO GmbH, Advanced Microelectronic Center Aachen (AMICA), Germany — [4]Research Center for Functional Material, Japan — [5]International Center for Materials Nanoarchitectonics, Japan

Bernal-stacked bilayer graphene (BLG) is a material that has a unique property: BLG is intrinsically a semimetal, but becomes a semiconductor under the applicaton of an out-of-plane displacement field. This controlled opening of a gate-tunable band gap makes it a promising material for realizing highly-tunable transistors and photodetectors. The limiting factor of BLG-based devices is disorder. Only by using graphitic bottom gates a true band insulating state was achieved in BLG, which exhibits a clean gap opening with faint signs of residual disorder. Using finite bias spectroscopy, we show that BLG devices with graphitic top and bottom gate electrodes exhibit extremely low disorder. We perform transport measurements down to the sub-Kelvin regime and analyse the temperature-dependent transport behaviour. For small displacement fields, where gap and disorder are expected to be of the same order of magnitude, the low-temperature hopping transport data are investigated concerning the dominant hopping mechanism.

15 min. break

HL 14.6 Tue 11:00 POT 81

high responsivity monolayer MoS_2 photodetectors on cyclic olefin copolymer-passivated SiO_2 gate dielectric — •Emad Najafidehaghani[1], Sirri Batuhan Kalkan[2], Ziyang Gan[1], Jan Drewniok[2], Michael F Lichtenegger[2], Uwe Hübner[3], Alexander S Urban[2], Antony George[1], Bert Nickel[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, Jena — [2]Ludwig Maximilian University of Munich, Faculty of Physics, Munich — [3]Leibniz Institute of Photonic Technology (IPHT), Jena

2D material-based photodetectors attracted significant research interest due to their high responsivity, flexibility and transparency. However, the trap states present at the surface of SiO_2 gate dielectrics diminishes the performance of 2D material-based photodetectors. To reduce the detrimental effect of SiO_2 surface traps, an ultrathin film (5 nm) of cyclic olefin copolymer (COC) layer is employed as a surface passivator. Due to the reduction of the interface trap density, the photoresponsivity of the MoS_2 devices on passivated SiO_2 is enhanced by four orders of magnitude compared to non-passivated MoS_2 devices. Under optimized conditions a record photoresponsivity of 3×10^7 A/W in combination with a short response time is observed. Our findings show that the ultrathin COC passivation of the gate dielectric enables to probe exciting properties of the atomically thin 2D semiconductors.

HL 14.7 Tue 11:15 POT 81

Atomic layer deposition of horizontal and vertical MoS_2/WS_2 heterostructures — •Christian Tessarek, Tim Grieb, Andreas Rosenauer, and Martin Eickhoff — Institut für Festkörperphysik, Universität Bremen

Beyond the properties of single two-dimensional (2D) layers, heterostructures made of 2D transition metal dichalcogenides promise new properties based on moiré physics and interlayer excitons.

Vertical and horizontal MoS_2 and WS_2 heterostructures were grown by atomic layer deposition (ALD) and analyzed by Raman and photoluminescence spectroscopy. The influence of the the ALD growth sequence, i.e. MoS_2/WS_2 vs. WS_2/MoS_2, was investigated. Elemental distribution of Mo and W in a horizontal heterostructure was studied by high resolution transmission electron microscopy and energy-dispersive X-ray spectroscopy. Additional high temperature annealing was performed to improve the structural and optical properties of the layers.

HL 14.8 Tue 11:30 POT 81

Fully automated platform for 2D material flake detection using real-time machine learning techniques — •Jan-Lucas Uslu, Timo Ouaj, Bernd Beschoten, Lutz Waldecker, and Christoph Stampfer — JARA-FIT and 2nd Institute of Physics A, RWTH Aachen University, Aachen, Germany

As of today, most of fundamental experimental 2D material research is based on mechanically exfoliated flakes, finding suitable flakes for the fabrication of van der Waal heterostructures is time-consuming and time-critical part requiring expert knowledge and manpower.

In order to mitigate this problem, we demonstrate a simple and robust real time-capable algorithm based on Gaussian mixture models, a machine learning technique, to allow for a fast automated search of exfoliated flakes of different 2D materials in a single run with an automated microscope setup to analyze batches of exfoliated material.

The algorithm solves the task of automatically detecting various flakes on Si++/SiO2 wafer dices, allows to index the location and segmentation of each flake and provides metrices such as size, thickness and shape.

The algorithm is evaluated on more than 500.000 images of different 2D materials including graphene and multilayer graphene, hexagonal boron nitride, transition metal dichalcogenides and 2D magnets.

HL 14.9 Tue 11:45 POT 81

CVD Growth of Hexagonal Boron Nitride on CMOS-compatible Substrates — •Max Franck[1], Jarek Dabrowski[1], Markus Andreas Schubert[1], Walter Batista Pessoa[2], Dominique Vignaud[2], Luc Henrard[3], Christian Wenger[1,4], and Mindaugas Lukosius[1] — [1]IHP - Leibniz-Institut für innovative Mikroelektronik, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]University Lille, CNRS, Centrale Lille, JUNIA ISEN, University Polytechnique Hauts de France, UMR 8520-IEMN F-59000 Lille, France — [3]Department of Physics, Namur Institute of Structured Materials, University of Namur, Rue de Bruxelles 61, 5000 Namur, Belgium — [4]Semiconductor Materials, BTU Cottbus-Senftenberg, Platz der Deutschen Einheit 1, 03046 Cottbus, Germany

Hexagonal boron nitride (hBN) is a two-dimensional insulator with a range of promising applications, including DUV optoelectronics and protection layers for high-mobility graphene. Most commonly, high-quality hBN is grown via CVD on catalytic transistion metal substrates. However, the hBN films require transfer to CMOS-compatible substrates, which leaves residual metal contaminations at concentrations unacceptable for Si technology integration.[1] Therefore, growth of hBN thin films directly on CMOS-compatible substrates, such as Si, Ge or dielectrics, is desirable. We present recent results regarding CVD synthesis of well-oriented, few-layer hBN films on such substrates using borazine as a single-source precursor. Morphology and crystallline quality were characterized using XPS, AFM, Raman spectroscopy and TEM. [1] G. Lupina, J. Kitzmann, et al. ACS Nano 2015, 9, 4776-4785.

HL 14.10 Tue 12:00 POT 81

Microwave plasma driven 2H-1T phase modulation of WSe2 for improving NO2 gas sensing performance — •Yu Duan[1,2], Sam Zhang[2], Huaping Zhao[1], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Center for Advanced Thin Films and Devices, School of Materials and Energy, Southwest University, Chongqing, 400715, China

Transition metal dichalcogenides (TMDs) have been widely used in recent years for gas sensors. Herein, we constructed a simple microwave plasma device by modifying a home microwave oven for surface treatment of WSe2. A 1T/2H hybrid phase structure was constructed by phase modulation and Se vacancies were introduced to effectively enhance its gas sensing performance. The sample after 60 s of treatment exhibited high response (52.24%), fast response rate (49.8 s), short recovery time (14.9 mins), and outstanding stability and selectivity for 1 ppm NO2 at room temperature. In addition, molecular model of the microwave plasma-treated sample is proposed, leading to the intrinsic mechanism of its performance enhancement. It is demonstrated that microwave plasma treatment is a promising method to enhance the gas sensing performance of TMDs.

HL 15: Spin phenomena in semiconductors

Time: Tuesday 9:30–10:30 Location: POT 361

HL 15.1 Tue 9:30 POT 361

Photoexcited charge carrier and spin dynamics in methylammonium lead bromide doped by magnetic transition metals. — •Stanislav Bodnar, Jonathan Zerhoch, Shangpu Liu, Andrii Shcherbakov, and Felix Deschler — PCI, Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg

One of the most challenging tasks for LED applications is emitting 100% polarized light from the device. Typically, this is achieved by introducing an additional layer of polarization filter which leads to losing half of the light intensity. To overcome this issue, one has to find a system with a high degree of photoluminescence (PL) polarization. A promising approach here is using magnetic metal doping in combination with a highly efficient semiconductor. We have chosen to use transient absorption (TA) spectroscopy at cryogenic temperatures to investigate changes in the optical properties induced by magnetic metal doping in CH3NH3PbBr3 since it gives spectral information about the energies of electronic states and dynamic properties of the photoexcited carriers. We find a change in the main ground state bleach (GSB) peak position in doped CH3NH3PbBr3, which depends on the transition metal used. The main GSB peak of pure CH3NH3PbBr3 at 4 K is at 2.32 eV. Doping CH3NH3PbBr3 with Mn leads to a shift of the main peak to lower energies by 0.04 eV. The modifications of the TA spectra are associated with changes in the bandgap energy, which is the result of doping-induced lattice expansion. Additionally, we observed changes in the spin lifetime by an order of magnitude which could be associated with modification of the Rashba field.

HL 15.2 Tue 9:45 POT 361

Mode locking of hole spin coherences in CsPb(Cl,Br)$_3$ perovskite nanocrystals — •Erik Kirstein[1], Nataliia E. Kopteva[1], Dmitri R. Yakovlev[1,2,3], Evgeny A. Zhukov[1,2], Elena V. Kolobkova[4,5], Maria S. Kuznetsova[6], Vasily V. Belykh[3], Irina A. Yugova[6], Mikhail M. Glazov[2], Manfred Bayer[1], and Alex Greilich[1] — [1]Experimental Physics 2, Department of Physics, TU Dortmund, 44227 Dortmund, Germany — [2]St. Petersburg, Russia — [3]Moscow, Russia — [4]St. Petersburg, Russia — [5]St. Petersburg, Russia — [6]St. Petersburg, Russia

The spin physics of perovskite nanocrystals is attracting increasing attention, both for fundamental studies and spintronic applications. Here, stable CsPb($Cl_{0.5}Br_{0.5}$)$_3$ lead halide perovskite nanocrystals embedded in a fluorophosphate glass matrix are studied by time-resolved optical spectroscopy to unravel the coherent spin dynamics of holes and their interaction with nuclear spins of the ^{207}Pb isotope. We demonstrate the spin mode locking effect and nuclear induced frequency focussing leading to the synchronization of the hole spin Larmor precession frequencies of the nanocrystal ensemble.

HL 15.3 Tue 10:00 POT 361

Spin-flip Raman scattering on resident electrons and holes in two-dimensional (PEA)2PbI4 perovskites — •Carolin Harkort[1], Dennis Kudlacik[1], Natalia E. Kopteva[1], Dmitri R. Yakovlev[1], Marek Karzel[1], Erik Kirstein[1], Oleh Hordiichuk[2,3], Maksym V. Kovalenko[2,3], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44221 Dortmund — [2]Laboratory of Inorganic Chemistry, Department of Chemistry and Applied Biosciences, ETH Zürich, CH-8093 Zürich, Switzerland — [3]Laboratory for Thin Films and Photovoltaics, Empa-Swiss Federal Laboratories for Materials Science and Technology, CH-8600 Dübendorf, Switzerland

Two-dimensional lead halide perovskites are promising material systems for photovoltaic and optoelectronic applications. They are attractive for optical control of carrier spins due to an increased chemical stability compared to bulk lead halide perovskites. With the technique of Spin-flip Raman scattering we investigated in 2D Ruddlesden-Popper type $(PEA)_2PbI_4$ perovskites the Zeeman splitting of carrier spins, resident electrons and holes, that can be detected through the exciton emission. The Landé-factors of these electrons and holes and their anisotropy are measured at a low temperature of 2 K. We show that the hole Zeeman splitting is affected by the Overhauser field resulting from the dynamic nuclear polarization which allows us to define the sign of the hole Landé-factor. In this structure the Overhauser field has a maximum value of 600 mT.

HL 15.4 Tue 10:15 POT 361

Microscopic origin of the effective spin-spin interaction in a semiconductor quantum dot ensemble — Fredrik Vonhoff[1,2], Andreas Fischer[1], •Kira Deltenre[1], and Frithjof B. Anders[1] — [1]Department of Physics, TU Dortmund University, D-44227 Dortmund — [2]Department of Physics, Technical University of Munich, D-85748 Garching

We present a microscopic model for a singly charged quantum dot (QD) ensemble to reveal the origin of the long-range effective interaction between the electron spins in the QDs. Wilson's numerical renormalization group (NRG) is used to calculate the magnitude and the spatial dependency of the RKKY interaction mediated by the growth-induced wetting layer.

Using the NRG results obtained from realistic parameters as input for a semiclassical simulation for a large QD ensemble, we demonstrate that the experimentally reported phase shifts in the coherent spin dynamics between single and two-color laser pumping can be reproduced by our model [1], solving a longstanding open problem of the microscopic origin of the inter-QD electron spin-spin interaction.

[1] F. Vonhoff, A. Fischer, K. Deltenre, and F. B. Anders, Phys. Rev. Lett. **129**, 167701 (2022)

HL 16: Quantum dots: Transport (joint session HL/TT)

Time: Tuesday 9:30–12:15 Location: POT 151

HL 16.1 Tue 9:30 POT 151

Contact formation analysis of nickel to SiGeOI to form Nickel-Germano-silicide using Flash lamp annealing — •Muhammad Moazzam Khan[1], Slawomir Prucnal[1], and Yordan M. Georgiev[1,2] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, D-01328 Dresden, Germany — [2]Institute of Electronics at the Bulgarian Academy of Sciences, 72, Tzarigradsko chaussee blvd, 1784-Sofia, Bulgaria

In CMOS technology, parasitic source/drain (S/D) resistance becomes more crucial in determining the overall device performance as the device dimensions get smaller. The contact resistance dominates this parasitic S/D resistance to a great extent, which limits the drive current. In order to have minimal impact on electrical performance, the contact should have linear Current-Voltage characteristics and negligible resistance in comparison to the device resistance. When replacing silicon with silicon-germanium as a channel material in future devices, it is necessary to investigate the contact formation mechanism in order to develop suitable contacts for energy-efficient devices. In this work, we are investigating metal semiconductor contact formation on SiGeOI using flash lamp annealing and studying their properties using structural and electrical characterization.

HL 16.2 Tue 9:45 POT 151

Predicting charge density maps in 2D nanostructures with machine learning techniques — •Amanda Teodora Preda[1,2,3], Calin Andrei Pantis-Simut[1,2,3], Nicolae Filipoiu[2,3], Lucian Ion[2], Andrei Manolescu[4], and George Alexandru Nemnes[1,2,3] — [1]Research Institute of the University of Bucharest (ICUB), Sos. Panduri 90, Bucharest, Romania — [2]University of Bucharest, Faculty of Physics, 077125 Magurele-Ilfov, Romania — [3]Horia Hulubei National Institute for Physics and Nuclear Engineering, 077126 Magurele-Ilfov, Romania — [4]Department of Engineering, Reykjavik University, Menntavegur 1, IS-102 Reykjavik, Iceland

Machine learning (ML) models have the potential to significantly improve and assist the design process of nanodevices that require precise control of the quantum states.

For 2D nanoelectronic structures, charge and spin densities are relevant observables and are also suited for ML techniques which employ image processing. The model systems that we considered are two dimensional quantum dots with multiple electrons and random confinement potentials. With convolutional neural networks, we built a ML model to predict whether a configuration displays singlet-triplet transitions in the ground state. For image translation problems, we used models based on conditional generative adversarial networks in order to predict the charge density distribution for arbitrary interacting systems taking as input either the non-interacting cases or just the shape of the confining potential.

HL 16.3 Tue 10:00 POT 151

Mesoscopic transport properties of individually prepared GaN-nanowire field-effect transistors — •Hannes Hergert[1,2], Matthias T. Elm[1,2,3], and Peter J. Klar[1] — [1]Institute of Experimental Physics I, Giessen, Germany — [2]Center for Materials Research, Giessen, Germany — [3]Institute of Physical Chemistry, Giessen, Germany

In order to keep the optimization of transistors within Moore's law new material systems as well as new transistor concepts such as GaN-nanowire field effect transistors (NW-FET) are needed. In this work we characterize the electrical transport properties of single NW-FET. Furthermore, we are able to obtain a deeper understanding of the mesoscopic transport processes. Unintentionally doped GaN-nanowires were fabricated using molecular-beam-epitaxy and device fabrication was performed by a combination of different lithographic methods and atomic layer deposition. After an annealing process the nanowire's resistance shows an ohmic behaviour. Electrical transport measurements were performed between 2 and 280 K. The investigated NW-FET exhibits a transfer characteristic identical to those of classical field-effect transistors. We show that the electrical transport is dominated by two transport processes: a transport within a metal-like impurity band at low temperatures and a hopping process at higher temperatures. Furthermore we were able to identify universal conductance fluctuations at temperatures below 140 K, which arise from the shift of the Fermi level when applying a topgate voltage.

HL 16.4 Tue 10:15 POT 151

Multi-Channel Kondo Effect in Few-Electron Quantum Dots — •Olfa Dani[1], Johannes C. Bayer[1], Timo Wagner[1], Gertrud Zwicknagl[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Germany — [2]Institut für Mathematische Physik, Technische Universität Braunschweig, Germany

The Kondo effect is a many particle entangled system, that involves the interaction between a localized spin in the quantum dot and free electrons in the electron reservoirs. This entanglement can be calculated using simplifying assumptions concerning the electronic structure of the quantum dot.

In this work we investigate a quantum dot device formed electrostatically in a two-dimensional electron gas using top-gates. A quantum point contact is used as a sensitive charge detector to detect single-electrons tunneling through the system. This enables us to know the exact number of electrons in the quantum dot (Ne). By changing the applied gate voltage, we are able to control Ne.

A Zero-bias anomaly is observed for a strong coupling to the leads and possible symmetrical tunnel barriers. This Kondo resonance appears for successive Ne showing a deviation from the conjectured odd-even behavior. The Kondo resonance is strongest for Ne=9 and displays a particle-hole symmetry for Ne =7,..,11. It is absent for Ne =6 and Ne = 12. These observations indicate the influence of the shell structure [1] of the electronic states in the quantum dot where orbital degeneracy is present.

[1] L. P. Kouwenhoven, et. al., Rep. Prog. Phys. 64, 701-736 (2001).

HL 16.5 Tue 10:30 POT 151

Highly Conductive Silicon Nanowires by Modulation-Doping via Aluminum-Induced Acceptor States in an SiO2-shell — •Daniel Hiller[1], Ingmar Ratschinski[1], Soundarya Nagarajan[2], Jens Trommer[2], Thomas Mikolajick[2,3], and Dirk König[4] — [1]Institute of Applied Physics, TU Bergakademie Freiberg, Germany — [2]Nanoelectronic Materials Laboratory gGmbH, Dresden, Germany — [3]Institute of Semiconductors and Microsystems, TU Dresden, Germany — [4]Integrated Materials Design Lab, ANU, Canberra, Australia

Silicon nanowires (Si NWs) enable maximum gate control over the source-drain current when configured in a gate-all-around FET-architecture. However, Si NWs with few nm in diameter suffer from severe difficulties with efficient impurity doping due to a multitude of physical and technological problems (diffusion, dielectric and quantum confinement, statistics of small numbers, etc.). Here, we present a novel doping concept for Si NWs comparable to the modulation doping approach of III-V semiconductors. Based on results from density functional theory (DFT) calculations, we use Al-doped SiO2 shells around the Si NWs, which contain unoccupied Al-induced acceptor states that are energetically located below the Si valence band edge. These states can capture electrons from the Si, creating free holes as majority charge carriers [1-5]. In this presentation, recent results from the experimental realization of this concept on Si NWs are shown. We demonstrate that modulation doping using SiO2:Al-shells allows for several orders of magnitude lower resistances when compared to undoped SiO2-shells.
[1] D. König et al., Sci. Rep. 7, 46703 (2017)

30 min. break

HL 16.6 Tue 11:15 POT 151

Carrier dynamics in quantum-dot tunnel- injection structures: microscopic theory and experiment — •Michael Lorke[1], Igor Khanonkin[2], Stephan Michael[1], Johann Peter Reithmaier[3], Gadi Eisenstein[2], and Frank Jahnke[1] — [1]Institute for Theoretical Physics, University of Bremen, Otto-Hahn-Allee 1, Bremen, 28359, Germany — [2]Electrical Engineering Department and Russel Berrie Nanotechnology Institute, Technion, Haifa, 32000, Israel — [3]Technische Physik, Institute of Nanostructure Technologies and Analytics, Center of Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Kassel, 34132, Germany

Among the challenges for the next generation of semiconductor lasers is the enhancement of their modulation speed to satisfy the need for

higher data transfer rates. For this purpose, tunnel injection lasers are an appealing concept, as they promise improved modulation rates and better temperature stability. Moreover, they eliminate a major detri- mental effect of quantum dot lasers, which is the gain nonlinearity caused by hot carriers. It is shown in this work how the aforementioned improvements depend on the design of tunnel-injection devices. We perform a theory-experiment comparison on scattering times in tunnel injection devices to highlight the importance of alignment between the injector well and the quantum dot ensemble. It is shown how differences in the coupling to the injector quantum well caused by the alignment lead to scattering times into the quantum dot ensemble that vary by an order of magnitude.

HL 16.7 Tue 11:30 POT 151

Electron transport through a quantum dot in controlled heat bath environment — •Hatef Ghannadi maragheh, Johannes C. Bayer, and Rolf J. Haug — Institute for Solid State Physics, Leibniz Universität Hannover, Appelstraße 2, 30167 Hannover, Germany

For optimizing any device, amongst them semiconductor-based qubit, one has to understand the effects of the environment on them. In this sort of devices, not just quantum states of the channel but also the state of the particles is affected [1-3]. The device consists of split-gate quantum dot in a GaAs/AlGaAs heterostructure. The temperature of the measurement ranged from 49.9 mK to 800 mK.

There have been several works on explaining how electron transport through the quantum dot system would behave for different temperatures [4-5]. As the temperature changes, the Fermi distribution of the lead*s changes. This influenced the conductivity of the dot since in the presence of the bias voltage the transport window gets altered. Besides, depending on the presence of energy levels in the transfer window, the conductivity is manipulated by changing the temperature. For low temperatures, due to the local density of states and coupling of the barrier gates to the leads, fluctuations start to emerge.

[1]*K. C. Nowack et al, Science 318, 1430-1433 (2007)
[2]*Pioro-Ladrière, et al, Nature Physics 4, 776*779 (2008)
[3]*Jan K Kühne, et al, physica status solidi (b) 256(6) (2019)
[4]*E. B. Foxman, et al, Phys. Rev. B 47, 10020(R) (1993)
[5]*O. Dani, et al, Communications Physics 5 (1), 1-7 (2022)

HL 16.8 Tue 11:45 POT 151

Manipulation of temporal correlations in single-electron tunneling — •Johannes C. Bayer, Adrian Schmidt, Timo Wagner, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover

Precisely timed single-particle operations are of critical importance for quantum technologies operating at fixed clock cycles. A detailed understanding of the interplay between an external drive and the response of the single-particle source is essential for achieving and improving the accuracy in the time domain. We here demonstrate a high level of control over the time domain of a driven single electron transistor (SET). Using a gate defined quantum dot connected to a highly sensitive charge detector [1] allows detecting electrons tunneling into and out of the SET in real-time [2, 3]. The tunneling rates of such devices are controllable by gate voltages. We drive the SET by modulating gate voltages periodically in time and use time-dependent tunneling rates [2] and waiting time distributions [4] to analyze the impact of the driving parameters on temporal correlations in the tunneling times.

[1] J. C. Bayer, T. Wagner, E. P. Rugeramigabo and R. J. Haug, Ann. Phys. 531, 1800393 (2019)
[2] T. Wagner, P. Talkner, J. C. Bayer, E. P. Rugeramigabo, P. Hänggi and R. J. Haug, Nat. Phys. 15, 330-334 (2019)
[3] R. Hussein, S. Kohler, J. C. Bayer, T. Wagner and R. J. Haug, Phys. Rev. Lett. 125, 206801 (2020)
[4] F. Brange, A. Schmidt, J. C. Bayer, T.Wagner, C. Flindt and R. J. Haug, Sci. Adv. 7, eabe0793 (2021)

HL 16.9 Tue 12:00 POT 151

Scalable integrated readout electronics for semiconductor quantum dots — •Jonas Bühler[1], Arun Ashok[1], Lammert Duipmans[1], Patrick Vliex[1], Christian Grewing[1], André Zambanini[1], and Stefan Van Waasen[1,2] — [1]Central Institute of Engineering, Electronics and Analytics, Electronics Systems (ZEA-2) Forschungszentrum Jülich GmbH, 52428 Jülich, Germany — [2]Faculty of Engineering, Communication Systems, University Duisburg-Essen, 47057 Duisburg, Germany

Quantum computing is one of the promising candidates to overcome the limitations of *classical* computing, e.g. von Neumann architecture. Nowadays much progress has been made on the implementation of scalable qubits. This work focuses on semiconductor qubits, which need operating temperatures near 0 K. Room temperature electronics for control and readout, which are limiting the bandwidth and the scalability due to parasitic elements and heat conduction, are still widely used. Some progress has been made to integrate the qubit control and readout in the direct vicinity of the qubit at cryogenic temperatures. Especially readout electronics still have a limited scalability because of circuit size and power consumption. This work tries to overcome those limitations by comparing different readout architectures and implement a multiplexed and integrated readout circuit with lower area and power consumption. This integrated circuit in a 22nm FD-SOI technology will be placed on top of scalable quantum computing architectures and therefore might be a crucial step on the way to a multi-million qubit quantum computer.

HL 17: THz and MIR physics in semiconductors

Time: Tuesday 9:30–12:45 Location: POT 251

HL 17.1 Tue 9:30 POT 251

Terahertz-induced anomalous currents after optical excitation of excitons in quantum wells — •Cong Ngo[1], Shekhar Priyadarshi[2], Huynh Thanh Duc[3], Mark Bieler[2], and Torsten Meier[1] — [1]Department of Physics, Paderborn University, Warburger Strasse 100, D-33098 Paderborn, Germany — [2]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany — [3]Institute of Applied Mechanics and Informatics, VAST, 1 Mac Dinh Chi, District 1, Ho Chi Minh City, Vietnam

We study transient anomalous currents in GaAs quantum wells by solving the multi-band semiconductor Bloch equations in the length gauge, including excitonic effects and carrier longitudinal-optical and acoustic phonons scattering process. The band structure is obtained by diagonalizing a 14-band $\mathbf{k}\cdot\mathbf{p}$ model within the envelope function approximation. To solve the random phase problem originating from the numerical diagonalization of the band structure model, we apply a smoothing gauge transformation [1]. Our numerical results show quite strong anomalous currents appear for optical excitation near the excitonic resonances and simultaneous Terahertz excitation. The current transients oscillate with a frequency corresponding to the inverse of the energy difference between the 1s and 2s exciton states. The numerical results including excitons are in good agreement with experiments [2].

[1] L. H. Thong, C. Ngo, H. T. Duc, X. Song, and T. Meier, *Phys. Rev. B* **103**, 085201 (2021).
[2] S. Priyadarshi, K. Pierz, and M. Bieler, *Phys. Rev. Lett.* **115**, 257401 (2015).

HL 17.2 Tue 9:45 POT 251

Generation of THz vortex beams and interferometric determination of their topological charge — •Samuel W. Pinnock, Seulki Roh, Tobias Biesner, Artem V. Pronin, and Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany

We developed and demonstrated the efficacy of 3D printed spiral phase plates for the generation of vortex THz beams with orbital angular momenta $\ell = \pm 1$ and $\ell = \pm 2$. The vortex beam generation was confirmed by means of frequency-domain transmission spectroscopy. The topological charge of the vortex beams was determined via phase-sensitive Mach-Zehnder interferometry, which enabled the superposition of a vortex beam with ℓ and its conjugate beam with $-\ell$. The resulting interference patterns were found to be consistent with the expected intensity distributions for a given ℓ, which provides strong confirmation of the spatial phase structure of the generated vortex beams in the THz regime. Such THz vortex beams could be used in spectroscopic studies of optical transitions with $\Delta\ell \neq 0$ in different condensed-matter systems, including semiconductors and topological materials.

HL 17.3 Tue 10:00 POT 251

Ultrafast Terahertz-Wave Emission from Photoconductive Antenna Arrays and Spin Emitters — •Osama Hatem[1], Thales V. A. G. de Oliveira[2], Susanne C. Kehr[1], and Lukas M. Eng[1,3] — [1]Institute of Applied Physics, Technische Universität Dresden, 01062 Dresden, Germany — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [3]ct.qmat: Würzburg-Dresden Cluster of Excellence - EXC 2147, Technische Universität Dresden, Dresden, Germany

For long time, terahertz (THz) radiation (0.1 THz to 10 THz) was little used in science and technology owing to the lack of efficient terahertz sources and detectors. However, recent advances in laser technology and semiconductors industry sparked the interest in exploring this spectral range further. Recently, THz radiation has shown great importance in a wide range of potential applications including THz time-domain spectroscopy and imaging [1-2].

In this work, we report the emission of THz waves from GaAs photoconductive antenna arrays and Fe/Pt spin emitters upon excitation with femtosecond laser pulses at 800 nm. THz waves with bandwidth of 0.1- 5 THz and SNR $>$ 500 below 1 THz were measured. Moreover, detection of THz waves by electro-optic sampling was investigated using ZnTe, GaP, and GaSe crystals of varying thickness. The results are of great significance for THz nanoscopy and imaging applications.

[1] M. Schall et al., Int. J. Infrared Millim. Waves 20, 595-604 (1999). [2] O. Hatem, J. Opt. Soc. Am. B 36, 1144-1149 (2019).

HL 17.4 Tue 10:15 POT 251

Characterization of semiconductors and their properties using terahertz TDS and the Drude-Lorentz model — •Joshua Hennig[1,2], Jens Klier[1], Stefan Duran[1], Kuei-Shen Hsu[3], Antje Hirsch[4], Christian Röder[3], Jan Beyer[3], Franziska Beyer[4], Georg von Freymann[1,2], and Daniel Molter[1] — [1]Center for Materials Characterization and Testing, Fraunhofer ITWM, Kaiserslautern — [2]Department of Physics and Research Center Optimas, Technische Universität Kaiserslautern (TUK), Kaiserslautern — [3]Institut für Angewandte Physik, TU Bergakademie Freiberg, Freiberg — [4]Department of Crystal Growth, Fraunhofer IISB, Freiberg

Semiconductors play an important role in our modern world enabling many of the technological advancements. Therefore, it is of vital interest for an ever-growing industry as well as scientifically to find techniques to characterize optical and electrical properties such as the refractive index as well as the resistivity of these materials. Here, first steps in such characterizations using terahertz time-domain spectroscopy, a nondestructive technology proven to be capable of these challenging tasks, are shown. First, measurements performed on silicon, one of the most commonly used semiconductors, are evaluated to show the measurement principle and confirm the Drude-Lorentz model to be suitable to describe the charge carrier behavior. Next, samples of silicon carbide, an important semiconductor material with applications e.g. in power electronics are examined. The knowledge of these important semiconductor properties can be helpful in quality checks in the production process and any future work with those materials.

HL 17.5 Tue 10:30 POT 251

Interband cascade infrared photodetectors based on Ga-free InAs/InAsSb superlattice absorbers — •Andreas Bader[1], Florian Rothmayr[2], Nabeel Khan[2], Fauzia Jabeen[1], Johannes Koeth[2], Sven Höfling[1], and Fabian Hartmann[1] — [1]Technische Physik, Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Am Hubland, D-97074 Würzburg, Germany — [2]nanoplus Nanosystems and Technologies GmbH, Oberer Kirschberg 4, D-97218 Gerbrunn, Germany

We present results on interband cascade infrared photodetectors (ICIP) based on Ga-free InAs/InAsSb superlattice (SL) absorbers. An alternative extraction path of photogenerated carriers is required when substituting the more standard InAs/Ga(In)Sb SL absorbers for Ga-free SLs. The device operates in the photovoltaic mode in the mid infrared spectral range with cut-off wavelengths between around 6.5 um at 100 K and 9 um at RT. At elevated temperatures, features of negative-differential-conductance (NDC) emerge. Under illumination, these NDC features can supply gain in the device leading to a peak responsivity of 0.45 A/W at room temperature. At 300 K the zero-bias detectivity D* of the presented device is around 1*10^8 Jones which compares well to similar ICIPs based on InAs/GaSb SL absorbers.

HL 17.6 Tue 10:45 POT 251

Assessment of epitaxially grown p-doped InAs on undoped GaSb exhibiting terahertz emission — •Cyril Salang[1], Dean Von Johari Narag[1], Rommel Jagus[1], Gerald Angelo Catindig[2], Mae Agatha Tumanguil[1], Alexander De Los Reyes[2], Ivan Cedrick Verona[2], Hannah Bardolaza[2], Armando Somintac[2], Elmer Estacio[2], and Arnel Salvador[2] — [1]Materials Science and Engineering Program, University of the Philippines Diliman, Philippines — [2]National Institute of Physics, University of the Philippines Diliman, Philippines

A p-InAs/undoped-GaSb thin film was grown via molecular beam epitaxy. The 260 Å p-InAs was grown on 260 nm undoped InAs over 10 periods of InGaAs(3 nm)/GaAs(3 nm) superlattice to minimize the surface roughness prior to the p-InAs growth. Three periods of 20-nm undoped GaAs/260-nm undoped InAs served as a buffer with growth interruption applied on the first 2 mins of deposition of each GaAs and InAs layer. X-ray diffraction shows a peak at 2θ $\sim 61^o$ corresponding to InAs. The sample's resistance was measured to be 43 Ω. The terahertz (THz) emission was evaluated using 1.55 μm femtosecond laser excitation in reflection geometry. The current sample emits at $\sim$20 times lower THz intensity compared to that of a previously investigated 1 ± 0.4 μm p-InAs/n-GaSb sample possibly due to the lesser thickness leading to a lower photo-Dember response, and differing crystal qualities from the different growth processes. Nonetheless, exploring growth techniques for producing thin InAs films is desired to realize photoconductive antennas for transmission geometry.

30 min. break

HL 17.7 Tue 11:30 POT 251

Coherent State Steering in Condensed Matter Systems with Strong Light-Matter Engineering — •Michael Spencer, Joanna Urban, Maxamillian Frenzel, and Sebastian Maehrlein — Department of Physical Chemistry, Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany

Physical properties of materials are derived largely from their chemical constituents, structural arrangement, and local properties such as temperature and dielectric environment. Next-generation materials science is increasingly focused on manipulation of structural properties in order to access material properties on-demand, in search of emergent, enhanced, or even hidden states of matter. One such method to transiently modify crystalline materials is the application of intense terahertz (THz) laser pulses. These pulses allow for resonant and selective excitation of infrared-active vibrational modes (phonons) of a crystal, allowing for coherent and ultrafast modulation of condensed-matter system properties. With the introduction of an electromagnetic cavity, the subsequent enhancement of this light-matter interaction between the intense THz radiation and the phonons will provide expanded control over excited-state steering, allowing access to exotic, transient states of matter. I will present our steps towards first realizations of such strongly-coupled light-matter interactions of phonons in crystalline materials within the THz frequency range. In addition, I will discuss our novel measurement techniques for the detection of strong light-matter interactions, where we utilize the unique technical capabilities of terahertz time-domain spectroscopy.

HL 17.8 Tue 11:45 POT 251

Terahertz cyclotron emission from HgTe QWs — •S. Gebert[1,2], C. Consejo[1], S. Ruffenach[1], J. Torres[2], B. Jouault[1], and F. Teppe[1] — [1]Laboratoire Charles Coulomb (L2C), UMR 5221 CNRS, Université de Montpellier, F-34095 Montpellier, France — [2]Institut d'Electronique et des Systèmes (IES), UMR 5214 CNRS, Université de Montpellier, F-34095 Montpellier, France

Motivated by the emergence of graphene, several concepts for Landau-level (LL) lasers, tunable by a magnetic field over the whole terahertz (THz) frequency range, have been proposed. One hoped in particular was, that the non-equidistance of the LLs from Dirac fermions could efficiently suppress the non-radiative Auger recombination, which typically prevails over the radiative recombination. However, despite this non-equidistance an unfavorable non-radiative process still persists in Landau-quantized graphene, and no cyclotron emission from Dirac fermions has yet been reported. To eliminate this last non-radiative process, it is sufficient to slightly modify the dispersion of the Landau levels, e.g. by opening a small gap in the linear band structure. A proven example of such gapped graphene-like materials are HgTe quantum wells (QWs) close to the topological phase transition. We here experimentally demonstrate spontaneous Landau emission from Dirac fermions in such HgTe QWs, where the emission is tunable be-

tween 0.5 THz and 3 THz by both the magnetic field and the carrier concentration [1].

[1] S. Gebert et al., Nat. Photon. (accepted); preprint is avaliable at doi.org/10.21203/rs.3.rs-1630601/v1

HL 17.9 Tue 12:00 POT 251

Coherent phonon dynamics in quasi-2D perovskites probed by THz-induced Kerr effect — •Joanna M. Urban[1], Marie Cherasse[1,2], Maximilian Frenzel[1], Michael Spencer[1], Gaelle Trippe-Allard[3], Emmanuelle Deleporte[3], Luca Perfetti[2], Martin Wolf[1], and Sebastian F. Maehrlein[1] — [1]FHI of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany — [2]LSI, Palaiseau, France — [3]Université Paris-Saclay, LuMIn, Gif-sur-Yvette, France

2D hybrid organic-inorganic perovskites (HOIP) are self-assembled multiple quantum well structures, formed by metal halide octahedral layers alternating with large organic spacer cations. They combine the intriguing properties of the 3D HOIP polar, anharmonic lattice with optoelectronic properties arising due to low dimensionality. We study a family of 2D HOIPs in the Ruddlesden-Popper phase $(PEA)_2(MA)_{n-1}Pb_nI_{3n+1}$ (n=1,2,3). Using intense, close to single-cycle THz fields we excite coherent optical phonons and probe the lattice dynamics via THz-induced Kerr effect (TKE). Strikingly, we observe long-lived coherent phonon oscillations at room temperature. Comparison with static Raman spectroscopy results as well as the measured fluence and temperature dependence confirm that the observed features in the 0.5-3 THz range correspond to Raman-active modes of the inorganic sublattice, excited via a nonlinear driving process. The nontrivial azimuthal angle dependence of the TKE signal can be explained considering the crystal structure and the symmetry of the Raman modes using the $\chi^{(3)}$ nonlinear susceptibility tensor formalism.

HL 17.10 Tue 12:15 POT 251

Optically excited charge-carrier dynamics in the antiferromagnetic semiconductor MnTe — •Changqing Zhu[1], Patrick Pilch[1], Anneke Reinold[1], Gunther Springholz[2], Mirko Cinchetti[1], and Zhe Wang[1] — [1]TU Dortmund University, Germany — [2]Johannes Kepler University of Linz, Austria

Room-temperature antiferromagnetic semiconductors are very interesting for possible spintronic applications. With a long-range antiferromagnetic order (T_N = 307 K) at room temperature, the hexagonal α-MnTe is a relevant candidate for those applications. Here we report on time-resolved measurements of ultrafast dynamics of optically excited charge carriers in α-MnTe thin film, by optical pump - optical probe and optical pump - THz probe spectroscopic techniques at room temperature. In contrast to a phononic oscillation mode at 5.3 THz as observed by 2.4 eV pump [1], our studies with an 1.5 eV pump pulse cannot reveal the optical phonon mode but rather low-energy acoustic phonon-like behavior at high pump fluence. Moreover, nonlinear dependence on pump fluence is observed both in our optical and terahertz probes, for a pump fluence above $\sim$ 2.0 mJ/cm^2. This indicates a different physical mechanism than in the previous studies. The observed relaxation processes can be associated to electron-hole recombination and electron-phonon scattering.

[1] D. Bossini et al. Phys. Rev. B 104, 224424 (2021).

HL 17.11 Tue 12:30 POT 251

Time-resolved nanospectroscopy on Si-doped GaAs-InGaAs core-shell nanowires — •Andrei Luferau[1,2], Maximilian Obst[2], Susanne Kehr[2], Lukas Eng[2], Stephan Winnerl[1], Alexej Pashkin[1], Emmanouil Dimakis[1], and Manfred Helm[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Institute of Applied Physics, Technische Universität Dresden, Dresden, Germany

High-quality epitaxial nanowires (NWs) based on III-V semiconductors offer the possibility to fabricate ultrafast optical devices due to their direct bandgap and the high electron mobility. Contactless investigation of photoexcited carriers within single NWs is enabled by optical-pump THz-probe scanning near-filed optical microscopy (SNOM) experiment. Here we report on first THz-pump MIR-probe SNOM studies on Si-doped GaAs-InGaAs core-shell NWs utilizing THz radiation from the free-electron laser FELBE. The experiment was carried out with SNOM setup from Neaspec equipped with nanoFTIR module, where a broadband MIR source (5-15μm) serves as a probe. Upon intraband THz-pump (25μm) we observed a red shift of amplitude and phase of the NW plasma resonance, while control interband optical pumping (780nm) induced a blue shift of the resonance, and in both cases an exponential decay with a time constant of 4-5ps is seen. We attribute the blue shift to the contribution of photogenerated carriers. The red shift is assigned to the heating of the electrons in the conduction band and the subsequent increase of the effective mass in the nonparabolic Γ-valley due to high peak electric fields of THz pulses.

HL 18: Optical Properties (joint session HL/CPP)

Time: Tuesday 9:30–13:00 Location: POT 112

HL 18.1 Tue 9:30 POT 112

Can Ge and Si be optoelectronic materials: Hexagonal polytypes — •Martin Keller[1], Abderrezak Belabbes[1,2], Jürgen Furthmüller[1], Friedhelm Bechstedt[1], and Silvana Botti[1] — [1]Friedrich-Schiller-Universität Jena, Institut für Festkörpertheorie und -optik, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Department of Physics, Sultan Qaboos University, P.O. Box 36, PC 123, Muscat, Oman

The group IV elements silicon and germanium crystallize in cubic diamond structure under ambient conditions and feature indirect bandgaps. Therefore they cannot emit light efficiently and are not applicable in active optoelectronic devices. Under high pressure, however, as well as using different growth techniques, several Si and Ge polymorphs, including hexagonal polytypes, have been observed. Lonsdaleite Ge as well as Ge-rich hexagonal alloys have even been found to have a direct bandgap and strongly emit light with varying frequency. Thus hexagonal systems have become of great interest for potential optical emitters that may be integratable with CMOS technology. We have performed extensive ab initio studies of the energetic, structural, elastic and electronic properties as well as the strengths of some dipole transitions of the hexagonal Si and Ge polytypes 2H, 4H and 6H using Density Functional Theory and approximate quasiparticle treatments, and trends between the different geometries are analysed. The results for cubic and hexagonal Si and Ge agree excellently with existing experimental findings. The electronic structures point to promising optical properties.

HL 18.2 Tue 9:45 POT 112

Many-body effects in the mid-infrared dielectric function of InSb from 80 to 800 K — Melissa Rivero Arias, Cesy Zamarripa, Jaden Love, Carlos Armenta, Carola Emminger, Sonam Yadav, and •Stefan Zollner — New Mexico State University, Las Cruces, NM, USA

We describe measurements of the mid-infrared dielectric function of bulk InSb near the direct band gap using Fourier-transform infrared spectroscopic ellipsometry from 80 to 800 K in an ultra-high vacuum cryostat. Indium antimonide is the zinc blende compound semiconductor with the smallest direct band gap (E_0=0.18 eV at 300 K) due to its heavy elements and the large resulting spin-orbit splitting and Darwin shifts. The band gap is extracted from the dielectric function by fitting with a parametric oscillator model. It decreases from 80 to 450 K following a Bose-Einstein model, then remains constant up to 550 K, and increases again at the highest temperatures. This is explained with a thermal Burstein-Moss shift: The onset of optical absorption increases as electron-hole pairs are thermally excited at the highest temperatures. The intrinsic carrier concentration determined from the Drude tail in the ellipsometry spectra agrees qualitatively with temperature-dependent Hall experiments and calculations based on degenerate Fermi-Dirac statistics.

HL 18.3 Tue 10:00 POT 112

Polarized Raman scattering study of epitaxially grown GeSn layers with various Sn content — •Agnieszka Anna Corley-Wiciak[1], Omar Concepción[2], Marvin Hartwig Zoellner[1], Detlev Grützmacher[2], Dan Buca[2], Giovanni Capellini[1,3], and Davide Spirito[1] — [1]IHP Leibniz-Institut für innovative Mikroelektronik, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany —

[2]Peter Grünberg Institute 9 (PGI-9) and JARA-Fundamentals of Future Information Technologies — [3]Dipartimento di Scienze, Università Roma Tre, V.le G. Marconi 446, 00146 Roma, Italy

$Ge_{1-x}Sn_x$ alloys are an excellent candidate for developing mid-infrared light sources integrated with CMOS technology. The challenges in the controlled growth with high crystal quality have highlighted the peculiarity of these alloys, which can be monitored by their vibrational properties. To this purpose, Raman spectroscopy is an effective experimental method to determine these properties, as this technique is non-destructive, contactless, fast, and locally resolved. We use Raman scattering with different polarization configurations to investigate $Ge_{1-x}Sn_x$ ($0.05 \leq x \leq 0.14$) alloys grown by Chemical Vapour Deposition on Ge/Si virtual substrates. Measurements were performed in backscattering geometry with parallel and cross polarizations. In this way, we identify multiple components in the vibrational modes and how they deviate from simplified models. Our results will help to understand the fundamental properties of $Ge_{1-x}Sn_x$ alloys to enable fast assessment for their applications in optoelectronic and thermoelectric.

HL 18.4 Tue 10:15 POT 112

Eigenmodes and Polarization Structure of Coupled Elliptical Microcavities — •Johannes Düreth[1], Simon Betzold[1], Monika Emmerling[1], Antonina Bieganowska[2], Jürgen Ohmer[3], Utz Fischer[3], Sven Höfling[1], and Sebastian Klembt[1] — [1]Technische Physik, RCCM and Würzburg-Dresden Cluster of Excellence ct.qmat, University of Würzburg, Germany — [2]Faculty of Problems of Fundamental Technology, Department of Experimental Physics, Laboratory for Optical Spectroscopy of Nanostructures, Wroclaw, Poland — [3]Department of Biochemistry, University of Würzburg, Germany

Elliptical potentials give rise to a set of eigenmodes called Ince-Gaussian modes. Contrary to hemispherical potentials, the geometric shape leads to a mode splitting of the otherwise degenerate fundamental mode. Theoretically, this behaviour can be exploited to realize interesting topological phenomena like non-reciprocal transport, the non-hermitian skin-effect or engineer artificial gauge fields. On the way to an experimental implementation of such systems, the singular building blocks of these photonic potentials - single and coupled elliptical potentials - have to be experimentally studied.

Here we present an investigation of the mode splitting and polarisation in single elliptical microcavities, as well as an examination of the coupling between differently angled ellipses.

15 min. break

HL 18.5 Tue 10:45 POT 112

Optical properties of $Ag_xCu_{1-x}I$ alloy thin films — •E. Krüger[1], M. Seifert[2], V. Gottschalch[3], H. Krautscheid[3], C.S. Schnohr[1], S. Botti[2], M. Grundmann[1], and C. Sturm[1] — [1]Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Germany — [2]Friedrich-Schiller-Universität Jena, Institut für Festkörpertheorie und Optik , Germany — [3]Universität Leipzig, Institut für Anorganische Chemie, Germany

Copper iodide (CuI) is a promising wide bandgap semiconductor for applications in transparent optoelectronic devices. In this context, the specific tuning of electrical and optical properties, which can potentially be achieved with ternary alloys such as $CuBr_xI_{1-x}$ [1] and $Ag_xCu_{1-x}I$ [2], is crucial for the development of novel CuI-based devices. In particular, $Ag_xCu_{1-x}I$ is of great interest because the intrinsic conductivity changes from p-type to n-type with increasing Ag content.

Here we present the bandgap energy and spin-orbit splitting in $Ag_xCu_{1-x}I$ alloys as a function of alloy composition and temperature, studied by a combination of experimental and computational methods. The non-linear bandgap dependence on Ag content can be described by a quadratic bowing parameter of 0.54 eV and is dominated by charge carrier redistribution effects in the presence of unequal element-specific bond lengths. The slight increase of the spin-orbit splitting from 640 meV for CuI to about 790 meV for AgI is discussed in terms of decreasing p-d hybridization of the valence bands at the Γ-point.

[1] N. Yamada et al., Adv. Funct. Mater. **30**, 2003096 (2020)
[2] A. Annadi and H. Gong, Appl. Mater. Today **20**, 100703 (2020)

HL 18.6 Tue 11:00 POT 112

Multipole theory of optical spatial dispersion in crystals — •Óscar Pozo — Centro de Física de Materiales, Universidad del País Vasco, 20018 San Sebastián, Spain

Natural optical activity is the paradigmatic example of an effect originating in the weak spatial inhomogeneity of the electromagnetic field on the atomic scale. In molecules, such effects are well described by the multipole theory of electromagnetism, where the coupling to light is treated semiclassically beyond the electric-dipole approximation. That theory has two shortcomings: it is limited to bounded systems, and its building blocks - the multipole transition moments - are origin dependent. In this work, we recast the multipole theory in a translationally-invariant form that remains valid for periodic crystals. Working in the independent-particle approximation, we introduce 'intrinsic' multipole transition moments that are origin independent and transform covariantly under gauge transformations of the Bloch eigenstates. Electric-dipole transitions are given by the interbank Berry connection, while magnetic-dipole and electric-quadrupole transitions are described by matrix generalizations of the intrinsic magnetic moment and quantum metric. In addition to multipole-like terms, the response of crystals at first order in the wave vector of light contains band-dispersion terms that have no counterpart in molecular theories. The rotatory-strength sum rule for crystals is found to be equivalent to the topological constraint for a vanishing chiral magnetic effect in equilibrium, and the formalism is validated by numerical tight-binding calculations.

HL 18.7 Tue 11:15 POT 112

Predicting bandgap in strain-engineered multinary III-V semiconductors — •Badal Mondal and Ralf Tonner-Zech — Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, 04103 Leipzig, Germany

The tuning of the type and size of bandgaps of III-V semiconductors is a major goal for optoelectronic applications. Varying the relative composition of several III- or V-components in compound semiconductors is one of the major approaches here. Alternatively, straining the system can be used to modify the bandgaps. By combining these two approaches, bandgaps can be tuned over a wide range of values, and direct or indirect semiconductors can be designed. However, an optimal choice of composition and strain to a target bandgap requires complete material-specific composition, strain, and bandgap knowledge. Exploring the vast chemical space of all possible combinations of III- and V-elements with variation in composition and strain is experimentally not feasible. We thus developed a density-functional-theory-based predictive computational approach for such an exhaustive exploration. This enabled us to construct the 'bandgap phase diagram' [1] by mapping the bandgap in terms of its magnitude and nature over the whole composition-strain space. Further, we have developed efficient machine-learning models to accelerate such mapping. We will show the application to binary [2], ternary and quaternary material combinations and the possible impact on device design.

[1] https://bmondal94.github.io/Bandgap-Phase-Diagram , 2022
[2] https://arxiv.org/abs/2208.10596

HL 18.8 Tue 11:30 POT 112

GeSn vertical p/n photodetectors formed by 2-step ion implantation — •Shuyu Wen[1,2], Saif Shaikh[1], Oliver Steuer[1], Yonder Berencen[1], Slawomir Prucnal[1], and Shengqiang Zhou[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany — [2]Institute of Semiconductors, Chinese Academy of Sciences, Bejing, China

Germanium (Ge) is a promising material in integrated circuit (IC) due to the high mobility of hole carrier and highly compatibility in the Si-base IC technology. However, the indirect band structure of Ge leads to the low radiative recombination efficiency, limiting the application in opto-electronics. Alloying Ge with Tin (Sn) is a promising method to obtain energy band modification even to a direct band. Here, high quality Ge0.97Sn0.03 and Ge0.955Sn0.045 alloy is obtained by CMOS-compatible ion implantation method. Tensile strain leads by Sn alloying and damage recovery after Flash annealing (FLA) are characterized by Raman and XRD measurements. A subsequently phosphors implantation is applied to obtain vertical pn photodetectors (PD). The device shows an extended spectral response comparing with commercial Ge PD. This work provides a new CMOS-compatible method to fabricate photodetectors in short-wave infrared.

15 min. break

HL 18.9 Tue 12:00 POT 112

Interplay between strain, Sn content and temperature in GeSn-based optoelectronic devices — •Ignatii Zaitsev[1], Agnieszka A. Corley-Wiciak[1], Dan Buca[2], Omar Concepción[2], Michele Virgilio[3], Giovanni Capellini[1,4], Costanza L.

Manganelli[1], and Davide Spirito[1] — [1]IHP - Leibniz-Institut für innovative Mikroelektronik, Frankfurt (Oder), Germany — [2]PGI 9, Jülich, Germany — [3]Università di Pisa, Pisa, Italy — [4]Università Roma Tre, Roma, Italy

Several works have shown the subtle interplay between thermomechanical strain, Sn content and band occupation in optoelectronic devices based on CMOS-integratable group-IV materials (Ge, SiGe, SiGeSn). This is especially the case when temperature plays a key role, e.g. devices operating at cryogenic temperature or in presence of high power. Here we provide a theoretical-experimental approach combining 3D FEM calculations, Raman and photoluminescence spectroscopy to fully capture the influence of mechanical and thermomechanical features on the optical properties. We apply this method to strained GeSn microdisks, a device geometry aimed at laser in the MIR range. With the presented methods, we can develop a thorough guidelines for the assessment and design of integrated light emitters.

HL 18.10 Tue 12:15 POT 112

Excitons in MoS_2 bilayers under pressure — •Jan-Hauke Graalmann[1], Paul Steeger[2], Robert Schmidt[2], Steffen Michaelis de Vasconcellos[2], Rudolf Bratschitsch[2], and Michael Rohlfing[1] — [1]Institute of Solid State Theory, University of Münster, 48149 Münster, Germany — [2]Institute of Physics, University of Münster, 48149 Münster, Germany

Theoretical and experimental studies have shown that the optical spectrum of the MoS_2 bilayer changes under pressure.

Our theoretical investigations are based on DFT, *GdW* and the Bethe-Salpeter equation. For the specific stress conditions of the experiment, our calculations show an effective shift of the excitation energies of the A exciton towards higher energies with increasing pressure. This behaviour can be explained with an approximately constant direct band gap at the K point while the binding energy decreases. Due to a growing valence band splitting for increasing pressures, the interlayer exciton shows a smaller shift. These results are substantiated by measurements using a piston type diamond anvil cell (DAC) to create pressures in the GPa range.

The reason for only small changes of the fundamental band gap is a significant influence of interlayer interaction. The effect of a decreasing gap by biaxial lateral shrinking of each single layer under an external pressure gets counterbalanced by the reduction of the interlayer distance. Furthermore, the real space distribution shows an increased interlayer character for the A and interlayer exciton under pressure.

HL 18.11 Tue 12:30 POT 112

Optical properties of a vacancy-related complex in 4H-SiC — •Maximilian Schober[1], Nicolas Jungwirth[1], Takuma Kobayashi[2], Johannes A. F. Lehmeyer[2], Michael Krieger[2], Heiko B. Weber[2], and Michel Bockstedte[1] — [1]Institute for Theoretical Physics, Johannes Kepler University Linz, Austria — [2]Lst. f. Angewandte Physik, Friedrich-Alexander-University Erlangen-Nürnberg, Germany

SiC is host to multiple color centers, such as the silicon vacancy, the divancy, and the carbon antisite-vacancy complex, with relevant applications as qubits, single photon sources and in quantum metrology. Recently, the carbon di-vacancy-antisite complex was identified as an annealing product of vacancy related defects [1], and is expected to feature favorable properties for quantum technology. The presence of strongly localized silicon and carbon dangling bonds points to rich photo- and spin physics that has so far not been explored in detail. In this work we probe the basal and axial configurations of $V_C C_{Si} V_C$ for their electronic-, optical- and radiative properties using a theoretical framework of hybrid density functional and many body approaches. We obtain the principal transitions, as well as the associated static- and transition dipole moments of the relevant charge states. Our results suggest a tentative identification of the carbon di-vacancy-antisite with the temperature-stable (TS) center [2].

[1] E. M. Y. Lee *et al.*, Nat. Commun. 12, 63 (2021).
[2] M. Rühl, C. Ott, S. Götzinger, M. Krieger, H. B. Weber, Appl. Phys. Lett. 113, 122102 (2018).

HL 18.12 Tue 12:45 POT 112

Defects or Dots – what semiconductor physics can bring into optical super-resolution imaging — •Philipp Kellner[1], Jana Sütterlin[1], Paul Konrad[2], Andreas Sperlich[2], and Christian Eggeling[1,3] — [1]Institut für angewandte Optik und Biophysik, FSU Jena, Philosophenweg 7, 07743 Jena — [2]Physikalisches Institut, Julius-Maximilians Universität Würzburg, Am Hubland, 97074 Würzburg — [3]Institut für physikalische Hochtechnologie, Albert-Einstein-Straße 9, 07745 Jena

Super-resolved optical microscopy is a widely used tool throughout the medicine and biology community. Mostly and routinely done with organic dyes super-resolution imaging has led to various insights into cell structures and diffusional dynamics. The fundamental problem occuring with organic dyes is their rather dim brightness and their lack of photostability paired with photo-toxicity. This presentation will shed light on novel semi-conductor-based chromophores, like NV-centers in diamond, defects in hBN and CdTe quantum dots, and their use in optical nanoscale sensing schemes like StED-imaging or fluorescence correlation microscopy.

HL 19: Organic Electronics and Photovoltaics I (joint session CPP/HL)

Time: Tuesday 9:30–13:00 Location: GÖR 226

HL 19.1 Tue 9:30 GÖR 226

Use of a multiple hydride donor to achieve an n-doped polymer with high solvent resistance — Farzaneh Saeedifard[1,2], Dominique Lungwitz[3], Zi-Di Yu[4], Sebastian Schneider[5], Ahmed E. Mansour[3,6], •Andreas Opitz[3], Stephen Barlow[1,2], Michael F. Toney[1], Jian Pei[4], Norbert Koch[3,6], and Seth R. Marder[1,2] — [1]University of Colorado Boulder, US — [2]Georgia Institute of Technology, Atlanta, US — [3]Humboldt-Universität zu Berlin, Germany — [4]Peking University, China — [5]Stanford University, US — [6]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany

Insolubilization of doped semiconducting polymer layers can help to fabricate efficient multilayer solution-processed electronic and optoelectronic devices. Here, we present a promising technique to simultaneously n-dope and largely insolubilize conjugated polymer films using tetrakis[4-(1,3-dimethyl-2,3-dihydro-1*H*-benzo[*d*]imidazol-2-yl)phenoxymethyl]methane (tetrakis-O-DMBI-H), which consists of four 2,3-dihydro-1*H*-benzoimidazole (DMBI-H) n-dopant moieties covalently linked to one another. [1] Doping a thiophene-fused benzodifurandione-based oligo(*p*-phenylenevinylene)-*co*-thiophene polymer (TBDOPV-T) with tetrakis-O-DMBI-H results in a highly n-doped film with bulk conductivity of 15 S/cm. Optical absorption spectra reveal a film retention of ∼93% after immersion in *o*-dichlorobenzene for 5 min. This is caused by multiple electrostatic interactions the multiple electrostatic interactions between each dopant tetra-cation and up to four nearby anionic doped polymer segments.

[1] F. Saeedifard et al., *ACS Appl. Mater. Interfaces* **14** (2022) 33598.

HL 19.2 Tue 9:45 GÖR 226

Numerical Simulation of Crystallization Kinetics in Binary Mixtures for Organic Photovoltaic Applications — •Maxime Siber, Olivier Ronsin, and Jens Harting — Helmholtz-Institute Erlangen-Nürnberg for Renewable Energies (HI-ERN), Germany

With the aim to understand the formation process of organic photoactive layers, and identify process-structure relationships in order to optimize their fabrication, a computational framework relying on the phase-field modelling approach has recently been developed. It is now sought to quantitatively compare numerical simulations of drying organic photovoltaic (OPV) films with corresponding experimental realizations.

Since the fabrication process involves the interplay of multiple physical phenomena, which separate characterization already is a challenging task from the simulative, as well as from the experimental side, this first study focusses on crystallization behaviour in isothermal, non-evaporating, binary OPV blends. In particular, this talk addresses crystalline structures that arise from different crystallization processes such as solution-triggered crystallization, diffusion-limited crystallization, or spinodal decomposition-assisted crystallization. Furthermore, crystallization kinetics quantified for several blend ratios and material parameters are also analyzed and compared. Finally, perspectives re-

garding validation against in-situ experiments and derivation of design rules for OPV film fabrication are also provided.

HL 19.3 Tue 10:00 GÖR 226

Optical properties of perfluorotetracene (PFT) crystal polymorphs — •Ana Maria Valencia[1,2] and Caterina Cocchi[1,2] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg — [2]Physics Dept., Humboldt-Universität zu Berlin und IRIS Adlershof

The family of perfluorinated acenes is gaining popularity among organic materials for optoelectronics. Since the electronic and optical properties of molecular solids are crucially dependent on their packing motifs, it is crucial to consider crystalline phases in the simulations to understand the structure-property relationships of these materials, especially regarding electronic correlations and excitations. Here, we investigate from first principles by means of density functional theory and many-body perturbation theory the electronic structure and the optical excitations of two crystal polymorphs of perfluorotetracene, considering for comparison tetracene and the corresponding isolated molecules. This way, we can assess the effects of fluorination as well as of the crystal periodicity. We find that the absorption spectra are only mildly influenced by the packing motif. However, our analysis gives insight into the exciton binding energies as well as the spatial distribution of the excitons. We inspect not only the first excitations but also the higher-energy ones, thus providing an all-around understanding of the optical excitations in these materials.

HL 19.4 Tue 10:15 GÖR 226

Controlling long-range order in dip coated piezo- and ferroelectric molecular materials — •Andrey Butkevich and Martijn Kemerink — Institute for Molecular Systems Engineering and Advanced Materials, Im Neuenheimer Feld 225, 69120 Heidelberg, Germany

Organic piezo- and ferroelectrics are of great interest due to their tunable properties. However, the extensive procedures that are often required to achieve saturation polarization limit their possible applications. A so far unexplored possible solution is to pre-align the molecules during the deposition from solution. Here, we analyzed the effect of dip coating parameters on the alignment of multiple supramolecular piezo- and ferroelectrics. Dip coated films were characterized for different material concentrations and dip coating velocities. The investigation revealed that morphologies with strong alignment along the dip coating direction are formed for both material types. For ferroelectrics, the changes in the ferroelectric switching behavior of the resulting thin films were investigated. The ferroelectric switching was investigated using the double wave method, revealing that dip coating perpendicular to the electrodes leads to an almost perfect in-plane alignment of the supramolecular polymers, which was confirmed by X-ray diffraction. The observed switching behavior was comparable to films that were aligned via conventional field-annealing. Hence, dip coating enhanced the ferroelectric switching in the investigated molecules, which we anticipate can be directly transferable to other molecular ferroelectrics.

HL 19.5 Tue 10:30 GÖR 226

In search of novel organic ferroelectrics — •Heiko Mager — IMSEAM, Heidelberg University

The switchable polarization and concomitant pyroelectric and piezoelectric properties of ferroelectric materials enable a variety of applications, ranging from memory devices over thermal and mechanical sensors to energy harvesters. Although current applications are dominated by inorganic materials, organic ferroelectrics offer a flexible, cheap and possibly non-toxic and biodegradable alternative.

Here, we present experimental research on the ferroelectric-like behavior of the novel liquid crystalline molecule C6H6F5O-C3-Amide and its molecular derivatives. To screen for a possible para- to ferroelectric phase transitions, dielectric spectroscopy was employed. While the for ferroelectric materials characteristic Curie-Weiß behavior was not directly observed, features in the dielectric suggest a possible phase transition coinciding with a peak in differential scanning calorimetry traces.
Polarization hysteresis loops were obtained via double wave measurements and characteristic capacitance- voltage "butterfly" loops measured. Comparisons between the different molecular derivatives allow insights into the molecular groups relevant for the switching process.

HL 19.6 Tue 10:45 GÖR 226

Implementation and simulation of drift-diffusion models for organic mixed conductor devices — •Andres David Peña Unigarro[1,2] and Florian Steffen Gunther[2,3] — [1]Institute of physics, TU Chemnitz, Chemnitz, Germany — [2]IFSC, University of São Paulo, Brazil — [3]UNESP, Rio Claro, Brazil

Organic electrochemical transistors (OECTs) have emerged as potential transducers in applications that require the conversion of ion fluxes to electronic current. For the understanding of the fundamental mechanism in OECTs and OECT-based applications, as well as for their rational optimization, however, it is essential to have theoretical models that agree with experimentally measured device responds. Most of the existing OECT models consider that the ion flux from the electrolyte into the organic, semiconducting layer takes place only due to an electrical field. These models are efficient to describe the steady state operations of OECTs, but are rather limited when compared to transient behaviors. Recently, more refined models which take a diffusion term into account, have been developed. The simplifications needed to use an analytical solution of the governing equation, however, reduces its generality, limiting the results to specific cases. In our work, we use numerical methods to solve the drift-diffusion equation in one dimension to overcome these limitations of the analytical solution. This allows us to go beyond the standard boundary conditions and to analyze the impact of other alterations.

HL 19.7 Tue 11:00 GÖR 226

Noise in Organics Semiconductors and Devices — •Priya Viji, Dorothea Scheunemann, Constantin Tormann, and Martijn Kemerink — Institute for Molecular Systems Engineering and Advanced Materials, Heidelberg University, Germany

Noise, typically considered an unwanted signal in measurements, can also contain information about the charge kinetics in organic semiconductors. Since the corresponding devices often show high resistances and capacitances, the measurement of -albeit very small- current fluctuations via voltage noise is most suitable. To quantify this noise and to eliminate noise from other devices in the measurement line, a cross-correlation technique is implemented and applied to P3HT doped with varying concentrations of F4TCNQ. The results compare quantitatively with kinetic Monte Carlo simulations in which noise calculations were implemented. To understand the effect of the electric field on the charge carriers, disentangling noise in directions parallel and perpendicular to the electric field is essential. The direction perpendicular to the electric field does show a gradual increase at high electric fields, which matches the concept of an Effective Temperature, as described by Marianer and Shklovskii, in which the effects of electric field and lattice temperature are combined. In the direction of the electric field, an additional contribution due to shot noise is observed. However, its magnitude deviates from the theoretical prediction of shot noise, which can be quantified as a non-unity Fano-factor.

15 min. break

HL 19.8 Tue 11:30 GÖR 226

Uniaxially Aligned Merocyanine Films by Graphene Nanoribbon Templated Growth — •Philipp Weitkamp, Lukas Böhner, Nora Gildemeister, Dirk Hertel, and Klaus Meerholz — Physikalische Chemie, Universität zu Köln, Deutschland

We herein report the unique and novel approach of achieving a polycrystalline thin film consisting of uniaxially aligned domains by using 7-armchair graphene nanoribbon (7-aGNR) monolayers as van-der-Waals template. For this purpose, a merocyanine dye was evaporated on 7-aGNRs, transferred on quartz glass substrates. The alignment of the formed molecular aggregate along the GNR alignment direction was proven by polarisation dependent absorbance spectroscopy. The J- and H-transition, formed by the dye aggregate, were correlated with distinct axes of the crystal structure. By combining this correlation with polarisation dependent absorbance measurements and X-ray diffraction experiments we elucidated the three-dimensional structure of the formed aggregate thin film. The growth mode of these films was investigated as a function of the applied layer thickness. Atomic force microscopy-based morphology analysis and X-ray diffraction experiments were used to reveal the anisotropic on-surface crystallisation along the 7-aGNR long axes direction. Furthermore, we found that the delocalisation length of the aggregate increases with increasing in-plane order. Finally, we demonstrated that the in-plane alignment leads to an anisotropic charge carrier transport by implementing the templated

merocyanine thin film as active layer in a top-gated organic field effect transistor.

HL 19.9 Tue 11:45 GÖR 226

Investigation on organic light-emitting diodes, fabricated by a self-developed and highly automated physical vapor deposition system — •Fabian Binder, Mona Löther, Pascal Schady, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg

Organic light emitting diodes (OLEDs) are most commonly produced in ultra-high vacuum by physical vapor deposition (PVD) of several organic and metallic layers on a carrier substrate. We developed an automated PVD system, mainly consisting of two vacuum chambers for organic and metal deposition, respectively. Stepper motors and sensor solutions ensure a smooth and precise positioning of the carrier substrate above the evaporation crucibles. The substrate is then rotated with a defined speed to achieve an even deposition of the material. In order to vapor-deposit material, a certain material-specific temperature range is required which is realized by a software-based temperature controller which manages the evaporation rate according to the user's specifications. A user interface facilitates planning of the desired OLED layer stack and provides information about the production progress. The capabilities of our new PVD system were tested by producing OLEDs based on multiple-resonance TADF emitters of the DABNA series. We performed electro-optical LJV-characterization and determined the devices'quantum efficiencies. The results of this investigation will enable us to optimize the production process with regard to evaporation rates and layer thicknesses.

HL 19.10 Tue 12:00 GÖR 226

improvement of electrical transport in organic semiconductor thin films by charge transfer doping — •Hongwon Kim[1], Andreas Opitz[2], Florian Fenzl[1], and Wolfgang Brütting[1] — [1]Experimentalphysik IV, Institut für Physik, Universität Augsburg — [2]Institut für Physik, Supramolekulare Systeme, HU zu Berlin

Charge carrier transport in organic semiconductor is based on the hopping mechanism. We have used in-situ charge transfer doping during film-growth to improve the electrical conductivity by simultaneously increasing the carrier density and reducing their thermal activation energy. By doping planar organic semiconductors, such as DBTTF, a-6T, and DIP, with strong acceptors (F6-TCNNQ & HATCN), hybridization of pi-orbitals occurs while generating new interphases (charge transfer complex, CTC). On the other hand, DBP, a non-planar molecule, forms an amorphous thin film without any CTC generation. To measure the characteristics of CTC, we used near-infrared transmission spectroscopy, which can detect the absorption peaks of CTCs and the energy gap. In addition, the activation energy is obtained from temperature-dependent conductivity measurements. We observe a correlation between the magnitude of the electrical conductivity and its activation energy, which can be ascribed to the binding energy of CTCs. Depending on the specific system, conductivity maxima are observed between 10 and 30% molar doping ratios.

HL 19.11 Tue 12:15 GÖR 226

Electrical transport dynamics of conducting polymers in nanoconfinement — Sukanya Das and •K.S. Narayan — Chemistry and Physics of Materials Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru- 560064, India

Inherently disordered conducting polymers consist of different characteristic lengths, defect distribution over the polymer chains and their microstructural modifications can alter the transport properties significantly. The electrical transport of conducting polymers such as poly(3,4-ethylene dioxythiophene): poly(styrenesulfonate) PEDOT:PSS has shown conductivity enhancement when confined in an array of nanochannels in the form of alumina nanopillars. The transverse conductivity along the nanopillar axis, which is an otherwise suppressed quantity, increases nonlinearly by approximately three orders in magnitude as the diameter of the scaffold-channel is decreased to 20 nm, when measured at single nanochannel level as well as at bulk-macroscopic level. This suggests the major role of dimensions and geometry in eliciting efficient electrical transport. Similarly, more than 3 orders of conductivity increase have been shown by in-situ polymerized poly(3,4-ethylenedioxythiophene):tosylate within the nanochannels which has similar electronic backbone PEDOT but a different dopant environment. The microscopic insight into PEDOT:Tos has shown higher degree of crystallinity and ordering as compared to PEDOT:PSS nanochannels. We utilize this property of PEDOT:PSS to fabricate hybrid organic-inorganic perovskite photodiode with efficient hole extraction and faster response times in the nanoconfined devices.

HL 19.12 Tue 12:30 GÖR 226

In-situ spectro-electrochemistry of N-type conjugated organic systems for opto-electronic and electro-optic applications — •Meenal Kataria and Sabine Ludwigs — IPOC-Functional Polymers, Institute of Polymer Chemistry, University of Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart, Germany

This talk will highlight our ongoing research on in-situ spectroelectrochemistry. We are developing functional organic conjugated materials and devices for opto-electronic and electro-optic applications. Here, one of our aims is to utilize an in-situ spectroelectrochemical approach to calculate the energy levels of blends of donor polymers (e.g. PM6) and non-fullerene acceptors (e.g. Y6) utilized for high performance organic solar cells. For relevant device information it is important to have precise values of energy levels of the same blend systems as used in devices. Thus, our absorption assisted electrochemistry technique proved be advantageous approach (1). In another research work discussing the effect of isomerism on conductivity of n-type polymers (e.g. P(NDI2OD-T2)), this above approach has been used to identify the redox states during electrochemical doping which helped to identify the charge transfer transport mechanism (2). In the last example, this technique has been utilized to calculate the frontier energy levels of push-pull D-π-A systems and to study the effect of acceptor strength on their energy levels (3).

Ref. (1) J. Mater. Chem. C 2022, 10, 11565. (2) Chem. Mater. 2019, 31, 3542. (3) Phys.Chem.Chem.Phys. 2020, 22, 2283.

HL 19.13 Tue 12:45 GÖR 226

Delocalization Enhances Conductivity at High Doping Concentrations — •Dennis Derewjanko[1], Dorothea Scheunemann[1], Emmy Järsvall[2], Anna I. Hofmann[2], Christian Müller[2], and Martijn Kemerink[1] — [1]IMSEAM, Heidelberg University, Im Neuenheimer Feld 225, 69120 Heidelberg, Germany — [2]Department of Chemistry and Chemical Engineering, Chalmers University of Technology, 41296 Gothenburg, Sweden

Many p-type organic semiconductors are experimentally found to follow a universal power-law trend between conductivity and charge carrier concentration at practically relevant high doping levels. This behavior cannot consistently be explained by conventional charge transport models. Here, we develop a physically transparent model based on the combination of a tight binding model and a variable range hopping model to show that the observed power-law trend can be explained by consideration of an energy dependent localization length. The underlying cause is an energetic lifting of the charge carriers to partly delocalized states due to the rising Fermi energy level at high charge carrier concentration. At low charge carrier concentrations, the well-known Mott-Martens model is recovered.

HL 20: Focus Session: Frontiers of Electronic-Structure Theory I (joint session O/HL)

Time: Tuesday 10:30–12:45 Location: TRE Ma

HL 20.1 Tue 10:30 TRE Ma

Two-component GW implementation for molecular valence excitations — •Qinglong Liu, Ramón L. Panadés-Barrueta, and Dorothea Golze — Chair of Theoretical Chemistry, Technische Universit at Dresden, 01062 Dresden, Germany

We present an all-electron GW implementation for the computation of charged molecular excitations, that includes scalar relativistic effects and spin-orbit coupling (SOC). Our method is based on a two-component (2c) approach, which can process 2c spinors and their corresponding eigenvalues from different levels of theory. The relativistic input for our 2c GW calculation is obtained in two ways: One approach is a non-self-consistent second variation SOC scheme, i.e. a scalar relativistic (SR) calculation is performed followed by an expansion of the spinors on top of the SR eigenvectors [1]. Another approach is the spinors and their eigenvalues are obtained by running a self-consistent relativistic DFT calculation with the X2C method [2]. Our algorithm has been implemented in the FHI-aims program package, which is based on numeric atom-centered orbitals (NAOs). In our 2c GW algorithm we combine the all-electron NAO scheme with the resolution of the identity technique based on the Coulomb metric (RI-V) and use the analytical continuation to evaluate the G_0W_0 self energy. We present results for the numerical validation of our implementation and for the influence of the relativistic input (second variation SOC vs X2C) on the valence excitations of small heavy molecules.

[1] W. Huhn and V. Blum, Phys. Rev. Materials 1, 033803 (2017)
[2] M. Iliaš and T. Saue, J. Chem. Phys. 126, 064102 (2007)

HL 20.2 Tue 10:45 TRE Ma

Screened potential in two-dimensional GW calculations within the LAPW framework — •Ben Alex, Sven Lubeck, and Claudia Draxl — Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

To calculate two-dimensional (2D) materials in a three-dimensional periodic code, one has to consider periodically repeated layers. The calculation of quasiparticle energies for 2D materials within the GW approximation requires the introduction of a 2D cutoff for the Coulomb potential as the layers would otherwise interact with each other. This cutoff leads to a stronger q dependence of the dielectric function around $q = 0$ which requires much denser sampling of the first Brillouin zone. In order to address this issue, an analytic expression for the dielectric function was previously derived for a plane-wave basis [1]. This expression is then integrated numerically in a small region around $q = 0$. The goal of this work is to adapt this technique to the linearized augmented planewave + local-orbital (LAPW+lo) basis as implemented in the full-potential all-electron code `exciting`. We show that also in our case, we obtain a significant computational speedup. Furthermore, this approach is compared with an approach where the dielectric function is interpolated to a denser q-grid.

[1] F. A. Rasmussen et al., Phys Rev B 94, 155406 (2016).

HL 20.3 Tue 11:00 TRE Ma

GW multipole approach for the frequency description of the dielectric screening — •Claudia Cardoso[1], Dario A. Leon[2], Andrea Ferretti[1], Daniele Varsano[1], and Elisa Molinari[1] — [1]S3 Centre, Istituto Nanoscienze, CNR, 41125, Modena (Italy) — [2]Department of Mechanical Engineering and Technology Management, Norwegian University of Life Sciences, 1430, Ås (Norway)

In the present work, we discuss a numerical approach for GW calculations that takes into account the frequency dependence of the screening via a multi-pole approximation (MPA), an accurate and efficient alternative to current full-frequency methods, that overcomes several limitations of the plasmon pole approximation (PPA).

MPA was recently developed and validated for semiconductors[1]. We now extend the use of MPA to metallic systems by optimizing the frequency sampling for these class of materials and propose a simple method to include the zero q limit of the intra-band contributions. The good agreement between MPA and full frequency results for the calculations of quasi-particle energies, polarizability, self-energy and spectral functions in different metallic systems confirms the accuracy and computational efficiency of the method. Finally, we discuss the physical interpretation of the MPA poles through a comparison with experimental electron energy loss spectra for Cu.

[1] D. A. Leon, C. Cardoso, T. Chiarotti, D. Varsano, E. Molinari, A. Ferretti, Phys. Rev. B 104, 115157

Topical Talk HL 20.4 Tue 11:15 TRE Ma

Towards low-scaling GW calculations for 2D materials — •Jan Wilhelm — Institute of Theoretical Physics, University of Regensburg

Semiconducting two-dimensional materials are an ideal platform to study excitons thanks to the strong exciton binding energy and good experimental accessibility of the excitons. The GW+Bethe-Salpeter approach (GW+BSE) has been successful in analyzing excitons in single-layer 2D materials [1], but the application of GW+BSE is challenging for 2D double layers and moiré structures [2]. This is because the large unit cells in these structures contain hundreds to thousands of atoms, resulting in a high computational cost for GW+BSE calculations. In this talk, I will present a low-scaling GW algorithm for 2D materials that potentially allows for the inclusion of more than a thousand atoms in the simulation [3]. This algorithm is based on localized basis functions and can handle periodic boundary conditions and the divergence of Coulomb interactions in the Brillouin zone. I will present first benchmark calculations.

[1] D. Y. Qiu, F. H. da Jornada, S. G. Louie, PRL 111, 216805 (2013). [2] Nat. Phys. 17, 720 (2021), Nature 608, 499 (2022), Science 376, 406 (2022), Nature 603, 247 (2022). [3] J. Wilhelm, D. Golze, L. Talirz, J. Hutter, C. Pignedoli, JPCL 9, 306 (2018), J. Wilhelm, P. Seewald, D. Golze, JCTC 17, 1662 (2021).

15 min. break

HL 20.5 Tue 12:00 TRE Ma

Accelerating core-level GW calculations by combining the contour deformation with the analytic continuation of W — •Ramón L. Panadés Barrueta and Dorothea Golze — Theoretische Chemie, Technische Universität Dresden, Bergstr. 66c, 01062 Dresden, Deutschland

Many-body methods, like the GW approximation, have recently proven to be a highly effective tool for computing core-level excitations [1]. In particular, the contour deformation (CD) is an efficient, scalable and numerically stable approach that has enabled core-level calculations on systems up to 100 atoms [2]. In this work, we reduce the scaling of CD applied to core-levels from $O(N^5)$ to $O(N^4)$, using an analytic continuation of the screened Coulomb interaction W [3]. The new method (CD-WAC) has been implemented in FHI-aims. CD-WAC has been extensively tested on well established benchmark sets like the GW100 and the CORE65, reporting MAEs of less than 5 meV with respect to CD. The theoretical scaling has been confirmed by performing scaling experiments on large acene chains and amorphous carbon. Speedups of 5 times have been attained with CD-WAC for the largest systems.

[1] D. Golze, M. Dvorak, and P. Rinke. Front. Chem., 7:377, 2019.
[2] D. Golze, J. Wilhelm, M.J. Van Setten, and P. Rinke. J. Chem. Theory Comput., 14(9):4856-4869, 2018.
[3] I. Duchemin and X. Blase. J. Chem. Theory Comput., 16(3):1742-1756, 2020.

HL 20.6 Tue 12:15 TRE Ma

Many-Body Effects of Metals Investigated by Means of the GW Method — •Zimo Zhou, Nakib Protik, and Claudia Draxl — Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

Even if semilocal exchange-correlation functionals of density-functional theory (DFT) can capture the overall band structure of many metals well, they fail to obtain the correct position of the d-bands. This leads, for instance, to the underestimation of the interband absorption onset in the corresponding optical spectra as shown for a set of elemental metals [1]. In this work, we provide a systematic investigation of the quasi-particle band structure and the optical properties of this set of materials. To this extent, the self-energy corrections to the DFT results are computed by the GW approach of many-body perturbation theory as implemented in the full-potential all-electron code exciting [2,3]. We show that the optical absorption spectra based on these quasi-particle bands remedy the shortcomings of semi-local DFT, accurately reproducing the experimental counterparts.

[1] W. S. M. Werner, K. Glantschnig, and C. Ambrosch-Draxl, J.

Phys. Chem. Ref. Data 38, 1013 (2009). [2] A. Gulans, S. Kontur, C. Meisenbichler, D. Nabok, P. Pavone, S. Rigamonti, S. Sagmeister, U. Werner, and C. Draxl, J. Phys: Condens. Matter 26, 363202 (2014). [3] D. Nabok, A. Gulans, and C. Draxl, Phys. Rev. B 94, 035418 (2016).

HL 20.7 Tue 12:30 TRE Ma

Separable Resolution-of-Identity in an all-electron numeric atom-centered basis set framework — •Francisco Delesma[1], Dorothea Golze[2], and Patrick Rinke[1] — [1]Department of Applied Physics, Aalto University, Espoo, Finland — [2]Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, Dresden, Germany

The resolution-of-identity (RI) is a common way in quantum chemistry and computational materials science to reduce the computational cost of two-electron Coulomb integrals, another central entity in computational quantum mechanics. In 2019, Duchemin and Blase proposed the separable-RI approach [1], which preserves the accuracy of the standard, global RI method with the Coulomb metric (RI-V) and permits the formulation of cubic-scaling random-phase approximation (RPA) and Green's function based GW approaches.

In this work, we present the first implementation of the separable-RI in an all-electron numeric atom-centered orbital framework. Separable-RI is implemented in the FHI-aims code [2] and optimized for massively parallel execution. We extend the separable-RI framework beyond the original Hartree-Fock (HF) and GW implementations of Duchemin and Blase to MP2 and RPA, SOSEX and CCSD. Our separable-RI total energies and GW quasiparticle energies for the Thiel test set of small organic molecules reproduce the exact two-electron Coulomb integral calculations within 1 meV or better.

[1] I. Duchemin and X. Blase, J. Chem. Phys. 150, 174120 (2019)
[2] V. Blum, et al, Comput. Phys. Commun. 180, 2175, (2009)

HL 21: Thermal properties

Time: Tuesday 11:00–11:45 Location: POT 361

HL 21.1 Tue 11:00 POT 361

Wigner thermal transport in rare-earth zirconates and their solid solutions — •Anees Pazhedath[1], Lorenzo Bastonero[1], Nicola Marzari[1,2], and Michele Simoncelli[3] — [1]U Bremen Excellence Chair, Bremen Center for Computational Materials Science, and MAPEX Center for Materials and Processes, University of Bremen, D-28359 Bremen, Germany — [2]Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [3]Cavendish Laboratory, Theory of Condensed Matter Group, University of Cambridge, England

Anharmonicity and disorder are both limiting factors for heat transport, and understanding how their interplay determines thermal conductivity is crucial to devise design strategies for thermal barrier coatings (TBC). Rare-earth (RE) zirconates are prospective TBC materials, owing to their strong anharmonicity and disorder tunable through alloying. Here, we use the Wigner transport equation in conjunction with state-of-the-art first-principles simulations to elucidate the microscopic physics underlying thermal transport in solid solutions of RE-zirconates, analyzing solutions of $La_2Zr_2O_7$ and $Yb_2Zr_2O_7$ as a paradigmatic test case. This work deepens our understanding on how the interplay between disorder and anharmonicity affects thermal transport in complex crystals with glass-like conductivity, also extending the reach of first-principles simulations to the description of thermal transport in RE-zirconate solid solutions

HL 21.2 Tue 11:15 POT 361

The Influence of Anharmonicity on Negative Thermal Expansion of α-Sn — •Reinhard K. Kremer[1], Paweel T. Jochym[2], Jan Lazewski[2], Andrzej Ptok[2], Przemyslaw Piekarz[2], Andrzej M. Olés[3], and Eva Brücher[1] — [1]MPI for Solid State Research, Stuttgart, Germany — [2]Institute of Nuclear Physics, Polish Academy of Sciences, Krakow, Poland — [3]Institute of Theoretical Physics, Jagiellonian University, Krakow, Poland

The lattice vibrational properties of α-Sn (gray tin) were investigated experimentally by temperature dependent x-ray diffraction and theoretically by density functional theory calculations. Similar to the other elements of group IV, α-Sn exhibits a lattice anomaly at low temperatures and negative thermal expansion, with a minimum at ~ 27 K and a magnitude three times larger than in Si. Influence of anharmonic effects up to 4th order potential terms on the phonon dispersion relations, the lattice parameters, and the thermal expansion coefficient have been tested. The performed analysis gives an excellent agreement with experiment when quartic potential terms are included in the theory. We point out that negative thermal expansion in α-Sn is not driven by anharmonicity of interatomic potential. This resolves the long-standing puzzle in the thermal behavior of α-Sn.

HL 21.3 Tue 11:30 POT 361

Origin of thermal anisotropy in monoclinic $\beta - Ga_2O_3$ — •Markus R. Wagner[1,2], Benjamin M. Janzen[2], Zbigniew Galazka[3], Bartlomiej Graczykowski[4], Kai Xu[5], Ricardo Rurali[5], and Juan Sebastian Reparaz[5] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]Technische Universität Berlin, Germany — [3]Leibniz-Institut für Kristallzüchtung, Berlin, Germany — [4]Faculty of Physics, Adam Mickiewicz University, Poland — [5]Institut de Ciència de Materials de Barcelona, ICMAB-CSIC, Spain

We present a comprehensive all-optical contact-free investigation of the anisotropy of GHz and THz phonon-mediated material properties in $\beta - Ga_2O_3$. The full thermal conductivity tensor is determined by a newly developed all-optical experimental technique that enables sub-degree angular resolution in the measurement of the in-plane anisotropy of the thermal conductivity based on anisotropic frequency-domain thermoreflectance. Using this novel approach we determine the in-plane anisotropy of the thermal conductivity and its anisotropy ratio with high precision. The anisotropy of the sound velocity, elasticity, and Young modulus is measured by polarized, angular-resolved Brillouin light scattering of GHz acoustic phonons. Based on the experimental anisotropy maps of acoustic phonon velocities and thermal conductivity in combination with calculations of the phonon density of states and phonon lifetimes, we discuss the individual contributions of phonon velocities and phonon lifetimes to the anisotropy of the thermal conductivity.

HL 22: 2D Materials IV (joint session HL/CPP)

Time: Wednesday 9:30–12:30 Location: POT 81

HL 22.1 Wed 9:30 POT 81

Nonlinear optical characterization of atomically thin layers of the transition metal dichalcogenides WSe_2 and MoS_2 — •Henry Volker Hübschmann[1], Gerhard Berth[1], Ioannis Caltzidis[1], Katharina Burgholzer[2], Alberta Bonanni[2], and Klaus D. Jöns[1] — [1]Department of Physics, Paderborn University, 33098 Paderborn, Germany — [2]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, 4040 Linz, Austria

In the field of quantum technologies functional 2D-structures based on transition metal dichalcogenides like WSe_2 and MoS_2 represent a novel material platform due to their specific optical and electronic properties. In contrast to semimetallic graphene they feature an electronic band gap and a strong spinorbit coupling. Applications of such layered 2D-materials in functional structures are to be found within photonics, spinorbitronics or nanoelectronics. In this work we present our fundamental nonlinear study on mechanically exfoliated atomically thin layers of the semiconductors WSe_2 and MoS_2. In this context, the second harmonic generation was determined for both van der Waals layered material systems as a function of the layer number. The respective nonlinear behavior was proven by a power-dependent characterization and supplemented by polarimetric analysis. Nonlinear imaging of the flakes was successfully performed by confocal SH-microscopy. In a further step the oxidation of MoS_2 layered systems was analyzed, here it was shown that for an even number of layers the oxidation leads to a break of their centrosymmetric structure, which is manifested in the clear presence of a relatively strong second harmonic signal.

HL 22.2 Wed 9:45 POT 81

Single Photon Emitters in hBN via ultra-low energy helium ion implantation — •Prokhor Tkhor[1,2], Minh Bui[1,2], Renu Rani[1], Thorsten Brazda[1], and Beata E. Kardynał[1,2] — [1]Peter Grünberg Institut-9, Forschungszentrum Jülich, Jülich — [2]Department of Physics, RWTH Aachen, Aachen

Properties of heterostructures of transition metal dichalcogenides depend strongly on the moire lattice configuration and on the strength of coupling between the constituent monolayers. The first one can be controlled by the lattice constant of the constituent monolayers and their relative orientation, while the latter can be tuned by changing the spacing between them. In this contribution, we study a heterostructure of monolayers of WSe2/ hBN/ WSe2 with a moire potential periodicity of around 5 nm. The insertion of a monolayer of hBN between the two WSe2 monolayers results in a weak coupling between them. We discuss the results of the measurements of the dependence of the photoluminescence on the doping and electric field in this system. In this system the lowest intralayer excitonic states are optically spin-forbidden and at low electron concentration the effect of the moire potential on scattering of electrons and excitons dominates the optical signal masking the effect of correlations. Further, we discuss the observed non-monotonic charge shifts between the monolayers as a function of applied electric field.

HL 22.3 Wed 10:00 POT 81

Thin hexagonal boron nitride in the deep-UV: The pursuit of single photon emitters and their properties — •Nils Bernhardt[1], Luka Choi[1], Felix Nippert[1], Angus Gentle[2], Milos Toth[2], and Markus R. Wagner[1,3] — [1]Technische Universität Berlin, Berlin, Germany — [2]University of Technology Sydney, Sydney, Australia — [3]Paul-Drude-Institut, Berlin, Germany

Interest in hexagonal boron nitride (hBN) continues to grow in optoelectronics with the discovery of an increasing number of quantum emitters in all spectral ranges. The wide band gap and chemical stability inherent to this material encourage hBN as a semiconductor substrate, while the possibility of reliably fabricating thin films entails unusual and unique properties. Consequently, room-temperature defect quantum emitters with reproducible emission properties from the UV to the near-IR can be engineered for applications such as quantum communication.

In this work, we investigate the recently observed luminescence of hBN at 4.1eV with a pulsed, frequency-tripled titanium-sapphire laser at 240nm. Experimental methods such as photoluminescence spectroscopy and time-resolved fluorescence spectroscopy are utilized alongside a Hanbury Brown and Twiss interferometer for correlation measurements in the deep UV as a means to identify single-photon emitters. Through this approach, we are able to establish a scientific basis for further investigation into the UV emission of hBN.

HL 22.4 Wed 10:15 POT 81

Electrical control of excitonic complexes in $MoSe_2$ homobilayers — •Bárbara Rosa[1], Chirag Palekar[1], Alisson Cadore[2], Yuhui Yang[1], Aris Koula-Simos[1], Sefaattin Tongay[3], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Berlin, Germany — [2]Brazilian Nanotechnology National Laboratory, Campinas, Brazil — [3]School for Engineering of Matter, Transport and Energy, Arizona State University, Tempe, USA

Effects of periodic Moiré potential in transition metal dichalcogenides (TMDs) bilayers are directly controlled by the twist angle between the monolayers. Novel features arising from intra- and interlayer excitons, such as their ultrafast formation and charger transfer, long population recombination lifetimes, and binding energy of dozens of meVs, turn TMD heterostructures into an attractive device for the study and manipulation of optical and transport properties via electrical fields. Moreover, such effects may appear even more pronounced at twisted homobilayers, since the absence of lattice mismatch promotes the appearance of larger Moiré superlattices. In this work, we explore the ability to control excitonic complexes in $MoSe_2/MoSe_2$ twisted bilayers (t-BLs) by performing gate-dependent microphotoluminescence (μPL) spectroscopy at room temperature. We observe the energy tunability of several meVs occurring at the emission of excitonic complexes derived from the t-BL region. In addition, other effects, such as the emergence of new excitonic features, are observed through μPL spectroscopy at cryogenic temperatures.

15 min. break

HL 22.5 Wed 10:45 POT 81

Tailoring Coulomb interactions in WS_2-graphene heterostructures — •David Tebbe[1], Marc Schütte[1], Kenji Watanabe[2], Takashi Taniguchi[3], Christoph Stampfer[1], Bernd Beschoten[1], and Lutz Waldecker[1] — [1]2nd Institute of Physics A, RWTH Aachen University — [2]Research Center for Functional Materials, Japan — [3]International Center for Materials Nanoarchitectonics, Japan

The exciton binding energy and the quasiparticle bandgap in two dimensional semiconductors depend on their dielectric environment.

We investigate the screening of Coulomb interactions in heterostructures of WS_2 and graphene, separated through thin spacer layers of hexagonal boron nitride (hBN). By using hBN spacers from one to 16 atomic layers, we experimentally determine the tuning of the exciton binding energy and the quasiparticle bandgap as a function of the WS_2-to-graphene interlayer spacing.

This change in both energies is well described by a one over distance dependence, which is consistent with a screening arising from an image charge induced by the graphene layer.

Additionally, by doping the graphene with a graphitic back gate, we show that the ability of the graphene to screen Coulomb interactions in neighbouring layers is strongly modified. We determine the change in screening strength to be approximately 20% at room temperature, demonstrating that Coulomb-interactions in WS_2 can be modified in-situ without changing the doping level of the material itself.

HL 22.6 Wed 11:00 POT 81

Evidence for equilibrium exciton condensation in monolayer WTe2 — •Massimo Rontani — CNR-NANO, Modena, Italy

We present evidence [1] that the two-dimensional bulk of monolayer WTe2 contains electrons and holes bound by Coulomb attraction, excitons, that spontaneously form in thermal equilibrium. On cooling from room temperature to 100 K, the conductivity develops a V-shaped dependence on electrostatic doping, while the chemical potential develops a step at the neutral point. These features are much sharper than is possible in an independent-electron picture, but they can be accounted for if electrons and holes interact strongly and are paired in equilibrium. Our calculations from first principles show that the exciton binding energy is larger than 100 meV and the radius as small as 4 nm, explaining their formation at high temperature and doping levels.

Below 100 K, more strongly insulating behaviour is seen, suggesting that a charge-ordered state forms. The observed absence of charge density waves in this state is surprising within an excitonic insulator picture, but we show that it can be explained by the symmetries of the exciton wavefunction. Therefore, in addition to being a topological insulator, monolayer WTe2 exhibits strong correlations over a wide temperature range.

This work is done in collaboration with Elisa Molinari, Daniele Varsano, Samaneh Ataei, Maurizia Palummo, Bosong Sun, David Cobden. It is partially funded by MUR PRIN2017 No. 2017BZPKSZ EXC-INS and MaX EU Center of Excellence.

[1] B. Sun et al., Nature Physics 18, 94-99 (2022).

HL 22.7 Wed 11:15 POT 81

Charge and exciton quenching at defect states in TMDC-graphene heterostructures — •Daniel Hernangómez-Pérez[1], Amir Kleiner[1], Andrea Donarini[2], and Sivan Refaely-Abramson[1] — [1]Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, 7610001 Rehovot, Israel — [2]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

In recent years, studies of charge transfer and excitonic properties of van der Waals heterostructures have revealed a fertile research arena, spanning Coulomb blockade physics [1], ultrafast interlayer charge separation [2] or graphene-quenched photoluminescence [3]. We theoretically study charge transfer and excitonic properties in XS_2-graphene (X = W, Mo) heterobilayers with monoatomic chalcogen vacancies [4-5]. We discuss the impact of the subgap defect-based features in the microscopic dynamics, as well as the interplay between spatial symmetries and the spin degree of freedom through the spin-orbit interaction. Finally, we report the electronic and optical properties computed by many-body perturbation theory and show how defects and graphene alter the absorption properties of the TMDC due to a combination of folding, commensuration and impact of defect in-gap energy bands.

[1] N. Papadopoulos, *et al.* Phys. Rev. B 101, 165303 (2020). [2] S. Aeschlimann, *et al.* Science Advances 6 (20)(2020). [3] E. Lorchat, *et al.*, Nat. Nano. 15, 283 (2020). [4] D. Hernangómez-Pérez, A. Donarini, and S. Refaely-Abramson, arXiv:2209.14420. [5] D. Hernangómez-Pérez, A. Kleiner, and S. Refaely-Abramson (in preparation).

15 min. break

HL 22.8 Wed 11:45 POT 81

The influence of anisotropy on excitons in magnetic semiconductors — •Marie-Christin Heissenbüttel, Thorsten Deilmann, and Michael Rohlfing — Institute of Solid State Theory, University of Münster, Germany

Understanding the peculiar interrelation between crystal structure, magnetic properties and light-matter interaction in semiconducting two-dimensional-like magnets is of fundamental interest. From our ab-initio *GW*/Bethe-Salpeter equation calculations, we are able to examine electronic and excitonic properties on the same footing.

Because of its large crystal anisotropy combined with in-plane ferromagnetism, the van-der-Waals stacked CrSBr has recently come to the fore e.g. to study correlated phenomena. Due to the unique interplay of anisotropy, two-dimensional magnetism and optoelectronic properties resulting in a quantum confinement, we observe very flat dispersions, different effective masses and a quasi-1D behaviour of excitons within a monolayer of CrSBr [1]. Moreover, we find that the Rydberg series of two excitonic states is intricately modified by the different extension of the wavefunctions within momentum space.

[1] https://arxiv.org/abs/2205.13456

HL 22.9 Wed 12:00 POT 81

From $MoSe_2$ to MoS_2 and everything in-between — •Jennifer Schmeink, Vladislav Musytschuk, Nicolas Hille, Erik Pollmann, Peter Kratzer, and Marika Schleberger — Universität Duisburg-Essen, Fakultät für Physik, Germany

Asymmetrical, or Janus transition metal dichalcogenide (TMDC) monolayers such as MoSSe are a current hot topic in the field of two-dimensional (2D) materials due to their unique properties. The most common approach of fabrication is to start off from one of the two base TMDCs' monolayer and selectively substitute the top-most layer of chalcogen atoms with another kind. However, if the substitution is partial, the resulting material resembles more an alloy than a Janus-type structure. These in-between materials show their own interesting features, as they allow for example a fluid optical bad-gap tuning from that of $MoSe_2$ at 1.54 eV over 1.70 eV for MoSSe up to 1.84 eV of MoS_2. In my talk I want to show off the varying optical and electronic properties of these $MoS_{2(1-x)}Se_{2x}$ ($0 \leq x \leq 1$) structures with a special focus on the Janus-type MoSSe monolayer. This talk will explore the fascinating question of what lies in between.

HL 22.10 Wed 12:15 POT 81

Optimized Irradiation Protocol for Quantum Sensors in Hexagonal Boron Nitride — •Paul Konrad[1], Andreas Gottscholl[1], Andreas Sperlich[1], Igor Aharonovich[2], and Vladimir Dyakonov[1] — [1]Experimental Physics 6, Julius-Maximilians-University of Würzburg, 97074 Würzburg — [2]School of Mathematics and Physical Sciences, University of Technology Sydney, Ultimo, NSW 2007, Australia

Colour centres in solid-state materials show great potential in quantum information technology and sensing applications. The lately discovered negatively charged boron vacancy (V_B^-) in hexagonal boron nitride (hBN)[1] has shown that the defect exhibits a spin-triplet ground state with spin-dependent photoluminescence. The system can be exploited in terms of its application as temperature, magnetic field, and pressure sensor [2,3] which extends the already known applications of e.g. NV-centers in diamond not only due to its 2D character but also by highly improved temperature sensing especially at low temperatures.

Here we present an irradiation protocol for creation of V_B^- by nitrogen ions, leading to optimized spin relaxation parameters and therefore improving quantum metrology limits. We also present tremendous improvement of ODMR contrast showing hyperfine interaction on flakes of down to 80nm thickness.

[1] Gottscholl et al., *Nat. Mat.*, **19**, 5, 540 (2020).
[2] Gottscholl et al., *Sci. Adv.*, **7** (14), eabf3630 (2021).
[3] Gottscholl et al., *Nat. Commun.*, **12**, 4480 (2021).

HL 23: Focus Session: Breakthroughs in wide-bandgap semiconductor laser diodes I

Recently, a number of significant breakthroughs have taken place in the area of wide-bandgap semiconductor laser diodes. The exploration of the limits of III-nitride materials, the improved understanding of the optical and electronic properties allowed to push the lasing wavelength towards the UV-B and UV-C spectral range with AlGaN-based laser diodes emitting at record short wavelength near 270 nm and 300 nm. In addition, advanced designs and fabrication technologies have led to the realization of novel devices in the blue-violet and even UV spectral range such as low-threshold VCSELs, narrow-linewidth GaN-based DFB laser diodes and photonic crystal lasers. In this focus session we will review these recent developments and discuss the future challenges and application for these devices.

Organized by Tim Wernicke, Ulrich Schwarz, and Michael Kneissl

Time: Wednesday 9:30–12:15 Location: POT 361

Invited Talk HL 23.1 Wed 9:30 POT 361

Vertical-cavity surface-emitting lasers – this is the way — •Å. Haglund[1], G. Cardinali[2], L. Persson[1], F. Hjort[1], J. Enslin[2], E. Torres[1], C. Kuhn[2], S. Graupeter[2], M. Grigoletto[2], M. A. Bergmann[1], N. Prokop[2], M. Guttmann[2], L. Sulmoni[2], N. Lobo Ploch[3], M. Cobet[2], T. Kolbe[3], J. Gustavsson[1], F. Nippert[2], I. Häusler[2], M. R. Wagner[2], J. Ciers[1], T. Wernicke[2], and M. Kneisl[2,3] — [1]Chalmers University of Technology, Göteborg, Sweden — [2]Technische Universität Berlin, Berlin — [3]FBH, Berlin

In recent years, there has been tremendous improvement in the performance of blue-emitting vertical-cavity surface-emitting lasers (VCSELs). Ultraviolet (UV)B (280-320 nm) and UVC (<280 nm) VCSELs have also been demonstrated, but so far only under optical pumping. All VCSELs require high reflectivity mirrors with an accurate cavity length control, but there is today no consensus on which is the best approach to realize this. We will summarize state of the art and then go into depth on our concept which is based upon using all-dielectric distributed Bragg reflectors where substrate removal is achieved by selective electrochemical etching. This approach has enabled the world's first UVB VCSEL at 310 nm. It also gives access to both sides of the cavity which allows for detuning postgrowth with drastically reduced lasing thresholds as well as an athermalized lasing wavelength. Thus, we believe that - this is the way - for nitride VCSELs. As a first step towards electrically injected UV VCSELs, we will demonstrate resonant cavity light emitting diodes with tunnel junctions.

Invited Talk HL 23.2 Wed 10:00 POT 361

Towards GaN-based diode lasers with narrow linewidth and high reliability — •Sven Einfeldt[1], Erik Freier[1], Ji-Hye Kang[1], Hans Wenzel[1], Anna Mogilatenko[1], Johannes Glaab[1], Asmaa Abou-Shewarib[1], Veit Hoffmann[1], Johannes Enslin[1], Martin Guttmann[1], Saad Makhladi[1], Jörg Fricke[1], Olaf Brox[1], Mathias Matalla[1], Maria Norman-Reiner[1], Christoph Stölmacker[1], Markus Weyers[1], Luca Sulmoni[2], Michael Kneissl[2], Lukas Uhlig[3], and Ulrich T. Schwarz[3] — [1]Ferdinand-Braun-Institut (FBH), Berlin, Germany — [2]Technische Universität Berlin, Institut für Festkörperphysik, Berlin, Germany — [3]Technische Universität Chemnitz, Institut für Physik, Chemnitz, Germany

Various applications require GaN-based diode lasers that not only operate in single-mode at well-defined wavelengths, but also exhibit a small linewidth and high reliability. Single-mode operation can be achieved via the distributed feedback (DFB) or distributed Bragg reflector (DBR) laser design, i.e. monolithic integration of gratings in the chip. We present here the current state of the art in fabrication technology and properties of DFB and DBR diode lasers with high-order laterally coupled surface gratings. These include continuous wave single-mode operation at room temperature with an optical power of up to 20 mW (DBR) and 70 mW (DFB), respectively, and spectral half widths of about 20 pm. We also show results of selected studies on the reliability of GaN-based lasers, in particular on the stability of the operating voltage, the evolution of spatial inhomogeneities in the current distribution in the chip, and the stability of the facets.

Invited Talk HL 23.3 Wed 10:30 POT 361

Use of wafer patterning for new functionalities of InGaN light emitters — •Anna Kafar[1,2], Ryota Ishii[3], Atsushi Sakaki[4], Kiran Saba[1], Conny Becht[5], Szymon Grzanka[1,2], Ulrich Schwarz[5], Mitsuru Funato[3], Yoichi Kawakami[3], and Piotr Perlin[1,2] — [1]Institute of High Pressure Physics PAS, Warsaw, Poland — [2]TopGaN Ltd., Warsaw, Poland — [3]Kyoto University, Kyoto, Japan — [4]Nichia Corporation, Tokushima, Japan — [5]Chemnitz University of Technology, Chemnitz, Germany

In this work we present the use of patterning of bulk GaN substrates to control the growth of InGaN layers by metalorganic vapour-phase epitaxy. We demonstrate that using local change of substrate miscut, it is possible to obtain a spatial shift of emission energy of above 25 nm. Synchrotron radiation microbeam X-ray diffraction reveals that a significant change of In content in the QWs is possible between 9% and 18%. This approach can be used for example in fabrication of micro-arrays of laser diodes with different lasing wavelength. Another application is the fabrication of superluminescent diodes with broadened emission spectra by utilizing a profile of indium content along the device waveguide. Furthermore, we use the same concept to demonstrate monolithic light-guides integrated with laser diodes on the same wafer and fabricated based on the same epitaxy. We also study the possibility to use substrate patterning in a form of micro strips and discs regions of improved quality InGaN which can be used for fabrication of the active regions of the micro LEDs and laser diodes.

30 min. break

HL 23.4 Wed 11:30 POT 361

Time-dependent intensity and wavelength dynamics of blue laser diodes with wide quantum wells — •Jannina Tepass[1], Lukas Uhlig[1], Mateusz Hajdel[2], Grzegorz Muziol[2], and Ulrich Theodor Schwarz[1] — [1]Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]Institute of High Pressure Physics, Polish Academy of Sciences, Poland

In this study, thick quantum wells with two different thicknesses of 10.4 nm and 25 nm are analyzed. The very low overlap of the electron and hole wavefunction in such QWs due to the quantum confined Stark effect would indicate inefficient devices. However, it has been shown that thick QWs can be more effective and achieve high optical gain. This can be explained by the electric field screening that leads to a high overlap of the excited electron and hole states, which enable lasing. In this work, a pulsed electrical excitation scheme is used in which carrier injection at forward voltage is largely separated from carrier recombination at zero or reverse voltage. Due to this effect, the interplay between the piezoelectric field and the built-in potential on the charge carrier recombination in dependence on an external bias voltage can be observed. In particular, a sharp increase in the radiative recombination rate after the trailing edge of the driving pulse is observed, as well as a wavelength shift.

HL 23.5 Wed 11:45 POT 361

Single-mode lasing in optically pumped UVB VCSELs with circular relief structures — •Giulia Cardinali[1], Filip Hjort[2], Johannes Enslin[1], Munise Cobet[1], Michael A. Bergmann[2], Johan Gustavsson[2], Joachim Ciers[2], Tim Kolbe[3], Felix Nippert[1], Markus R. Wagner[1], Tim Wernicke[1], Åsa Haglund[2], and Michael Kneissl[1,3] — [1]Institute of Solid State Physics, Technische Universität Berlin, Berlin, Germany — [2]Department of Microtechnology and Nanoscience, Chalmers University of Technology, Gothenburg, Sweden — [3]Ferdinand-Braun-Institut (FBH), Berlin, Germany

Extending the emission wavelength of vertical-cavity surface-emitting lasers (VCSELs) in the ultraviolet (UV) range would allow advances in many applications, e.g. in medical diagnostics, material curing, and sterilization. UV VCSELs have been demonstrated only under optical pumping and they suffer from strong filamentation (i.e. spatially inhomogeneous emission), resulting in multimode lasing. In this work, we

study the emission characteristic of optically pumped UVB VCSELs with circular reliefs dry-etched on the bottom cavity. Single-mode lasing near 312 nm was achieved for VCSELs with 25 nm-deep reliefs with diameters smaller than 5 μm, when pumped up to 80 MW/cm^2. Here, the lateral size of the cavity was reduced below the dimension of one filament. VCSELs with 5 nm-deep reliefs did not show single mode lasing. 50 nm-deep structures did not lase for diameters below 6 μm. The higher thresholds in this sample are due to defect generation in the quantum-well by the dry etching, which was confirmed by time-resolved photoluminescence measurements of the carrier lifetimes.

HL 23.6 Wed 12:00 POT 361

Use of wafer patterning for new functionalities of InGaN light emitters — •Anna Kafar[1,2], Kiran Saba[1], Ryota Ishii[3], Atsushi Sakaki[4], Szymon Grzanka[1,2], Conny Becht[5], Ulrich Schwarz[5], Mitsuru Funato[3], Yoichi Kawakami[3], and Piotr Perlin[1,2] — [1]Institute of High Pressure Physics PAS, Warsaw, Poland — [2]TopGaN Ltd., Warsaw, Poland — [3]Kyoto University, Kyoto, Japan — [4]Nichia Corporation, Tokushima, Japan — [5]Chemnitz University of Technology, Chemnitz, Germany

In this work we present the use of patterning of bulk GaN substrates to control the growth of InGaN layers by metalorganic vapour-phase epitaxy. We demonstrate that using local change of substrate miscut, it is possible to obtain a spatial shift of emission energy of above 25 nm. Synchrotron radiation microbeam X-ray diffraction reveals that a significant change of In content in the QWs is possible * between 9% and 18%. This approach can be used for example in fabrication of micro-arrays of laser diodes with different lasing wavelength. Another application is the fabrication of superluminescent diodes with broadened emission spectra by utilizing a profile of indium content along the device waveguide. Furthermore, we use the same concept to demonstrate monolithic light-guides integrated with laser diodes on the same wafer and fabricated based on the same epitaxy. We also study the possibility to use substrate patterning in a form of micro strips and discs regions of improved quality InGaN which can be used for fabrication of the active regions of the micro LEDs and laser diodes.

HL 24: Quantum dots: Optics

Time: Wednesday 9:30–13:15 Location: POT 151

HL 24.1 Wed 9:30 POT 151

Raman spectroscopic structure analysis of colloidal semiconductor core-shell quantum dots for the achievement of near-unity quantum efficiency — •Sandra Zech[1,2], Sonja Krohn[2], Hannes Van Avermaet[3], Zeger Hens[3], Jan Steffen Niehaus[4], Janina Maultzsch[1], and Holger Lange[2] — [1]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Institute of Physical Chemistry, University of Hamburg, Hamburg, Germany — [3]Physics and Chemistry of Nanostructures, Ghent University, Ghent, Belgium — [4]Fraunhofer IPA Center for Applied Nano-Technology CAN, Hamburg, Germany

State of the art applications of quantum dots (QDs) require near-unity photoluminescence quantum yield (PLQY). This demand is rarely achieved and therefore the synthesis process is under constant optimization and nanocrystals consisting of a core with one or more shells of different materials are paving the way to achieve high PLQY. As those components have diverse lattice parameters, the induction of strain within the QDs is inevitable. Recently, we applied Raman spectroscopy for in depth structure characterization and a strain minimization approach to optimize the synthesis of InP/ZnSe/ZnS QDs towards near-unity PLQY. A similar effect plays a role in CdSe/CdS QDs when aiming for high PLQY. In these QDs, the formation of an alloyed interface between the CdSe core and CdS shell is assumed. By Raman spectroscopy, we are able to monitor the formation of these alloyed domains for different QD parameters and correlate it with the PLQY.

HL 24.2 Wed 9:45 POT 151

Collective Excitation of Spatio-Spectrally Distinct Quantum Dots Enabled by Chirped Pulses — •Florian Kappe[1], Yusuf Karli[1], Thomas Bracht[2], Saimon Covre da Silva[3], Tim Seidelmann[4], Vollrath Martin Axt[4], Armando Rastelli[3], Gregor Weihs[1], Doris Reiter[2,5], and Vikas Remesh[1] — [1]Institute für Experimentalphysik, Universität Innsbruck, Innsbruck, Austria — [2]Institut für Festkörpertheorie, WWU Münster, Münster, Germany — [3]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, Linz, Austria — [4]Theoretische Physik III, Universität Bayreuth, Bayreuth, Germany — [5]Condensed Matter Theory, TU Dortmund, Dortmund, Germany

To boost the communication rate in quantum communication devices, it is desirable to have an ensemble of single photon sources that can be collectively excited, despite their spectral variability. Rabi rotation, the most popular method for resonant excitation of the quantum dot, cannot assure a highly efficient state preparation, due to its sensitivity to the excitation parameters. Here, we demonstrate the robustness of Adiabatic Rapid Passage, using chirped laser pulses and collectively excite biexciton states [1] in energetically and spatially distinct quantum dots. We also demonstrate a regime of phonon contribution that widens the detuning range. Being able to generate high-purity photons from spatially multiplexed quantum dot sources with high efficiency is a big step towards the implementation of high photon rate quantum key distribution protocols. [1] Kappe et al, https://arxiv.org/abs/2209.08972 (in peer review)

HL 24.3 Wed 10:00 POT 151

Prospects of atomic vapor-based storage of single photons emitted by a deterministically fabricated quantum dot device — •Avijit Barua[1], Benjamin Maass[2], Norman Vincenz Ewald[2], Suk-in Park[3], Sung-yul Park[3], Jin-Dong Song[3], Janik Wolters[2], and Stephan Reitzenstein[1] — [1]Technische Universität Berlin, Berlin, Germany — [2]German Aerospace Center (DLR), Berlin, Germany — [3]Korea Institute of Science and Technology, Seoul, Republic of Korea

Semiconductor quantum dots (QDs) are extensively investigated as single-photon sources for applications in photonic quantum technology. Here, we develop bright and strain-tunable QD single-photon sources at the Cs D1 transition wavelength and explore the storage ability of semiconductor QD in atomic quantum memories. The devices are designed and numerically optimized to maximize extraction efficiency using the finite element method. By considering circular Bragg resonators with integrated QDs and Au-backside mirror, we numerically demonstrate a photon extraction efficiency of 65% and a Purcell factor of 0.72. In the experimental development, we implement in-situ electron-beam lithography to precisely integrate selected single QDs at 894 nm in such structures to create bright single-photon sources. The emission from the developed quantum devices is studied by means of photon autocorrelation measurements. Furthermore, we explore the prospects of interfacing the QD single photons with a vapor-based quantum memory by employing a ladder-type EIT configuration that allows for low-noise storage and retrieval at high repetition rates.

HL 24.4 Wed 10:15 POT 151

Double pulse excitation schemes for enhanced multiphoton interference — •Yusuf Karli[1], Florian Kappe[1], Julian Munzberg[1], Thomas Bracht[2], Saimon Covre da Silva[3], Armando Rastelli[3], Doris Reiter[2,4], Robert Keil[1], Vikas Remesh[1], and Gregor Weihs[1] — [1]Institute für Experimentalphysik, Universität Innsbruck, Innsbruck, Austria — [2]Institut für Festkörpertheorie, WWU Münster, Münster, Germany — [3]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, Linz, Austria — [4]Condensed Matter Theory, TU Dortmund, Dortmund, Germany

High-efficiency generation multiphoton states is an important prerequisite for linear quantum computing applications. Semiconductor quantum dots are high-brightness sources of highly indistinguishable single photons, which can then be used to generate multiphoton states via active temporal-to-spatial demultiplexing. Resonant s-shell excitation is the most popular method to generate high-indistinguishability single photons from a quantum dot [1], however, at the cost of brightness from cross-polarization filtering. Here, we advocate the versatility of novel double-pulse excitation schemes by demonstrating an 8-fold enhancement in four-photon coincidence rates. [1] APL Photonics 7.7 (2022)

HL 24.5 Wed 10:30 POT 151

Towards deterministic generation of time-bin entangled photons from GaAs quantum dots — •Florian Kappe[1], Yusuf Karli[1], Thomas Bracht[2], Saimon Covre da Silva[3], Armando Rastelli[3], Vikas Remesh[1], Doris Reiter[2,4], and Florian Kappe[1] — [1]Institut für Experimentalphysik, Universität Innsbruck, Innsbruck, Austria — [2]Institut für Festkörpertheorie, WWU Münster, Münster, Germany — [3]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, Linz, Austria — [4]Condensed Matter Theory, TU Dortmund, Dortmund, Germany

Semiconductor quantum dots are bright, on-demand single photon sources suitable for realising quantum communication devices. Here, we present our first results towards the deterministic generation of time-bin entangled photon states via dark exciton states from GaAs/AlGaAs quantum dots. Our schemes employ chirped laser pulses and an external magnetic field that enables the coupling of bright and dark exciton states in the quantum dot [1,2]. Based on numerical methods we analyze the quantum dot dynamics and state preparation fidelity and identify that the preparation schemes are quite robust against the phonon influence.

[1] Phys. Rev. B. 92(20), (2015). [2] Phys. Rev. B 104.7 (2021).

HL 24.6 Wed 10:45 POT 151

Generation of indistinguishable and entangled photons at telecom frequencies using tailored cavity designs — •David Bauch, Dustin Siebert, Jens Förstner, Klaus D. Jöns, and Stefan Schumacher — Department of Physics, Electrical Engineering and CeOPP, Paderborn University, Germany

The commonly utilized biexciton-exciton cascade yields photons with intrinsically limited indistinguishability [1]. By tuning the biexciton-exciton lifetime ratio, large increases in single photon indistinguishability can be achieved [1,2]. Using the cavity-induced Purcell enhancement is a simple method for radiative lifetime tuning. Employing a circular Bragg reflector at telecom wavelengths for suitable quantum dots allows for a Purcell enhanced biexciton-exciton transition, while still maintaining high extraction efficiency for the exciton-ground state transition. The decreased lifetime of the biexciton results in a faster emission of then indistinguishable single photons. Here, we demonstrate this effect numerically and determine the theoretically required parameters for the biexciton-exciton transition to yield highly indistinguishable single photons, which are also entangled with their exciton-ground state emission counterpart. We guide our calculations using Maxwell simulations for the cavity design, allowing for close-to real-life system predictions. Our simulation demonstrates the robust increase of the indistinguishability of the emitted photons even when accounting for electron-phonon coupling at low temperatures.

[1] E. Schöll, et al., Physical Review Letters 125, 233605 (2020) [2] F. Sbresny, et al., Physical Review Letters 128, 093603 (2022)

HL 24.7 Wed 11:00 POT 151

Exciton diffusion in a quantum dot ensemble — •Karol Kawa and Paweł Machnikowski — Wrocław University of Science and Technology, 50-370 Wrocław, Poland

We study theoretically Förster transfer [1] of an exciton in an ensemble of quantum dots (QDs) randomly distributed on a circular mesa. In such a system energy transfer was observed experimentally within a spatially resolved photoluminescene sprectroscopy [2]. The analytical form of Förster coupling in the general ensemble of quantum dipole emitters is known [3–5]. It is a sum of three power-law terms diminishing with distance, each multiplied by an oscillating factor. The fundamental transition energy in each QD is randomized. We solve the equation of motion for the density matrix using the stochastic simulation method with a given exciton decay rate. Then, we present the evolution of the exciton mean square displacement (MSD) from the initially excited QD. It runs in three time stages. First, a ballistic motion, followed by a standard diffusion, which ends at saturation. Using an approximate analytical approach [6], we provide formulas that qualitatively reproduce all stages of the MSD.

[1] T. Förster, Ann. Phys., 437, 55 (1948)
[2] F.V. de Sales et al., Phys. Rev. B 70, 235318 (2004)
[3] M.J. Stephen, J. Chem. Phys. 40, 669 (1964)
[4] R.H. Lehmberg, Phys. Rev. A 2, 883 (1970)
[5] F. Miftasani and P. Machnikowski, Phys. Rev. B 93, 075311 (2016)
[6] K. Kawa and P. Machnikowski, Phys. Rev. B 102, 174203 (2020)

30 min. break

HL 24.8 Wed 11:45 POT 151

Preparation of spin qubits in droplet-etched GaAs quantum dots using quasi-resonant excitation — •Caspar Hopfmann[1], Nand Lal Sharma[1], Weijie Nie[1], Robert Keil[1], Fei Ding[2], and Oliver G. Schmidt[1,3,4] — [1]Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstr. 20, 01069 Dresden — [2]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, 30167 Hannover — [3]Material Systems for Nanoelectronics, Technische Universität Chemnitz, 09107 Chemnitz — [4]Nanophysics, Faculty of Physics and Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, 01062 Dresden

Optically accessible quantum memories are fundamental for implementations of quantum networks as they facilitate the synchronization required for schemes of long-distance quantum information exchange. In order to use GaAs quantum dots, which so far has proven to be bright on-demand sources of entangled photon pairs, deterministic preparation of specific spin states is necessary. We present a comprehensive study on heralded spin preparation employing excited state resonances of droplet etched GaAs quantum dots. By observation of excitation spectra for a range of fundamental excitonic transitions the properties of different quantum dot energy levels, i.e. shells, are revealed. The innovative use of polarization-resolved excitation and detection in the context of quasi-resonant excitation spectroscopy of quantum dots greatly simplifies the determination of the spin preparation fidelities. By employing this method, spin preparation fidelities of quantum dot ground states of up to 85 % are found.

HL 24.9 Wed 12:00 POT 151

Effect of tunnel barrier thickness on optical properties of GaAs quantum dots embedded in Schottky diode structures — •Nand Lal Sharma[1], Moritz Langer[1], Ankita Choudhary[1], Oliver G. Schmidt[2], and Caspar Hopfmann[1] — [1]Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany — [2]Material Systems for Nanoelectronics, Technical University Chemnitz, 09107 Chemnitz, Germany

GaAs quantum dots (QDs) are promising candidates for on demand generation of single and entangled photon pair sources for quantum communication applications. In these QDs, the charge stability and optical linewidth depend on the solid-state environment, which can be controlled by embedding them in a diode structure [1]. In this work we investigate the effect of tunnel barrier thickness on the optical properties of droplet etched GaAs/AlGaAs QDs [2], embedded in Schottky diode structures. The QD photoluminescence from different charge states is controlled by application of an external bias. The effects of quantum dot charging, quantum confined Stark effect and photon coherence are investigated as a function of tunnel barrier thickness.

HL 24.10 Wed 12:15 POT 151

Size-dependence of the Auger process in self-assembled quantum dots — •Hendrik Mannel[1], Marcel Zöllner[1], Fabio Rimek[1], Arne Ludwig[2], Andreas Wieck[2], Martin Geller[1], and Axel Lorke[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Duisburg, 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 (QD), where short Auger recombination times $\tau_{Au} < 1\,ns$ quench the radiative recombination. In self-assembled QDs, an Auger recombination rate of $\tau_{Au} \approx 1\,ms$ has been observed [1].

We use resonance fluorescence to measure the Auger rate of differently sized self-assembled QDs having exciton recombination energies in the range of 920 to 980 nm [2]. The dots are charged with one electron before driving the trion transition to observe the quenching of this transition time-resolved on the investigated sample structure without a wetting layer.

Independently we can change the charge carrier occupation of the dot by gate voltage-dependent electron tunneling from the reservoir. This is a step to further understand the Auger effect and hopefully supress this unwanted effect in future application of quantum information processing.

[1]*A. Kurzmann et al., Nano Lett. 16, 3367 (2016). [2]*M. Löbl et al., Commun. Phys. 2, 93 (2019).

HL 24.11 Wed 12:30 POT 151

Single Mode Coupled Emission of Resonant Excited GaAs Quantum Dots — •Martin Kernbach[1,2], Julian Siller[1], Sophia

Fuchs[1], and Andreas W. Schell[1,2] — [1]Leibniz Universität Hannover, Deutschland — [2]Physikalisch-Technische Bundesanstalt, Braunschweig, Deutschland

Quantum technologies like computing, QKD, or sensing demand for deterministic bright sources of single indistinguishable photons. In order to provide quantum light of isolated systems properly usable for quantum information science, an efficient excitation and extensive collection in a single mode is required. Single molecules and cavity confined quantum dots are convenient sources. The coupling to the excited state is maximized on resonance, but challenges the usability of the emitter due to the costs for the separation of the optical excitation mode from the mode of emission. A temporal, spacial, spectral, or combined method for separation is typically used. Here we present a realization of a single emitter under resonant excitation in a confocal setup coupled into a single mode fiber with the emission mode filtered by polarization. So far, a free beam is directed on the objective mounted with the scanning stages on a 1 m long stick in a liquid helium reservoir. For resonant cw excitation of GaAs semiconductor quantum dots a SNR of polarization suppression up to 100 and count rates of 280 kcps are archived by using a collecting lens with NA 0.68 only. Under this scheme further investigations regarding the blinking behavior are possible as well as probing alternative emitters like single molecules.

HL 24.12 Wed 12:45 POT 151

The role of charge transfer for light emission from excitonic complexes in a single quantum emitter — •Marcel Zöllner[1], Fabio Rimek[1], Hendrik Mannel[1], Andreas D. Wieck[2], Arne Ludwig[2], Martin Geller[1], and Axel Lorke[1] — [1]University of Duisburg-Essen, Germany — [2]Ruhr-University Bochum, Germany

Due to the non-radiative Auger recombination in self-assembled quantum dots [1], the light emission of the trion X^- is reduced. However, for devices and statistical analyses, such as random telegraph signals, the amount of quantum dot photons is of great importance.
With time-resolved resonance fluorescence (RF) measurements, we investigate a comparatively small quantum dot, where we can tune the rate of the electron tunneling from the back contact into the quantum dot by increasing the gate voltage. This results in an up to two orders of magnitude higher trion intensity. Due to the large gate voltages (i.e. energetically strongly tilted conduction band) the electrons can easily overcome the tunnel barrier. Thus, the electron tunneling becomes the dominant effect and charges the quantum dot significantly faster than the Auger effect can discharge it.
Our results indicate that thin tunneling barriers, which can quickly equilibrate states in a quantum dot, make its radiative recombination more resilient against spurious charge transfer (Auger, electron capture, internal photoemission). However, this improvement goes along with a short coherence time.
[1] P. Lochner et al., Phys. Rev. B 103, 075426 (2021).

HL 24.13 Wed 13:00 POT 151

Single photon source in a topological cavity — Jonathan Jurkat[1], Sebastian Klembt[1], Marco De Gregorio[1], •Moritz Meinecke[1], Quirin Buchinger[1], Tristan Hader[1], Johannes Beierlein[1], Oleg Egorov[3], Monika Emmerling[1], Constantin Krause[1], Christian Schneider[2], Tobias Huber-Loyola[1], and Sven Höfling[1] — [1]Technische Physik, Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, 97074 Würzburg, Germany — [2]Lehrstuhl für Physik, Universität Oldenburg, 26129 Oldenburg, Germany — [3]Lehrstuhl für Kondensierte Materietheorie und Optik, Friedrich-Schiller-Universität Jena, 07743 Jena, Germany

The introduction of topological physics into the field of photonics has led to the development of photonic devices endowed with robustness against structural and photonic disorder. While a range of platforms have been successfully implemented demonstrating topological protection of light in the classical domain, the implementation of quantum light sources in photonic devices harnessing topologically non-trivial resonances is largely unexplored. Here, we demonstrate a single photon source based on a single semiconductor quantum dot coupled to a topologically non-trivial Su-Schrieffer-Heeger (SSH) cavity mode. We provide an in-depth study of Purcell enhancement for this topological quantum light source and demonstrate its emission of non-classical light on demand. Our approach is a promising step towards the application of topological cavities in quantum photonics.

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

Time: Wednesday 9:30–13:00 Location: POT 251

Invited Talk HL 25.1 Wed 9:30 POT 251

Interfaces in perovskite optoelectronics: role of energy level alignment and interface chemistry — •Selina Olthof — Universität zu Köln, Institut für Physikalische Chemie

Optoelectronic devices, such as perovskite solar cells, are typically multi-layer stacks in which the absorber layer is sandwiched between metal oxide and/or organic transport layers in order to facilitate charge extraction or ensure charge selectivity. As the perovskite absorber layer has been extensively optimized in the past years, the awareness is rising that device efficiency and stability is limited by the interfaces present in the device. However, in perovskite-based devices, the role of this energy level alignment remains to be elusive and rather inconclusive studies can be found in literature, which I will briefly outline. More important for the device seems to be the perovskite composition at the interface which can be significantly influenced by chemical reactions taking place, in particular next to metal oxides. I will summarize our work on a variety of metal oxides in which we use photoelectron spectroscopy to analyze which components are responsible for the strong interface chemistry. We show that the reactivity strongly depends on the choice of perovskite and that different metal oxides show fundamentally different reaction/degradation pathways. Intriguingly, we are able to introduce surface treatments which change the surface defect density and thereby affect the degree of perovskite degradation significantly.

HL 25.2 Wed 10:00 POT 251

Silver-nanoclusters and -vacancies influence the optical properties of Cs2AgBiCl6 nanocrystals — •Fei He[1], Yiou Wang[1], Quinten A. Akkerman[1], Markus Döblinger[2], Amrita Dey[1], and Jochen Feldmann[1] — [1]Chair for Photonics and Optoelectronics, Nano-Institute Munich and Department of Physics, Ludwig-Maximilians-Universität, Königinstraße 10, 80539 Munich, Germany — [2]Department of Chemistry, Ludwig-Maximilians-Universität München, Butenandtstrasse 5-13 (E), 81377 München, Germany

Though being indirect semiconductors Cesium-Silver-Bismuth-Halides (so-called double perovskites) have attracted much attention as a non-toxic alternative to Lead Halide Perovskites. Novel applications for solar cells and X-ray detectors have already been developed.

Here, we report on the successful synthesis of spherical Cs2AgBiCl6 nanocrystals showing good stability and characteristic photoluminescent spectra. In transmission electron microscopy (TEM) images we observe Ag-clusters on the surface of the nanocrystals. It is known that silver ions are easily reduced into metallic Ag leading to silver vacancies in the double perovskite material and probably to Ag-clusters on the surface. We discuss how silver-nanoclusters and -vacancies influence the luminescent behavior of the double perovskite nanocrystals and explain possible microscopic origins.

HL 25.3 Wed 10:15 POT 251

Accelerating research on solar cell materials with NOMAD — •Jose Marquez[1], Lauri Himanen[1], Markus Scheidgen[1], Claudia Draxl[1], Jens Hauch[2], Christoph Brabec[2], and Thomas Unold[3] — [1]Humboldt Universität zu Berlin — [2]Helmholtz Institute Erlangen-Nürnberg for Renewable Energy — [3]Helmholtz-Zentrum Berlin

New solar cell technologies need decades to overcome the 20% power conversion efficiency threshold needed to make them commercially viable. With thousands of possible chemical compositions for new absorber layer materials and an unlimited number of possible device architectures, it becomes impossible to navigate this material space without the help of data science. To radically accelerate and democratize this development process, FAIR data management activities involving experimental solar cell data are needed. The NOMAD Laboratory (https://nomad-lab.eu) is a platform and open-source software

driven by the NFDI consortium FAIRmat (https://fairmat-nfdi.eu) for making materials-science data FAIR. We show how the NOMAD infrastructure is evolving to support this task in the context of solar cells, demonstrated by an app for visualizing and searching rich and AI-ready experimental big solar cell data. NOMAD also provides an electronic lab notebook (ELN) which can be customized by research labs for AI-ready data/metadata entry, transfer, and processing in a FAIR-database context.

HL 25.4 Wed 10:30 POT 251

Interdiffusion of Cu(In,Ga)Se2 and Ag(In,Ga)Se2 investigated by In-Situ X-Ray Diffraction — •Julia Horstmann[1], Roland Mainz[2], Karsten Albe[3], Heiko Kempa[1], Torsten Hölscher[1], and Roland Scheer[1] — [1]Martin-Luther-Universität Halle-Wittenberg, Germany — [2]Helmholtz-Zentrum Berlin, Germany — [3]Technische Universität Darmstadt, Germany

The partial substitution of Ag with Cu in the chalcopyrite-based absorber of thin film solar cells is a promising approach towards higher power conversion efficiencies. The resulting (Ag,Cu)(In,Ga)Se2 (ACIGSe) alloy achieves a bandgap widening up to 0.2 eV, increased grain growth and a lower melting temperature. The latter might reduce structural defects and therefore recombination losses in the absorber. This is favorable especially for wide-bandgap solar cells, used as top subcells in tandem devices, whose device performance is mainly limited by deep defects. To gain a better understanding of the diffusion on the (I) sublattice, we experimentally explored the interdiffusion of Cu(In,Ga)Se2 and Ag(In,Ga)Se2 layers by in-situ X-ray diffraction (IS-XRD) and glow discharge optical emission spectroscopy. Besides the positive aspects of Ag-alloying, thermodynamic simulations have shown a miscibility gap for temperatures between 100°C and 400°C. It is theoretically proposed, that ACIGSe with a high Ga content and with a [Ag]/([Ag]+[Cu]) ratio between 0.25 and 0.75 decomposes into Ag-rich and Ag-poor phases. We have studied the phase stability of Ga-free and Ga-rich samples using IS-XRD during post-annealing processes.

HL 25.5 Wed 10:45 POT 251

NiO in perovskite solar cells: a peculiar interplay of degradation, passivation and device performance — •John Mohanraj[1], Bipasa Samanta[2], Maytal Caspary Torokar[2], and Selina Olthof[1] — [1]University of Cologne, 50939 Cologne, Germany — [2]Technion - IIT, Haifa, 3200003 Israel

The degradative interactions at the NiO/perovskite interface are notorious in the perovskite community as they lead to significant Voc and stability losses in p-i-n type perovskite solar cells (PSCs). So far, various Lewis bases have been introduced at this interface to passivate the metal oxide surface defects. Despite this process being successful in minimizing Voc and stability losses in PSCs, in-depth understanding of surface passivation and consequent suppression of the chemical processes at the NiO/perovskite interface are still elusive. This calls for a comprehensive surface investigation. To address these issues, we investigated solution processed NiO surfaces, their treatment with a series of passivating compounds, and the interface towards MAPbI3 in order to systematically probe the interface stability. Our methods include X-ray and UV photoelectron spectroscopy (XPS/UPS), XRD, SEM and UV-Vis absorption techniques. In parallel, first principle DFT calculations on differently treated NiO/MAPbI3 interfaces were carried out. These complementary investigations reveal changes in surface composition of the treated NiO and help us to suggest possible mechanisms for the degradative interactions. Finally, PSCs were fabricated using the stabilized NiO interfaces, and the impact on photovoltaic characteristics and device stability have been investigated.

30 min. break

HL 25.6 Wed 11:30 POT 251

Resonant coupling of spin-flip excitations with phonons in BiFeO3 — •Aseem Rajan Kshirsagar and Sven Reichardt — Department of Physics and Material Science, University of Luxembourg, Luxembourg

BiFeO3 is a technologically relevant multiferroic perovskite. While a vast literature exists on its electronic, optical, and multiferroic properties, some of its optically active electronic excitations remain to be understood or have been interpreted in ambiguous ways. This applies in particular to features below the absorption onset that feature prominently in resonant Raman scattering [1]. Here we present a detailed study of the electronic structure and resonant Raman spectrum of BiFeO3 from first principles. Using many-body perturbation theory on top of density functional theory, we first analyze and characterize its optical absorption spectrum in terms of excitons and atomic orbitals, focusing in particular on spin-flip excitations that are strongly localized. We then use the state-of-the-art method for the ab initio calculation of resonant Raman intensities [2,3] to analyze the resonant coupling of these finite-spin excitations with phonons. Our results show that these only weakly optically active excitations still leave a clear imprint on the resonant Raman spectrum, making the latter an even more powerful tool to probe "darker" electronic excitations.

[1] M. C. Weber, et al. Phys. Rev. B, 93, 125204 (2016).
[2] S. Reichardt and L. Wirtz, Phys. Rev. B, 99, 174312 (2019).
[3] S. Reichardt and L. Wirtz, Sci. Adv., 6, eabb5915 (2020).

HL 25.7 Wed 11:45 POT 251

Coherent Phonons in Halide Perovskite Nanocrystals — •Julian Georg Mann[1], Fei He[1], Quinten Akkerman[1], Tushar Debnath[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]Centre for Nanotechnology, Indian Institute of Technology Guwahati, Guwahati-781039

Halide perovskite nanocrystals are gaining increasing attention in contemporary research due to their promising performance in both light-emitting and solar technologies. We recently showed that photoexcitation of halide-perovskite nanocrystals with ultrashort laser pulses produces coherent phonons (Nat. Comm. 12, 2629 (2021)). We report femtosecond pump-probe spectroscopy studies on the formation and dynamics of coherent phonons in formamidine lead-halide ($FAPbX_3$) nanocrystals in terms of higher harmonic vibrational modes. In addition, we investigate the dynamics of vibrational wave packets in spherical $Cs_2AgBiBr_6$ double perovskite nanocrystals. Here, we observe that optically launched vibrational wave-packets alter spectral positions of excitonic resonances or oscillator strength of particular electronic transitions. Our results show that electron-phonon couplings (polaronic effects) need to be considered to fully understand the optoelectronic properties of halide-perovskite semiconductors.

HL 25.8 Wed 12:00 POT 251

Phonon-driven Intra-exciton Rabi Oscillations in Halide Perovskites — •Katrin Winte[1], Xuan Trung Nguyen[1], Daniel Timmer[1], Davide Ceratti[2], Caterina Cocchi[1], Michael Lorke[3], Frank Jahnke[3], David Cahen[2], Christoph Lienau[1], and Antonietta De Sio[1] — [1]University of Oldenburg, Germany — [2]Weizmann Institute of Science, Israel — [3]University of Bremen, Germany

There is increasing consensus that in halide perovskites (HaPs) the interaction of electronic excitations with the phonon modes of their flexible polar lattice is crucial for the unique optoelectronic and transport properties of these materials. Here we show that coherent low frequency phonon of the lead-halide lattice induce Rabi oscillations between 1s and 2p excitons in $CsPbBr_3$ crystals. Ultrafast two-dimensional electronic spectroscopy reveals an excitonic peak structure oscillating with a 100-fs period up to 2 ps at 20 K. This frequency does not match any phonon modes of the crystals. Only after 2 ps, slow coherent phonon oscillations dominate the dynamics. We rationalize these findings as off-resonant intra-exciton Rabi oscillations induced by the Pb-Br phonon fields of the HaP crystals. We show that the slow motion of Pb-Br sublattice induces electric fields at THz frequencies that are sufficiently strong to drive off-resonant population oscillations between 1s and 2s excitons. Model simulation of the nonlinear optical response support this interpretation. This goes beyond prevailing models for the electron-phonon coupling in HaPs. It suggests that the coupling of characteristic low frequency phonon to intra-excitonic transitions may be the key to control their anharmonic response.

HL 25.9 Wed 12:15 POT 251

Determining (almost) all optoelectronic properties of halide perovskites by transient photoluminescence — •Hannes Hempel[1], Martin Stolterfoht[2], Fangyuan Ye[2], and Thomas Unold[1] — [1]Helmholtz Zentrum Berlin, Germany — [2]Institute of Physics and Astronomy, University of Potsdam, Germany

Time-resolved photo luminescence (trPL) is probably the most common technique to quantify lifetimes of photogenerated charge carriers in semiconductors. However, the usual fitting of exponential decays to estimate lifetimes is a rather crude phenomenological approach since it ignores quenching processes that are not connected to carrier re-

combination and disregards the absolute amplitude of the luminescence. Here, we present an analysis of injection-dependent absolute trPL transients of bare triple-cation lead halide perovskite thin films. The presented analysis reveals a doping concentration of 3x1013cm-3 and a charge carrier mobility of 0.8 cm2/Vs, which are confirmed by Hall measurements. Further, we determine the injection-dependence of external radiative lifetimes, of the external radiative coefficient, and of the effective charge carrier lifetime. Based on the properties, an implied current-voltage curve is constructed that reveals the potential performance of the material in solar cell. Our trPL-based approach agrees well with the results of injection-dependent photoluminescence quantum yield measurements. However, it is superior in attributing losses, e.g. in the radiative ideality factor or the implied open circuit voltage, to the internal optoelectronic properties and thereby indicates the path to overcome these losses.

HL 25.10 Wed 12:30 POT 251

Characterization of optoelectronic properties of CsSnI3 perovskite thin film as a function of chemical composition. — •Fatima Akhundova, Hannes Hempel, Marin Rusu, Elif Hüsam, Marcus Bär, and Thomas Unold — Helmholtz-Zentrum Berlin

The performance of lead-based halide perovskites as a next generation solar cell rises every year, however toxicity of Pb is a major obstacle for commercialization. Tin is the immediate substitute for Pb in perovskite crystal structure as both metals possess the same electronic configuration. However, Sn-perovskite solar cells have significantly lower efficiencies which is partially caused by poor stability of Sn(II). We report a systematic study of structural and optoelectronic properties of co-evaporated CsSnI3 thin films with regard to lateral compositional gradient. Elemental compositions are confirmed by X-ray fluorescence and X-ray photoelectron spectroscopy techniques. Grazing-incidence X-ray diffraction reveals orthorhombic gamma phase with different preferred orientation for the excess Sn and Cs content. Moreover, Cs-rich regions shows better phase stability than the Sn-rich parts which undergo a phase transition to non-perovskite phase. The optical band gap, work function, and ionization energy are measured as a function of the Cs:Sn ratio to characterize the band diagram. The photoluminescence quantum yield, the charge carrier lifetime and mobility present these properties are rather robust against changes in composition. Our work emphasizes the impact of chemical composition on optoelectronic properties of Sn-based perovskites and demonstrates agile strategy for compositional engineering in materials research.

HL 25.11 Wed 12:45 POT 251

FAIR Cesium Lead Halide Perovskites Data by High-Throughput Investigation of Co-Evaporated Combinatorial Libraries — •Hampus Näsström[1], Pascal Beblo[2], Fatima Akhundova[2], Oleksandra Shargaieva[2], Jose A. Marquez[1], Hannes Hempel[2], Andrea Albino[1], Sebastian Brückner[1], Claudia Draxl[1], Eva Unger[2], and Thomas Unold[2] — [1]Humboldt-Universität zu Berlin — [2]Helmholtz-Zentrum Berlin

Artificial intelligence presents new possibilities in experimental materials research but typically require large well-characterized datasets. High-throughput technologies, including combinatorial synthesis, provide one method for obtaining such datasets. In this work, we show how such a dataset can be created through combinatorial co-evaporation and high-throughput characterization of $Cs_yPb_{1-y}(Br_xI_{1-x})_{2-y}$ perovskites. The evaporated films were investigated with a multitude of contact-less characterization methods such as hyperspectral photoluminescence imaging, time-resolved photoluminescence mapping, and grazing-incidence wide-angle X-ray scattering mapping. The results were combined to estimate the potential of the material in terms of the photovoltaic power conversion efficiency as a function of the Cs to Pb and Br to I ratio. Finally, a generalized data schema for combinatorial thin films was developed, and the data of the 3456 individual samples was disseminated in a Findable, Accessible, Interoperable and Reusable (FAIR) way within the Novel Materials Discovery (NOMAD) laboratory (nomad-lab.eu) that is operated by the NFDI consortium FAIRmat (fairmat-nfdi.eu).

HL 26: Focus Session: Frontiers of Electronic-Structure Theory IV (joint session O/HL)

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

HL 26.1 Wed 10:30 TRE Ma

A systematic DFT+U and Quantum Monte Carlo benchmark of magnetic two-dimensional (2D) CrX_3 (X = I, Br, Cl, F) — •Daniel Wines, Kamal Choudhary, and Francesca Tavazza — Materials Science and Engineering Division, National Institute of Standards and Technology (NIST), Gaithersburg, MD 20899, USA

The search for two-dimensional (2D) magnetic materials has attracted a great deal of attention because of the experimental synthesis of 2D CrI_3, which has a measured Curie temperature of 45 K. Often times, these monolayers have a higher degree of electron correlation and require more sophisticated methods beyond density functional theory (DFT). Diffusion Monte Carlo (DMC) is a correlated electronic structure method that has been demonstrated successful for a wide variety of systems, since it has a weaker dependence on the Hubbard parameter (U) and density functional. In this study we designed a workflow that combines DFT+U and DMC in order to treat 2D correlated magnetic systems. We chose monolayer CrX_3 (X = I, Br, Cl, F), with a stronger focus on CrI_3 and $CrBr_3$, as a case study due to the fact that they have been experimentally realized and have a finite critical temperature. With this DFT+U and DMC workflow and the analytical method of Torelli and Olsen, we estimated an upper bound of 43.56 K for the T_c of CrI_3 and 20.78 K for the T_c of $CrBr_3$, in addition to analyzing the spin densities and magnetic properties with DMC and DFT+U. We expect that running this workflow for a well-known material class will aid in the future discovery and characterization of lesser known and more complex correlated 2D magnetic materials.

Topical Talk HL 26.2 Wed 10:45 TRE Ma

TREX: an integrated HPC software platform for quantum Monte Carlo calculations — •Claudia Filippi — University of Twente, Enschede, The Netherlands

I will present the software development strategy and current achievements of the European Center of Excellence TREX "Targeting Real chemical accuracy at the EXascale" [1]. TREX focuses on methods at the high-end in the accuracy ladder of electronic structure approaches and, in particular, on quantum Monte Carlo methods which are uniquely positioned to fully exploit the massive parallelism of upcoming architectures. The main objective of TREX is the development of a user-friendly and open-source software suite, which integrates quantum Monte Carlo codes within an interoperable, high-performance platform. Core of our software efforts is the creation of the following two libraries:

- TREXIO: A common I/O library and file format for easily exchanging data between applications, facilitating high-throughput computing workflows [2];
- QMCkl: A library of computational kernels, written together by quantum Monte Carlo and HPC experts, to perform common CPU-intensive quantum Monte Carlo tasks [3].

[1] https://trex-coe.eu
[2] https://github.com/trex-coe/trexio
[3] https://trex-coe.github.io/qmckl

HL 26.3 Wed 11:15 TRE Ma

Exciton-phonon coupling in luminescence of indirect band-gap materials — Matteo Zanfrognini[1,2], Fulvio Paleari[1], Daniele Varsano[1], and •Ludger Wirtz[3] — [1]Centro S3, CNR-Istituto Nanoscienze, Modena, Italy — [2]Università di Modena e Reggio Emilia, Modena, Italy — [3]Department of Physics and Materials Science, University of Luxembourg, Luxembourg

Layered, quasi-2D materials, such as hexagonal boron nitride (hBN) are known to display very strong excitonic effects due to the concentration of excitons in two dimensions and due to the relatively weak dielectric screening. If the band-gap of the material is indirect, the dispersion of the lowest lying exciton can have a minimum at a finite wave vector q. Upon absorption of a photon and excitation to a vertical (q=0) exciton, the system will relax to the finite-q exciton. Luminescence then entails the absorption/emission of a phonon

with wave vector q. We present a computational approach for phonon-assisted luminescence in the presence of strong excitonic effects using two approaches: (i) a finite-displacement approach for the exciton-phonon coupling and (ii) a diagrammatic approach, calculating the q-dependent exciton-phonon coupling from the exciton eigenvectors and electron/hole-phonon scattering matrix elements. We show that the methodology quantitatively explains recent measurements of different stackings of BN layers. [1]

[1] A. Plaud, I. Stenger, F. Fossard, L. Sponza, L. Schué, F. Ducastelle, A. Loiseau, J. Barjon, to be published.

HL 26.4 Wed 11:30 TRE Ma

A combined G_0W_0/BSE scheme of characterizing photoexcitations in hydroxylated rutile TiO_2(110) — •Savio Laricchia, Andrea Ferretti, Daniele Varsano, and Claudia Cardoso — Centro S3, CNR-Istituto Nanoscienze, 41125 Modena, Italy

In reduced TiO_2, electronic transitions originating from polaronic excess electrons in surface-localized band-gap sta tes (BGS) are known to contribute to the photoabsorption and to the photocatalytic response of TiO_2 in the visible region. Recent state-selective studies using two-photon photoemission (2PPE) spectroscopy have also identified an alternative photoexcitation mechanism contributing to the photoabsorption of the reduced surface (110) of rutile TiO_2. This process involves *d-d* excitations from BGS arising from surface and subsurface defects, including bridging hydroxyls and oxygen vacancies. Density Functional Theory (DFT) has been used to determine the character of the electronic excited states involved in a $d_{t_{2g}}$-$d_{t_{2g}}$ transitions, but its accuracy is questioned by its theoretical framework: DFT is in principle exact for ground state systems and does not describe interacting photogenerated electron-hole pairs, i.e. the excitons. This has highlighted the need to move beyond the DFT formalism, by working within a many-body perturbation theory (MBPT) framework. It will be shown how a G_0W_0 method, combined with the solution of the Bethe-Salpeter equation (BSE), provides a powerful tool for characterizing from first principles the optical excitations from BGS identified by 2PPE experiments on hydroxylated TiO_2(110).

15 min. break

HL 26.5 Wed 12:00 TRE Ma

Scaling the Way for All-Electron XPS Simulations to CalculateAbsolute Binding Energies of Surface Superstructures — •Dylan Morgan[1], Sam Hall[1], Benedikt Klein[1,2], Matthew Stoodley[1,2], and Reinhard Maurer[1] — [1]Department of Chemistry, University of Warwick, United Kingdom — [2]Diamond Light Source, Harwell Science and Innovation Campus, United Kingdom

First principles simulations of x-ray photoemission spectroscopy (XPS) and near-edge x-ray absorption fine-structure (NEXAFS) crucially support the assignment of surface spectra composed of many overlapping signatures. Core-level constrained Density Functional Theory calculations based on the Δ-SCF method are commonly used to predict relative XPS binding energy (BE) shifts but often fail to predict absolute BEs. The all-electron numeric atomic orbital code FHI-aims enables an accurate prediction of absolute BEs, but the legacy code lacked computational scalability to address large systems and robustness with respect to localisation of the core hole. We present a redesign of the core-hole constrained code in FHI-aims that delivers improvements to the scalability and robustness of core-hole constrained calculations in FHI-aims. We demonstrate the improved scaling behaviour and employ the new code to simulate core-level spectroscopic fingerprints of graphene moire superstructures. The code refactorisation forms the basis to expand the code towards improved core hole localisation methods and the rigorous treatment of relativistic effects for core-level spectra beyond the 1s shell.

HL 26.6 Wed 12:15 TRE Ma

Efficient diagonalization of BSE electron-hole Hamiltonian using group theory — •Jörn Stöhler[1,2], Dmitrii Nabok[1], Stefan Blügel[1], and Christoph Friedrich[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany — [2]RWTH Aachen University, Germany

The Bethe-Salpeter equation (BSE) is the state-of-the-art method for the calculation of optical absorption and electron-energy loss spectra including excitonic effects. We solve the BSE by diagonalizing an effective electron-hole Hamiltonian. Often, a high number of **k**-points is needed to converge the BSE spectra, which leads to a large size of the Hamiltonian matrix and makes its diagonalization very expensive. In this work [1], we use the full spatial symmetry group to transform the electron-hole product basis into a symmetry-adapted product basis, which brings the Hamiltonian into a block-diagonal form and speeds up the subsequent diagonalization. The basis transformation is sparse and causes little overhead. We provide an implementation of our method in the FLAPW code `Spex` and demonstrate speedups of 36, 52, 12 for Si, BN, and monolayer MoS_2, respectively.

We acknowledge financial support by MaX CoE funded by the EU through H2020-INFRAEDI-2018 (project: GA 824143).

[1] J. Stöhler, C. Friedrich, *Unpublished*

HL 26.7 Wed 12:30 TRE Ma

Excitonic effects on quadratic optical photoresponse tensors of semiconductors — •Peio Garcia-Goricelaya[1] and Julen Ibañez-Azpiroz[1,2] — [1]Centro de Física de Materiales, University of the Basque Country UPV/EHU, Spain — [2]IKERBASQUE Basque Foundation for Science, Spain

We present a general ab initio scheme for including many-body excitonic effects in the non-linear optical photoresponse up to second order. Our practical implementation starts from the length-gauge formulation of the single-particle non-interacting optical photoresponse tensors [1] that are efficiently calculated using Wannier interpolation [2]. Subsequently, excitonic corrections are included in the many-body interacting current-density response tensors by means of Dyson-like equations derived within TD-CDFT. These equations allow a natural connection with the formalism of the single-particle picture and the Wannier-interpolation scheme respecting the tensorial character of the response. We employ this scheme to assess the impact of excitonic effects on several quadratic optical processes as the second-harmonic generation and the shift-current bulk photovoltaic effect in technologically appealing semiconductors.

Funding provided by the European Union*s Horizon 2020 research and innovation programme under the European Research Council(ERC) grant agreement No 946629.

[1] J. E. Sipe and A. I. Shkrebtii, Phys. Rev. B 61, 5337 (2000).
[2] G. Pizzi et al., J. Phys. Cond.Matt. 32, 165902 (2020)

HL 26.8 Wed 12:45 TRE Ma

Electronic and optical properties of $CoFe_2O_4$ from density functional theory calculations, including many-body effects — •Shohreh Rafiezadeh[1], Vijaya Begum-Hudde[1,2], and Rossitza Pentcheva[1] — [1]Department of Physics University of Duisburg-Essen, Germany — [2]University of Illinois at Urbana-Champaign, USA

$CoFe_2O_4$ is a ferrimagnetic semiconductor that finds application as an anode material in photocatalytic water splitting. We present a comprehensive study of the electronic and optical properties of bulk $CoFe_2O_4$ using density functional theory calculations and many-body perturbation theory to clarify the broad range of reported band gaps both experimentally (0.55-4.1 eV)[1] and theoretically (0.9-1.90 eV). Starting with different exchange-correlation functionals, we obtain a direct band gap of 1.38 [PBE+(U=4 eV)], 1.69 eV [SCAN+(U=3 eV)], and an indirect gap of 2.02 eV (HSE06). Including quasiparticle corrections within G_0W_0 enhances and renders indirect band gaps for all functionals of 1.78, 1.95 and 2.17 eV, respectively. Excitonic effects are accounted for by solving the Bethe Salpeter equation and result in the lowest threshold for optical transitions at 1.50 eV (SCAN) and 1.61 eV (HSE06), followed by peaks at $\sim$ 2.0, 3.5 and 5.0 eV, in agreement with experiment highlighting the importance of electron-hole interactions. Support by DFG- within CRC/TRR 247, project B04, and computational time at MagnitUDE is gratefully acknowledged. [1] S. Singh and N. Khare, Sci. Rep. **8**, 6522 (2018).

HL 27: Focus Session: Wissenschaftskommunikation / Outreach (joint session HL/O/TT)

Im wissenschaftlichen Umfeld wird Maßnahmen der Öffentlichkeitsarbeit eine zunehmend größere Bedeutung zugemessen, - aus der Gesellschaft heraus und auch durch die großen Fördereinrichtungen und die DPG. Dabei geht es nicht nur um die Ergebnisse der Forschung, sondern auch darum, Prozesse und Methoden von wissenschaftlicher Arbeit transparent abzubilden – eine Aufgabe, die prinzipiell alle Forschenden übernehmen können. In diesem Symposium sollen erfolgreiche Projekte der Wissenschaftskommunikation, insbesondere aus dem Bereich der Festkörperphysik, vorgestellt werden. In ihrer Gesamtheit sollen sie das Spektrum der Wissenschaftskommunikation hinsichtlich des finanziellen und zeitlichen Aufwands aufzeigen und Methoden für unterschiedliche Zielgruppen vorstellen.

So dient diese Session sowohl als Ideengeber und Inspiration als auch als eine Art Netzwerk-Treffen zum Austausch über die Wissenschaftskommunikation in unterschiedlichen Kontexten.

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

Invited Talk HL 27.1 Wed 15:00 POT 81

experimentamus! Forschendes Lernen von Physik und Chemie in der Grundschule — •Sebastian Schlücker — Universität Duisburg-Essen, Campus Essen

Der Sachunterricht in der Primarstufe ist ein Konglomerat aus allen Natur- und Gesellschaftswissenschaften, erst in der Sekundarstufe findet eine Aufspaltung in die einzelnen Fächer statt. Zudem unterrichten viele Grundschul-Lehrkräfte fachfremd. Auch der Zeitaufwand für die Vorbereitung von Experimenten ist nicht unerheblich. Wie also kann man trotz dieser Hürden kindgerechte physikalische und chemische Experimente bereits in der Grundschule einführen?

Ich berichte aus 10 Jahren Erfahrung mit dem Projekt experimentamus!. Dabei handelt es sich um einen Kanon aus ca. 40 Experimenten für die Klassen 2 bis 4, welcher die Themen Licht, Wärme, Magnetismus, Wasser, Luft, Feuer und Elektrizität mit einem kindgerechten Alltagsbezug abdeckt. Anstelle des darlegenden Lernens wird auf das Forschende Lernen gesetzt: Frage - Hypothese - Experiment - Beobachtung - Erklärung; diese fünf Stationen des wissenschaftlichen Erkenntnisprozesses werden immer wieder durchlaufen. Ganz im Sinne Martin Wagenscheins wird dabei nach der exemplarischen und sokratischen Methode vorgegangen. Die praktische Implementierung umfasst 1. Materialkisten für alle Themen, 2. kompakte und leicht verständliche Informationshefter für die Lehrkräfte, sowie 3. Lernheftchen für alle SuS. Am Ende möchte ich über Erfahrungen und Herausforderungen im Rahmen dieses Projektes berichten und Ideen für eine mögliche weitere Verbreitung vorstellen.

HL 27.2 Wed 15:30 POT 81

Internal interfaces - goals and realisation of a scientific image film — •Ulrich Höfer[1,2] and Michael Dürr[2,3] — [1]Fachbereich Physik, Philipps-Universität Marburg — [2]SFB 1083, www.internal-interfaces.de — [3]Institut für Angewandte Physik, Justus-Liebig-Universität Giessen, Germany

Funded by the German Science Foundation (DFG), a professional film maker has produced an image film about the research conducted in the Collaborative Research Center SFB 1083 "Structure and Dynamics of Internal Interfaces". The six-minute video clip takes the non-specialist on a journey down to atomic scale to show the progress at the forefront of research at solid/solid interfaces. It is not a demanding educational film. Rather, it is a visually stunning piece that looks like science fiction taken straight out of a movie, with tracking shots that take the viewer down to the nanometer scale, with flights through luminous molecules, exotic excitons, and space-filling laser labs. The film also has a very impressive soundtrack. Gustav Holst's (1874-1934) composition "The Planets" was re-orchestrated especially for this film. It is available on the youtube channel of the DFG (https://www.youtube.com/watch?v=_-mDt0NzHrc). Visitors of Chemikum Marburg can watch the German version on a 4K OLED screen, a device actually based on microscopic processes at interfaces investigated by SFB 1083.

The idea behind the creation of a professional film, its conceptional design and the necessary steps towards its realization will be outlined.

HL 27.3 Wed 15:45 POT 81

Outreach activities of SFB 1083 @ Chemikum Marburg — •Christof Wegscheid-Gerlach, Luise Cleres, Ina Budde, Karl-Heinz Muth, and Marion Enssle — Chemikum Marburg / SFB1083

The diffusion of concepts, methods, and visions of the SFB 1083 on Structure and Dynamics of Internal Interfaces into the general public is our general goal. To this end project Ö makes use of the institution Chemikum Marburg e.V., whose basic idea is to fascinate the public excited about natural sciences. The experiments offered here, stand for chemical, biological, pharmaceutical, and physical subjects related with daily phenomena or beyond. We will give an overview about the introduction of basic ideas and methods of SFB 1083 to the public as well as the institution Chemikum Marburg. The contents of the individual offers, such as experiments within the regular workspace, the workshops for the Girls' Day and the compilation of special workshops that are offered to give high-school students an understanding of the research content of the SFB 1083 are presented. An additional topic is the linking of basic research to applications for regenerative energy resources. Hydrogen fuel cells are well-known to the general public and rely on functional internal interfaces. An additional workshop which was prepared in cooperation with the district Marburg-Biedenkopf gives an overview about production, storage, and application of hydrogen as a new energy resource. We will also share various occasions at Chemikum Marburg where further outreach activities represent SFB 1083.

Invited Talk HL 27.4 Wed 16:00 POT 81

Under the Microscope – spotlighting materials and nano science — •Svenja Lohmann and Pranoti Kshirsagar — The Science Talk, Germany

Real Scientists Nano is a science communication project dedicated to materials and nano science. Despite the widespread relevance of materials science to everyday life, we feel that dedicated science communication in this area is much rarer than in other fields. Our aim is to provide a platform for active materials and nano scientists to directly communicate their science and life as a scientist to the public. The use of social media thereby provides a very low threshold to science communication as basically the only requirement is to have an account. We have the goal to showcase the scientific community in all its diversity, and so far (12/2022) had guest scientists from more than 30 countries of origin as well as various fields and career stages. The two main pillars of the Real Scientists Nano project are the @RealSci_Nano Twitter account and the Under the Microscope podcast. Our guest scientists are interviewed for one podcast episode, and subsequently get to tweet from the account for one week following the rotation curation concept. We let curating scientist decide for themselves what they would like to tweet about. The form and content therefore vary greatly. Many of our scientists report from their everyday life, and are for example live-tweeting from a conference, uploading videos or photos from the lab or sending the occasional "stuck in meetings, will return later" tweet. Science communication on social media thus gives the opportunity to open a direct and real-time window into the scientist's life.

30 min. break

Invited Talk HL 27.5 Wed 17:00 POT 81

Phyphox – A pocketful of physics — •Christoph Stampfer — JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany

Most smartphones are used to make phone calls, to write short messages, surf the Internet or check e-mails. However, they can do much more: With the help of the integrated sensors and the free app "phyphox" (abbreviation for Physical Phone Experiments), pupils, stu-

dents, and teachers and interested others can independently perform and develop physics experiments. For example, the app can use the accelerometer to record pendulum movements and determine the rotational acceleration in a salad spinner, or the air pressure sensor to determine time-resolved differences in altitude and thus the speed of an elevator. The didactic potential of the app is great, as the students are picked up on ground that is very familiar and attractive to them (smartphones) and are introduced to experimental natural sciences in a playful way and with an extremely low barrier (zero cost, i.e. only one click away). The app helps to get students excited about scientific and technical questions and contexts at an early age. The app is available free of charge for Android and iOS (more information can be found at www.phyphox.org). In my presentation, I will go into the concept of phyphox, introduce the range of functions and show a number of application examples.

HL 27.6 Wed 17:30 POT 81

Chair PR representative as a doctoral student's secondary task: A field report — •Paula M. Weber, Felix Friedrich, and Manuel Seitz — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Especially in recent years, it has become more important to communicate one's scientific work and methods to the public in order to show that in the scientific world, knowledge can only be created through research and the scientific process. Yet, extra time besides research is often limited and it is thus difficult to get into science communication. In this talk, I would like to present how PhD students can use their interest in science communication to benefit their own research group as a part-time PR representative.

In the first part of my talk, I will report on our efforts to attract new bachelor and master students. This advertising is focused on an audience with a scientific background, such that lab tours and advertising posters may contain scientific language and references. The second part is about communication with the general public, who usually know physics from their school days. Here, I will report on how we presented our research activities at the Night of Science in Physics and at the "Highlights der Physik" in Würzburg.

Working part-time as a PR representative could encourage doctoral students to try their hand at science communication and develop the associated communication skills.

HL 27.7 Wed 17:45 POT 81

Real or Fake - A format in science communication that encurages critical thinking — •Tobias Löffler — Institut für Angewandte Physik Düsseldorf

The outreach format "Real or Fake" aims to train the audience in an critical approach to credible-sounding facts.

It is aimed at the general public and specifically at young people. At the same time, it offers an easy introduction for scientists to audience-oriented communication of science on stage. The format can be performed in front of a live audience or as an interactive online event. It has been proven to work as implemented into science festivals, nights of sciences, as a public individual event and also as part of events with constrained settings - such as outreach events at schools or as part of conferences.

"Real or Fake" was developed in 2017 by scientists around the Berlin March for Science who later founded Besserwissen e.V. with the goal to promote the format and support new organisers. I do cooprate with them since 2019 and have organized more than ten "Real or Fake" events since then.

In my talk, I will present the concept and its origins, give an overview of successful events and show what to do and what support one can get, if one wants to organize a "Real or Fake" event.

Invited Talk HL 27.8 Wed 18:00 POT 81

Physics for school and the public at the LMU — •Dr. Cecilia Scorza-Lesch — Fakultät für Physik der LMU, München

Germany lives from research and technology. Physics, as the basis of all empirical sciences and technologies, has a very special, fundamental role to play. The Faculty of Physics at LMU, the largest in Germany, comprises nine research areas, three centres and two excellence clusters. In this talk we will present the approach we use to successfully communicate our various topics of modern research, the role of physics in our daily lives and in the fight against global warming to the schools and the public in a participatory way.

HL 28: Focus Session: Breakthroughs in wide-bandgap semiconductor laser diodes II

Time: Wednesday 15:00–16:45 Location: POT 361

Invited Talk HL 28.1 Wed 15:00 POT 361

Fabrication of AlGaN-based UV-B laser diodes on lattice-relaxed high-quality AlGaN — •Motoaki Iwaya[1], Sho Iwayama[1,2], Tetsuya Takeuchi[1], Satoshi Kamiyama[1], and Hideto Miyake[2] — [1]Meijo Univ., Nagoya, Japan — [2]Mie Univ., Tsu, Japan

Recently, AlGaN-based ultraviolet (UV) light-emitting devices have been achieving remarkable performance. Highly efficient UV light-emitting diodes are finding applications in many fields, such as water and air sterilization. Meanwhile, room-temperature oscillation of laser diodes in the UV-C and UV-B region has also been realized in recent years by current injection. In this presentation, we show our realization of UV-B laser diode. To realize UV-B laser diodes, it is essential to fabricate them on lattice-relaxed AlGaN because the lattice mismatch between AlN and AlGaN active layers is at least 1.2%. We have obtained various methods for improving the quality of lattice-relaxed AlGaN, and would like to report on the methods and effects. As specific methods to fabricate lattice-relaxed high-quality AlGaN, we explain AlGaN fabricated by the spontaneous nucleation method and the AlN nanopillar method. We will also discuss the correlation between lattice defects such as dislocations, V-shaped pits, and hillocks and device properties. And we would like to present the characteristics of UV-B laser diodes fabricated on such AlGaN templates.

Invited Talk HL 28.2 Wed 15:30 POT 361

Breakthrough technologies to realize room-temperature continuous-wave deep-ultraviolet laser diodes — •Maki Kushimoto — Nagoya University, Nagoya, Japan

AlGaN-based UVC laser diodes operating at wavelengths are expected to be a low-cost, environmentally friendly, and highly efficient laser light source for a variety of applications. Although the pulsed operation of AlGaN-based laser diodes at UV-C wavelengths has been confirmed in the previous studies, continuous wave lasing without cooling was difficult because of the high operating voltage. In this study, we further reduced the threshold gain by improving the optical confinement and improved the threshold current density while lowering drive voltage by modification of device designs. The new design improved the optical confinement factor to the quantum wells from 4% to 6% , which has led to a significant reduction in threshold current density. Furthermore, A reduction in threshold voltage was achieved by reducing the lateral distance between the n- and p-electrodes by tapering the sides of the LD mesa. In the conventional structure, the presence of process-induced crystal defects forced a distance between the n and p electrodes, which was a major factor in increasing the operating voltage. This tapered mesa performs the role of suppressing crystal defects by controlling shear stress of mesa edge. As a result, room temperature CW lasing at a wavelength of 274 nm with a threshold current density of 4.2 kA/cm^2 and a voltage of 8.7 V was successfully achieved.

HL 28.3 Wed 16:00 POT 361

Spectral dynamics of lateral modes and filaments in InGaN broad-ridge laser diodes — •Lukas Uhlig[1], Dominic J. Kunzmann[1], Anna Kafar[2,3], Szymon Grzanka[2,3], Piotr Perlin[2,3], and Ulrich T. Schwarz[1] — [1]Chemnitz University of Technology, Chemnitz, Germany — [2]Institute of High Pressure Physics, Polish Academy of Sciences, Warsaw, Poland — [3]Top-GaN Ltd., Warsaw, Poland.

Blue InGaN broad-ridge laser diodes are versatile, efficient, and compact high power emitters, which are demanded for copper welding, white light generation, and other applications. Compared with standard narrow-ridge laser diodes, in case of the broad-ridge devices the ridge width is increased from around 2 μm to tens of micrometers,

leading to lateral multi-mode operation or filamentation.

We investigate a series of devices with ridge widths from 2.4 μm to 20 μm and study their lateral-spectral-temporal behavior as well as high-resolution spectra. With increasing ridge width, we observe the transition from lateral single-mode to multi-mode operation and in the case of the 20 μm wide ridge, filamentation occurs. In the multi-mode regime, the dynamic onset behavior as well as the spectral-lateral mode distribution are governed by competition of lateral and longitudinal modes for gain. Filaments form in the case of strong nonlinear interaction between intensity, charge carrier density, temperature, and refractive index. Using high-resolution spectroscopy, we can clearly differentiate between different lateral modes, which occur in parallel and form multiple longitudinal mode combs.

HL 28.4 Wed 16:15 POT 361

Temperature dependent electroluminescence studies of the carrier transport in multi colour deep ultraviolet light emitting diodes — •Jakob Höpfner[1], Florian Kühl[1], Marcel Schilling[1], Anton Muhin[1], Gregor Hofmann[2], Friedhard Römer[2], Tim Wernicke[1], Bernd Witzigmann[2], and Michael Kneissl[1] — [1]Technische Universität Berlin, Institute of Solid State Physics, Berlin, Germany — [2]Lehrstuhl für Optoelektronik, Department EEI, Friedrich-Alexander-Universität, Erlangen-Nürnberg, German

Earlier studies have shown that a drop in current injection efficiency (CIE) is partly responsible for the poor external quantum efficiencies (EQE) of AlGaN-based deep ultraviolet light emitting diodes (DUV-LEDs). In particular, the hole injection and the carrier distribution in the AlGaN multi quantum well (MQW) active region is not well understood. In order to get a better insight we have performed temperature dependent electroluminescence (EL) investigations of three-fold AlGaN MQW LEDs with two of the QWs emitting at 233 nm and one QW emitting at 250 nm. In addition, the position of the 250 nm QW with the MQW structure was varied. From temperature dependent EL measurements we observe a strong shift in the intensity distribution over wavelength and temperature. We were able to correlate this with a change in the hole injection into the different QWs suggesting an efficient hole transport over the barriers between the QWs at room temperature. These experimental results are also supported by devices simulations and enable us to further improve the LED heterostructure.

HL 28.5 Wed 16:30 POT 361

265 nm LEDs and laser heterostructures with p-type distributed polarization doping AlGaN layers — •Massimo Grigoletto[1,2], Sarina Graupeter[1], Verena Montag[1], Jakob Höpfner[1], Luca Sulmoni[1], Tim Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics, 10623 Berlin, Germany — [2]Ferdinand-Braun-Institut (FBH), Berlin, Germany

Efficient hole injection in AlGaN-based LEDs and lasers emitting in the ultraviolet (UV) spectral range remains a great challenge. Distributed polarization doped (DPD) p-type AlGaN heterostructures have been developed to overcome this hurdle. By introducing a constant piezoelectric polarization charge along compositionally graded $Al_xGa_{1-x}N$ layers a high density of free hole carriers can be established even in the absence of Mg dopants. In this study we have investigated the influence of the DPD design on the structural properties and electro-optic characteristics of AlGaN-based LEDs and laser heterostructures emitting near 265 nm. For efficient hole injection p-type $Al_xGa_{1-x}N$ layers with different Al gradients and thickness have been incorporated and grown by metal organic vapor phase epitaxy. On-wafer measurements of UV-LEDs exhibit forward voltages of 6 V at a dc current of 20 mA and output power of 1 mW comparable to conventionally Mg-doped heterostructures. The LEDs could be operated at high current densities up to 12 kA/cm^2 in pulsed mode, which shows the DPD is a promising approach for achieving low resistance p-type AlGaN layers with high al mole fractions.

HL 29: Materials and devices for quantum technology I

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

HL 29.1 Wed 15:00 POT 151

Mapping of the local valley splitting in a Si/SiGe qubit shuttle device — •Bingjie Chen[1], Mats Volmer[1], Tom Struck[1], Ran Xue[1], Inga Seidler[1], Joachim Knoch[2] und Lars R. Schreiber[1] — [1]JARA-FIT Institute for Quantum Information, Forschungszentrum Jülich GmbH and RWTH Aachen University, Germany — [2]Institut für Halbleitertechnik, RWTH Aachen University, Germany

Qubits based on the electron spin in gate-defined ^{28}Si/SiGe quantum dots (QD) are one of the major candidates for the quantum information processing. Due to weak spin-orbit coupling and low hyperfine interaction, their fidelity threshold for quantum error correction is reached. However, valley-state excitations [1-3] have implications for spin dephasing during qubit shuttling [4]. In our experiment, we map the valley splitting energy (E_{VS}) originating from the quantum well confinement at different locations of a qubit shuttle device [5]. We measure their orbital splitting and spin-polarization as a function of various electron fillings and magnetic fields [6]. We fit the local singlet-triplet splitting energy as a lower boundary of the relevant E_{VS}, which is distributed in a range of 11...73 μeV. The correlation length is approximatly the QD size and small dependence on the electric field perpendicular to the quantum well is found. [1]Dodson, J.P. ea., arXiv:2103.14702.[2]McJunkin, T. ea., Phys. Rev. B 104, 085406.[3]Hollman, A. ea., Phys. Rev. Applied 13, 034068.[4]Langrock, V. ea., arXiv: 2202.11793.[5]Seidler, I. ea., npj Quantum Inf. 8, 100.[6]Friessen. M. ea., Phys. Rev. B 75, 115318. This work has been funded by the German Research Foundation (DFG) within the project KN 545/28-1.

HL 29.2 Wed 15:15 POT 151

Accessing broad-band quantum dynamics in the low photon regime — •Markus Sifft[1], A. Kurzmann[2], J. Kerski[2], R. Schott[1], A. Ludwig[1], A. D. Wieck[1], A. Lorke[2], M. Geller[2], and D. Hägele[1] — [1]Ruhr University Bochum, Germany — [2]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany

The analysis of quantum dynamics from measurement records $z(t)$ poses a fundamental challenge in many fields of science and engineering. Measurement records are notoriously difficult to analyze due to inherent or additional background noise, loss of e.g., probe photons, and finite measurement times. We recently introduced quantum polyspectra as a tool to analyze $z(t)$ in terms of higher order spectra whose shapes can be predicted within a quantum master equation approach [1,2]. Here, we solve the problem of analyzing the blinking (charging) dynamics of a semiconductor quantum dot in the regime of low photon rates or high photon loss [3]. The usual telegraph noise of binned photon click events changes to rare single clicks in case of high photon loss. Fitting theoretical quantum polyspectra to their measured counterparts gives full access to the in- and out-tunneling rates $\gamma_{\rm in}$, $\gamma_{\rm out}$ of electrons despite low average photon rates $\gamma_{\rm p} \ll \gamma_{\rm in}+\gamma_{\rm out}$. We demonstrate the successful evaluation of tunneling rates at up to 99.9 % loss of photons surpassing a previous scheme that handled a 98 % loss using the same data. [1] Hägele et al., PRB 98, 205143 (2018), [2] Sifft et al., PRR 3, 033123 (2021), [3] Sifft et al., arXiv:2109.05862

HL 29.3 Wed 15:30 POT 151

Generation of V_{Si} color centers in 4H-SiC using He and Li focused ion beam — •Christian Gobert[1], Shravan Kumar Parthasarathy[1], Fedor Hrunski[2], Roland Nagy[2], and Patrick Berwian[1] — [1]Fraunhofer Institute for Integrated Systems and Device Technology (IISB), 91058 Erlangen, Germany — [2]Group of Applied Quantum Technologies, University Erlangen-Nuremberg (FAU), 91058 Erlangen, Germany

The silicon vacancy (V_{Si}) color center in 4H-SiC is a promising candidate as a qubit for quantum sensing, communication, and computing, due to its excellent spin and optical properties[1,2], scalability and mature semiconductor technology platform[3]. V_{Si} color centers can be fabricated by means of high energetic irradiation, e.g., using electrons, ions, neutrons, or laser pulses[4]. In this contribution, we report on a direct comparison of 3 different irradiation techniques, i.e. He- Li- and electron irradiation, for the first time on the very same sample material. Characterization is accomplished using confocal photoluminescence (PL) measurements on two perpendicular crystal orientations. We investigate the optical and spin properties of generated V_{Si} color

centers and employ PL mappings to judge the scalability of the irradiation technique. To evaluate the quality of the generated V_{Si} color centers, PL excitation spectroscopy (PLE) is applied.

[1] R. Nagy et al., Nat. Commun. 10, 1954 (2019)
[2] R. Nagy et al., Appl. Phys. Lett. 118, 144003 (2021)
[3] C. Babin et al., Nat. Mater. 21, 67-73 (2022)
[4] S. Castelletto, A. Boretti, J. Phys.: Photonics 2 (2020) 022001

HL 29.4 Wed 15:45 POT 151

1.*Quantum Vector Magnetometry of Magnetic Nanoparticles in Living Tissue — •Andre Pointner[1], Philipp Kunze[2], Regine Schneider-Stock[2], Bernhard Friedrich[3], Christoph Alexiou[3], Rainer Tietze[3], and Roland Nagy[1] — [1]Chair of Electron Devices, FAU Erlangen-Nuremberg — [2]Experimental Tumor Pathology, University Hospital Erlangen — [3]Experimental Oncology and Nanomedicine, University Hospital Erlangen

Developing an understanding of the underlying processes of cancer dissemination is to this day a pressing topic in medical research, due to the lack of observation techniques capable of resolving single cell behavior in living tissue. Widefield imaging with ensembles of nitrogen-vacancy centers (NV-Centers) in diamond as a quantum sensor allows the observation of individual cells by mapping selectively attached superparamagnetic iron oxide nanoparticles (SPIONs) on cells of interest. Application of a magnetic bias field results in a magnetic dipole emitted by the SPIONs, which adds onto the known bias field. The magnetic field causes a lift of the degeneracy of the NV-Centers spin states. Evaluating the spin transitions via optically detected magnetic resonance (ODMR) and comparison to the ground state hamiltonian enables the reconstruction of the magnetic field vector. By applying this measurement scheme pixelwise to a sequence of widefield images of the diamond sample, we calculate the corresponding dipole vector for the SPIONs and map the resulting magnetic field over the field of view. This enables single cell tracking in living tissue inside a homemade integrated widefield microscope over the span of multiple days.

HL 29.5 Wed 16:00 POT 151

Fabrication and pre-characterization of 10 μm long single-electron shuttling devices. — •Max Beer[1], Ran Xue[1], Inga Seidler[1], Jhih-Sian Tu[2], Lino Visser[1], Hendrik Bluhm[1], and Lars R. Schreiber[1] — [1]JARA-FIT Institute for Quantum Information, Forschungszentrum Jülich GmbH and RWTH Aachen University, Aachen, Germany — [2]Helmholtz Nano Facility (HNF), Forschungszentrum Jülich, Jülich, Germany

The electron-spin in gate-defined quantum dots in a Si/SiGe quantum well is one of the most promising qubits for scalable quantum computing. Scalability can be achieved by coherent coupling such as conveyor-mode single electron-spin shuttling [1]. Aiming at a shuttle distance of 10 μm, we fabricate a shuttling device with three patterned metal-gate layers forming an array of >140 gates. Al_2O_3 deposited by atomic layer deposition (ALD) isolates the gates, but also induces potential disorder in the quantum well. This disorder can be reduced by minimizing the oxid thickness [1]. We investigate two strategies: (I) Reduction of oxide thickness towards the ALD limit and (II) replacement of MOS-gates with Pd-Si Schottky-gates wherever applicable. Shuttling devices are selected by a transport measurement-protocol operating at 4.2 K on single electron transistors, which are operated as charge sensors for electron shuttling at 10 mK [2].

[1] Langrock, V. *et al.*, arXiv: 2202.11793 (2022).
[2] Seidler, I. *et al.*, npj Quantum Inf. 8: 100 (2022).

Work funded by the DFG under project number EXC 2004/1-390534769.

30 min. break

HL 29.6 Wed 16:45 POT 151

Coupling of solid-state quantum emitters to low-loss plasmonic waveguides — •Paul Steinmann, Hans-Joachim Schill, and Stefan Linden — Physikalisches Institut, Universität Bonn, Nussallee 12, 53115 Bonn, Germany

Plasmonic waveguides with integrated single photon emitters (SPEs) offer an attractive platform for nanophotonic quantum circuit applications. Here, we report on the coupling of strain-induced SPEs in an MoSe2 monolayer to low-loss plasmonic waveguides. For this purpose, we used electron beam lithography with the negative-tone resist Medusa82 to fabricate dielectric-loaded surface plasmon polariton waveguides (DLSPPWs) on top of a chemically prepared monocrystalline silver platelet. Additional gratings placed at the ends of the waveguides serve as in- and out-coupling structures. An MoSe2 monolayer was deposited on the centre of one of the waveguides by a dry-transfer technique. Operating at 4 Kelvin, surface plasmon polaritons (SPPs) are launched by a green laser at the in-coupling port of the waveguide. The SPPs travel through the waveguide and lead to the excitation of the monolayer. In addition to the exciton and trion signal, we observe sharp emission lines that we attribute to strain-induced trap states. The second-order correlation function of one of the spectrally filtered emission lines was measured with an HBT setup. The measured value g(2)(0)=0.4 indicates the single-photon nature of the emitter. Our findings indicate that TMDC monolayers can be used as integrated SPEs in efficient plasmonic circuits, and thus further pave the way towards plasmonic-based single photon networks.

HL 29.7 Wed 17:00 POT 151

Sensing of electrolytes with nitrogen-vacancy centers in nanodiamonds — •Maximilian Hollendonner[1,2], Sanchar Sharma[2], Durga Dasari[3], Silvia Viola Kusminskiy[2,4], and Roland Nagy[1] — [1]Chair of Electron Devices, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Max Planck Institute for the Science of Light, Staudtstraße 2, Erlangen, Germany — [3]3rd Institute of Physics, University of Stuttgart and Institute for Quantum Science and Technology (IQST), Stuttgart, Germany — [4]Institute for Theoretical Solid State Physics, RWTH Aachen University, Aachen, Germany

Today's batteries suffer from performance losses with increasing cell age which is caused by irreversible degradation processes at a molecular level. To understand these processes, it is important to measure them *in-situ* and *in-operando*. Up to now there exists no sensor which can perform this task with sub-micrometer resolution. We propose to use nanodiamonds containing single NV-centers as such sensors inside the liquid electrolyte of a battery. It has been shown that NV-centers are excellent electric field sensors [1,2]. From theoretical considerations we found out that by performing repeated FID pulse sequences it is not only possible to measure the electric field components generated by the ions inside the electrolyte but also the local ionic concentrations at the position of the nanodiamond with nanometer-resolution.

Sources: [1] F. Dolde *et al.*, *Nature Phys* **7**, 459-463 (2011) [2] J. Michl *et al.*, *Nano Lett.* 2019, 19, 8, 4904-4910

HL 29.8 Wed 17:15 POT 151

Interplay of Pauli Blockade with Electron-Photon Coupling in Quantum Dots — •Florian Ginzel and Guido Burkard — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

Both quantum transport measurements in the Pauli blockade regime and microwave cavity transmission measurements are important tools for spin-qubit readout and characterization. In our work [1] we theoretically investigate how a double quantum dot in a transport setup interacts with a coupled microwave resonator while the current through the DQD is rectified by Pauli blockade. We show that the output field of the resonator can be used to infer the leakage current and thus obtain insight into the blockade mechanisms without additional components such as charge or current sensors for each dot. In the case double quantum dot realized in silicon, we show how the valley quasi-degeneracy can impose limitations on this scheme. We also demonstrate that a large number of unknown double quantum dot parameters including (but not limited to) the valley splitting can be estimated from the resonator response simultaneous to a transport experiment, providing more detailed knowledge about the microscopic environment of the dots. Furthermore, we describe and quantify a back-action of the resonator photons on the steady state leakage current.

[1] F. Ginzel and G. Burkard, arxiv:2210.02982 (2022)

HL 29.9 Wed 17:30 POT 151

Structural and electrical characterization of the InAs/CdSe core/shell NWs — •Mane Kalajyan[1], Marvin Marco Jansen[1,2], Nils von den Driesch[3], Erik Zimmermann[1], Nataliya Demarina[4], Anton Faustmann[1], Gerrit Behner[1], Christoph Krause[1], Benjamin Bennemann[1], Jan Karthein[1], Detlev Grützmacher[1,3], Thomas Schäpers[1], and Alexander Pawlis[1,3] — [1]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich, Jülich, Germany — [2]Eindhoven University of Technology, Eindhoven, Netherlands — [3]Peter Grünberg Institut (PGI-10), Forschungszentrum Jülich, Jülich, Germany — [4]Peter Grünberg Institut (PGI-2), Forschungszentrum Jülich, Jülich, Germany

InAs nanowires (NWs) are a well-known basis for field-effect transistors (FETs), light-emitting diodes and lasers, quantum devices and biosensors. The larger band gap material CdSe, having a negligible lattice mismatch to InAs, allows for tailoring the conductive channel at the CdSe/InAs core/shell interface, thus making CdSe an excellent candidate for the InAs surface states passivation.

Here, we present the fabrication, structural, and electrical characterization of a unique InAs/CdSe core/shell NW system. The interface between the core and the shell is proven to be flawless by means of HR-TEM micrographs. Moreover, electrical characterization reveals a high-mobility two-dimensional transport channel in the InAs core. Finally, magnetotransport measurements show clear signs of weak antilocalization. These results make the novel InAs/CdSe hybrid NWs a promising basis for the quantum device applications.

HL 29.10 Wed 17:45 POT 151

Electrical excitation of color centers in phosphorus-doped diamond Schottky diodes — •Florian Sledz[1], Igor A. Khramtsov[2], Assegid M. Flatae[1], Stefano Lagomarsino[1], Navid Soltani[1], Shannon S. Nicley[3], Rozita Rouzbahani[3], Paulius Pobedinskas[3], Ken Haenen[3], Jin Qun[4], Xin Jiang[4], Paul Kienitz[5], Peter Haring Bolivar[5], Dmitry Yu. Fedyanin[2], and Mario Agio[1] — [1]Laboratory of Nano-Optics, University of Siegen, Germany — [2]Moscow, Russian Federation — [3]Institute for Materials Research (IMO) & IMOMEC, Hasselt University & IMEC vzw, Belgium — [4]Institute of Materials Engineering, University of Siegen, Germany — [5]Institute of Graphene-based Nanotechnology, University of Siegen, Germany

A robust single-photon source operating upon electrical injection at ambient condition is desirable for quantum technologies. Silicon-vacancy color centers in diamond are promising candidates as their emission is concentrated in a narrow zero-phonon line with a short excited-state lifetime of ˜1 ns. Creating the color centers in n-type diamond (phosphorus-doped) allows the implementation of a Schottky-diode configuration. This provides a simpler approach than the traditional complex diamond semiconductor junctions e.g., p-i-n. Selective optical excitation allows addressing of single silicon-vacancy color centers while suppressing background from mainly nitrogen-vacancy defects created during Si ion implantation. This paves a way for the realization of the predicted bright electroluminescence of color centers.

HL 30: Quantum transport and quantum Hall effects II (joint session HL/TT)

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

HL 30.1 Wed 15:00 POT 251

Aharonov-Bohm-type oscillations in phase-pure core/shell GaAs/InAs nanowires — •Farah Basaric[1,2], Anton Faustmann[1,2], Erik Zimmermann[1,2], Gerrit Behner[1,2], Alexander Pawlis[1,2], Christoph Krause[1,2], Hans Lüth[1,2], Detlev Grützmacher[1,2], and Thomas Schäpers[1,2] — [1]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology, Jülich-Aachen Research Alliance, Forschungszentrum Jülich and RWTH Aachen University, Germany

Epitaxially grown phase-pure GaAs/InAs core/shell nanowires offer uniformity in their electrical, mechanical and optical properties due to the absence of a crystallographic disorder. Magnetotransport measurements were carried out at variable temperatures and for different gate voltages, under an applied in-plane magnetic field. Pronounced Aharonov-Bohm-type oscillations in the conductance are observed for this nanowire type. In measurements at different gate voltages, significantly higher oscillation amplitudes are observed in comparison to the corresponding measurements on polymorphic core/shell nanowires. Furthermore, measurements at different temperatures show robustness of these oscillations against high temperatures as a result of reduced disorder. Finally, strong indications of a quasi-ballistic transport regime could be recognized for the phase-pure nanowire type. Obtained results indicate a strong effect of disorder reduction in GaAs/InAs nanowire transport properties, manifested in superior transport properties.

HL 30.2 Wed 15:15 POT 251

Spin valves based on bilayer graphene quantum point contacts — •Eike Icking[1,2], Christian Volk[1,2], Christopher Schattauer[3], Luca Banszerus[1,2], Kenji Watanabe[4], Takashi Taniguchi[5], Florian Libisch[3], Bernd Beschoten[1], and Christoph Stampfer[1,2] — [1]RWTH Aachen University, Germany — [2]Forschungszentrum Jülich, Germany — [3]TU Vienna, Austria — [4]Research Center for Functional Material, Japan — [5]International Center for Materials Nanoarchitectonics, Japan

Bernal bilayer graphene (BLG) is a unique material as it allows opening and electrostatically tuning a sizeable band gap by applying a perpendicular electric field. Recently, charge carriers have been confined successfully in one dimension to form quantum point contacts (QPC) based on split gates separated by a channel of a few hundred nanometers. Moreover, spin-polarized quantum transport through such structures has been demonstrated up to 6 e^2/h using a high in-plane magnetic field. The threshold magnetic field at which the lowest modes become spin-polarized depends on the subband spacing and thus on the width of the split gate channel. In this work, we combine two QPCs of different geometric widths, resulting in different threshold magnetic fields, to spin-polarize the first QPC and use it as a filter for the second QPC. In particular, we report on a spin-valve achieving spin-polarized channels with a total conductance of up to 10 e^2/h.

HL 30.3 Wed 15:30 POT 251

Optical and electrical tuning between the normal insulating and topological insulating phase of InAs/GaSb bilayer quantum wells — •Manuel Meyer[1], Tobias Fähndrich[1], Sebastian Schmid[1], Sebastian Gebert[1], Gerald Bastard[1,2], Fabian Hartmann[1], and Sven Höfling[1] — [1]Technische Physik, Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Am Hubland, D-97074 Würzburg, Germany — [2]Physics Department, École Normale Supérieure, PSL 24 rue Lhomond, 75005 Paris, France

Topological insulators (TI) based on InAs/GaSb bilayer quantum wells (BQW) are appealing due to their rich phase diagram with a TI and normal insulating (NI) phase[1]. The switching between both phases can be achieved by external electric fields using a top and back gate (TG and BG)[2]. However, especially a fully functional BG is difficult to realize in antimonides due to leakage issues. To overcome this bottleneck we present another tuning knob using optical excitation to switch from the NI to the TI phase over the TI gap[3]. By monitoring the charge carrier densities we can identify the hybridized band structure and in-plane magnetic field measurements evidence the TI gap. Furthermore, a top-gated sample is investigated. Without a back gate we find properties from both phases for magnetransport measurements which points to a mixing of NI and TI states. This is further indicated by the resistance peak evolutions with temperature for both samples.

[1] C. Liu et al., PRL 100, 236601 (2008)
[2] F. Qu et al., PRL 115, 036803 (2015)
[3] G. Knebl et al., PRB 98, 041301(R) (2018)

30 min. break

HL 30.4 Wed 16:15 POT 251

Transport in high mobility HgTe heterostructures — •Michael Kick, Lena Fürsst, Johannes Kleinlein, Saquib Shamim, Hartmut Buhmann, and Laurens W. Molenkamp — Experimentelle Physik III, Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

The Fractional Quantum Hall Effect (FQHE) has not yet been observed in the material system of HgTe. Due to recent progress in MBE growth, routinely charge carrier mobilities of HgTe heterostructures of over $\mu > 1{\cdot}10^6$ cm^2/Vs are obtained which is in the same order of magnitude as in the first reported experimental observation of the FQHE in GaAs/GaAlAs heterostructures. This opens up new prospects for transport investigations into the long time still open question of fractional states in this material system.

In 2-dimensional HgTe quantum wells, transport measurements show well pronounced quantum Hall plateaus for all filling factors, but no indication of any fractional state. High magnetic field measurements show a prolonged $\nu = 1$ plateau and a transition to an

insulating state. Intriguingly, the $\nu = 1$ plateau exhibits a transition to an insulating state for filling factor $\nu = 1/2$.

Another possibility to observe the FQHE in HgTe is provided by the 2D surface states of a 3D topological insulator. High mobility layers, $\mu > 1 \cdot 10^6\,\mathrm{cm}^2/\mathrm{Vs}$, of tensil strained HgTe are subject of extensive magneto-transport investigations. First results reveal a good and detailed correspondence to recent k.p band structure calculations for non-interacting electron systems.

HL 30.5 Wed 16:30 POT 251

Electron Density Depended Giant Negative Magnetoresistance — •Lina Bockhorn and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany

Ultra-high mobility two-dimensional electron gases not only show an increasing number of new fractional filling factors, but also an astonishing robust negative magnetoresistance at zero magnetic field [1 -5]. The theoretical description of this negative magnetoresistance is still an open issue due to its complex dependencies on several parameters.

The behavior of the giant negative magnetoresistance is affected by different scattering events, e. g. interface roughness, oval defects, background impurities and remote ionized impurities, which leads to a strong dependence on different parameters. Here, we take a closer look on the temperature dependence of the giant negative magnetoresistance for different electron densities. At low temperatures we observe the predicted temperature dependence of $T^{1/2}$ [6].

[1] L. Bockhorn et al., Phys. Rev. B 83, 113301 (2011).
[2] A. T. Hatke et al., Phys. Rev. B 85, 081304 (2012).
[3] R. G. Mani et al., Scientific Reports 3, 2747 (2013).
[4] L. Bockhorn et al., Phys. Rev. B 90, 165434 (2014).
[5] L. Bockhorn et al., Appl. Phys. Lett. 108, 092103 (2016).
[6] I. V. Gornyi et al., Phys. Rev. B. 69, 045313 (2004).

HL 30.6 Wed 16:45 POT 251

Massless Dirac fermions on a space-time lattice with a topologically protected Dirac cone — •Michal Pacholski[1], Alvaro Donís Vela[3], Gal Lemut[3], Jakub Tworzydlo[2], and Carlo Beenakker[3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Warsaw University, Warsaw, Poland — [3]Lorentz Institute, Leiden, The Netherlands

The symmetries that protect massless Dirac fermions from a gap opening may become ineffective if the Dirac equation is discretized in space and time, either because of scattering between multiple Dirac cones in the Brillouin zone (fermion doubling) or because of singularities at zone boundaries. Here we introduce an implementation of Dirac fermions on a space-time lattice that removes both obstructions. The quasi-energy band structure has a tangent dispersion with a single Dirac cone that cannot be gapped without breaking both time-reversal and chiral symmetries. We show that this topological protection is absent in the familiar single-cone discretization with a linear sawtooth dispersion, as a consequence of the fact that there the time-evolution operator is discontinuous at Brillouin zone boundaries.

HL 31: Focus Session: Frontiers of Electronic-Structure Theory V (joint session O/HL)

Time: Wednesday 15:00–17:30 Location: TRE Ma

HL 31.1 Wed 15:00 TRE Ma

Phase transitions in the two-dimensional Su-Schrieffer-Heeger model — •Changan Li[1], Songbo Zhang[2], Sangjun Choi[1], Jan Budich[3], and Björn Trauzettel[1] — [1]Institute for theoretical physics and astrophysics, University of Würzburg, Wuerzburg, Germany — [2]Department of Physics, University of Zürich, Winterthurerstrasse 190 8057, Zürich, Switzerland — [3]Institute of Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany

The 2D Su-Schrieffer-Heeger (SSH) model is endowed with rich topological physics. First we show that the random flux can induce a metal-band insulator transition in the 2D SSH, thus reporting the first example of such a transition. Remarkably, we find that the resulting insulating phase can even be a higher-order topological insulator with zero-energy corner modes and fractional corner charges. Employing both level statistics and finite-size scaling analysis, we characterize the metal-band insulator transition and numerically extract its critical exponent. By proposing another inclined 2D SSH model, a deformed one, we show that a pair of Dirac points protected by space-time inversion symmetry appear in the semimetallic phase. Interestingly, the locations of these Dirac points are not pinned to any high-symmetry points of the Brillouin zone but highly tunable through parameter modulations. Moreover, the merging of two Dirac points undergoes a topological phase transition, which leads to either an anisotropic topological insulating phase or a nodal-line metallic phase.

HL 31.2 Wed 15:15 TRE Ma

Ab initio embedding approach for carbon defects in hexagonal boron nitride: A new platform to probe environmental screening — •Danis Badrtdinov[1], Magdalena Grzeszczyk[2], Alexander Hampel[3], Cyrus Dreyer[3,4], Maciej Koperski[2], and Malte Rösner[1] — [1]Radboud University, Nijmegen, The Netherlands — [2]National University of Singapore, Singapore — [3]Flatiron Institute, USA — [4]Stony Brook University, USA

Correlated defects in layered van der Waals hosts hold high promises for realizing quantum technologies, as they allow for various possibilities to control defect properties, e.g., via altering the host thickness or by changing the substrate material. A quantitative description of the defect ground and excited states taking the details of the impurity environment into account is, however, a considerable challenge for conventional density-functional theory (DFT) based methods as the impurities might be correlated and dielectric environmental screening is not fully accounted for in DFT. To tackle these challenges we apply and extend an embedding approach that treat the defect states within exact many-body theory, while DFT is used as a starting point to describe the bulk host material. We study various carbon defects embedded in hexagonal boron nitride (hBN), allowing us to disentangle all mechanisms responsible for the alteration of defect properties including modifications to the impurity structure and changes in the environmental screening upon thinning down the hBN host. Our new embedding approach paves the way for improved identification of defects in layered materials and to tailor their properties.

HL 31.3 Wed 15:30 TRE Ma

Nonequilibrium electron dynamics in a two-sites Hubbard model — •Jakub Wronowicz and Yaroslav Pavlyukh — Department of Theoretical Physics, Wrocław University of Science and Technology

Electron dynamics in a two-sites Hubbard model is studied using the nonequilibrium Green's function approach using formalism developed in [1]. We focus on the electron dynamics arising in the adiabatic switching scenario. Many-body approximations are classified according to the channel of the Bethe-Salpeter equation in which electronic correlations are explicitly treated. They give rise to the so-called second Born, T-matrix and GW approximations. In each of these cases, the model is reduced to a system of ordinary differential equations, which resemble equations of motion for a driven harmonic oscillator with time-dependent frequencies. We discuss transient solutions for the off-diagonal density matrix. Analytical result for the steady state in second Born approximation is compared with the exact solution. It is further shown numerically that in the large Hubbard-U limit the T -matrix in the particle-hole channel and spin-adapted GW approximations converge to the same solution.

[1] Y. Pavlyukh, E. Perfetto, and G. Stefanucci, *Photoinduced dynamics of organic molecules using nonequilibrium Green's functions with second-Born, GW, T-matrix, and three-particle correlations*, Phys. Rev. B **104**, 035124 (2021).

HL 31.4 Wed 15:45 TRE Ma

Time-linear quantum transport simulations with correlated nonequilibrium Green's functions — •Riku Tuovinen[1], Yaroslav Pavlyukh[2], Enrico Perfetto[3], and Gianluca Stefanucci[3] — [1]Department of Physics, Nanoscience Center, University of Jyväskylä, Finland — [2]Department of Theoretical

Physics, Wroclaw University of Science and Technology, Poland — [3]Dipartimento di Fisica, Università di Roma Tor Vergata, Italy

We present a time-linear scaling method for open and correlated quantum systems. The method inherits from many-body theory [1] the possibility of selecting the most relevant scattering processes, thereby paving the way for real-time characterizations of correlated ultrafast phenomena in quantum transport. The open system dynamics is described in terms of an embedding correlator from which the transient current can be calculated via the Meir-Wingreen formula [2]. We efficiently implement the method through a combination with recent time-linear schemes for closed systems [3]. Electron-electron and electron-phonon interactions can be treated on equal footing while preserving all fundametal conservation laws. We employ the method by studying transport of correlated electron-hole pairs in semiconductors [4].

[1] G. Stefanucci and R. van Leeuwen, Nonequilibrium Many-Body Theory of Quantum Systems (CUP 2013).

[2] Y. Meir and N. S. Wingreen, PRL 68, 2512 (1992).

[3] N. Schlünzen, J.-P. Joost, and M. Bonitz, PRL 124 (2020) 076601.

[4] R. Tuovinen, Y. Pavlyukh, E. Perfetto, and G. Stefanucci, arXiv:2211.15635 (2022).

15 min. break

Topical Talk HL 31.5 Wed 16:15 TRE Ma

Challenges in modelling correlated electronic matter — •Roser Valenti — Institute of Theoretical Physics, Goethe University Frankfurt, Frankfurt, Germany

The microscopic modelling of correlated electronic matter from first principles poses a fundamental theoretical challenge due to the many-body character of the systems. In recent years there have been a few internationally coordinated efforts in theoretical method development to generate a common platform of benchmarked software tools including dynamical mean field theory and extensions.

In this talk I will present some of the challenges we face in such an endeavour and illustrate them with some examples on models and materials.

Funding from the DFG through QUAST FOR 5249-449872909 is acknowledged.

HL 31.6 Wed 16:45 TRE Ma

Electron-Phonon Interactions from DFPT within an All-Electron Framework — •Sebastian Tillack, Pasquale Pavone, and Claudia Draxl — Humboldt-Universität zu Berlin and IRIS Adlershof, 12489 Berlin, Germany

The interplay between electrons and the motions of nuclei in solids, described in terms of phonons, play a crucial role in the modeling of functional materials, particularly for understanding temperature dependent effects. We present an implementation of density-functional perturbation theory (DFPT) within a full-potential all-electron framework as implemented in the code `exciting` [1]. Our implementation allows one to compute phonons as well as the linear response to external electric fields. We use DFPT calculations to study lattice vibrations and electron-phonon interactions (EPIs) by means of many-body perturbation theory in β-Ga_2O_3. The electron self-energy contribution is computed as a function of temperature from which various properties such as quasi-particle energies, electron linewidths, and spectral functions are derived. We further incorporate many-body electron-electron interactions described by the GW method. Beyond that, our work creates the foundation for a fully *ab initio* study of the effect of EPIs on optical excitations.

[1] A. Gulans, et al. J. Phys.: Condens. Matter 26, 363202 (2014).

HL 31.7 Wed 17:00 TRE Ma

Calculation of phonon spectra with the FLAPW method using Density Function Perturbation Theory — •Alexander Neukirchen, Christian-Roman Gerhorst, Gregor Michalicek, Daniel Wortmann, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Computing phonons applying density functional perturbation theory (DFPT) within all-electron DFT methods is a well-known challenge due to the displacement of muffin-tin spheres and sphere-centered basis functions. In this talk, we present our current results of the phonon dispersion based on our implementation of the DFPT approach in the FLEUR code [1] (www.flapw.de), an implementation of the full-potential linearized augmented plane wave (FLAPW) method. We highlight the good agreement of our preliminary results with phonon dispersions obtained with the finite displacement method for which the FLEUR code has been combined with the phonopy tool (www.phonopy.github.io/phonopy/). We discuss the numerical challenges involved in calculating meV quantites on top of large ground state energies typical for all-electron methods and how we addressed them.

This work has been supported by the Helmholtz Postdoc Programme (VHPD-022) and by the MaX Center of Excellence funded by the EU through the H2020-INFRAEDI-2018-1 767 (Grant No. 824143).

[1] A. Neukirchen, C.-R. Gerhorst, D. A. Klüppelberg, M. Betzinger, D. Wortmann, G. Michalicek, G. Bihlmayer, S. Blügel, to be published.

HL 31.8 Wed 17:15 TRE Ma

Electron-phonon interaction using a localized Gaussian basis set — •Gerrit Johannes Mann, Thorsten Deilmann, and Michael Rohlfing — Institute of Solid State Theory, University of Münster, Germany

Electron-phonon interaction is a crucial mechanism in solid state physics that is responsible for a multitude of phenomena. However, in electronic structure calculations it is usually neglected. We developed an ab-initio implementation on top of density functional theory that combines finite differences calculations with the perturbative Allen-Heine-Cardona framework in order to calculate the temperature-dependent renormalization of the electronic bandstructure due to electron-phonon interaction using a basis set of localized Gaussian orbitals.

This implementation circumvents the limiting problems of previous implementations while maintaining a good agreement with the literature. The calculated Fan-Migdal zero-point renormalization of the direct band gap of silicon amounts to about 15 meV compared to 20 meV in the literature. Also the temperature-dependence of the renormalization agrees similarly well.

HL 32: Organic Electronics and Photovoltaics II (joint session CPP/HL)

Time: Wednesday 15:00–17:30 Location: GÖR 226

HL 32.1 Wed 15:00 GÖR 226

Charge-carrier dynamics across seven orders of magnitude in double-cable polymer-based single-component organic solar cells — •Yakun He[1,2], Bingzhe Wang[1], Larry Lueer[1], Dirk Guldi[1], Ning Li[1], and Christoph Brabec[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Martensstrasse 7, 91058 Erlangen, Germany — [2]KAUST Solar Center, King Abdullah University of Science and Technology, Thuwal 23955, Saudi Arabia

Single-component organic solar cells (SCOSCs) with intrinsically high stability have witnessed efficiencies from 2-3% to 6-11%. For boosting higher efficiencies of SCOSCs, essential information of charge-carrier dynamics as a function of microstructure is highly demanded, requesting systematical investigation on photophysics. In this work, for the first time, the charge-carrier dynamics of a representative double-cable polymer, which achieves efficiencies of over 6% as an active layer in SCOSCs, is investigated across seven orders of magnitude in time scale, from fs-ps TAS and ps-ns TRPL for probing charge generation to ns-us TAS for charge recombination. Specific emphasis is placed on understanding the impact of thermal post-treatment on the charge dissociation, transport, and recombination dynamics. By increasing the thermal annealing temperature, geminate recombination is reduced accompanied by more efficient charge dissociation and suppressed bimolecular recombination. Annealing the photoactive layer at 230 oC results in the highest photovoltaic performance correlating well with the findings from transient studies. This work intends to present a complete picture of the charge-carrier dynamics in SCOSCs.

HL 32.2 Wed 15:15 GÖR 226

What determines the Recombination Order in Organic Solar Cells? — •Kathrin Brocker, Jana Seiler, Dorothea Scheunemann, Clemens Göhler, and Martijn Kemerink — Institute for Molecular Systems Engineering and Advanced Materials, Heidelberg University

Organic Solar Cells provide an interesting and low-cost alternative to conventional inorganic photovoltaics. Upon illumination, excitons are created that separate into free electrons and holes at the donor-acceptor-interface and can be extracted to deliver electricity. The opposing loss mechanism is the recombination of charge carriers, which happens in the bulk both prior to and after charge separation. To understand these processes, the recombination order is crucially important. Experimentally, orders around or above 2 are typically found. Surprisingly, kinetic Monte Carlo (kMC) simulations that otherwise accurately reproduce experimental observations, yield values closer to 1. Here, we investigate the factors that might lead to higher recombination orders. Apart from the influence of morphology and contacts, special focus is laid on the effect of charge carrier delocalisation, which is shown to facilitate charge carrier separation and increase the fraction of bimolecular recombination. Simulation results are compared to experimental data obtained via the Steady State Bias Assisted Charge Extraction (BACE) method on P3HT:PCBM and PM6:Y6 solar cells.

HL 32.3 Wed 15:30 GÖR 226

Modeling of the photoluminescence of geminate pairs using a hopping based Monte Carlo simulation — •Maik Schwuchow, Angela Thränhardt, Carsten Deibel, and Sibylle Gemming — TU Chemnitz, Institut für Physik, 09126 Chemnitz, Deutschland

The investigation of the transport and recombination characteristics of optically excited charge carriers in organic materials is an on-going research topic. Studying the underlying effects is crucial for understanding and improving practical applications, e.g. organic solar cells (OSCs). A main step in the process of free charge carrier generation in OSCs is the formation of geminate pairs, so called charge transfer complexes, consisting of spatially separated, Coulomb-bound charges. The radiative recombination of geminate pairs yields a photoluminescence (PL) decay $\propto t^{-3/2}$ (t is time) on long time scales which arises due to a combination of thermally activated diffusion and attractive Coulomb interaction. While a continuous drift-diffusion model is able to theoretically explain this experimentally observed decay, weak molecular interaction and disorder are known to cause charge carrier localization. Therefore, a hopping model, based on tunneling between localized states, is usually more appropriate to describe charge transport in organic materials. We simulate the diffusion and recombination of hopping charge carriers using the Monte Carlo method and investigate the influence of different parameters, e.g. temperature and energetic disorder, on the PL data and the asymptotic slope.

HL 32.4 Wed 15:45 GÖR 226

Time-consistent hopping, transient localization, and polarons - new insights and approaches for carrier transport in organic crystals — Sebastian Hutsch, Michel Panhans, and •Frank Ortmann — Technische Universität München, Germany

Charge transport in organic semiconductors is affected by the complex interplay of electronic degrees of freedom and molecular vibrations. This is further complicated due to the rich vibrational spectrum of these materials with mode energies covering two orders of magnitude. If the electronic coupling between molecules is small, hopping approaches are a popular choice to model charge transport for which we have recently derived a time-consistent hopping theory. [1]

Similarly, for high-mobility materials a recent improvement has been realized based on a mode-specific treatment of molecular vibrations. This leads to an unprecedented level of accuracy for the prediction of the carrier mobility for a large number of systems. [2] I will finally discuss physically motivated predictors with a very good correlation to the mobility and low computational costs.

[1] S. Hutsch, M. Panhans and F. Ortmann, Phys. Rev. B. 104, 054306 (2021).

[2] S. Hutsch, M. Panhans and F. Ortmann, npj Comput. Mater. 8, 228 (2022).

HL 32.5 Wed 16:00 GÖR 226

Analysis of industrial viability for single-component organic solar cells — •Yakun He[1,2], Ning Li[1], Thomas Heumüller[1], Jonas Wortmann[1], and Christoph Brabec[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Martensstrasse 7, 91058 Erlangen, Germany — [2]KAUST Solar Center, King Abdullah University of Science and Technology, Thuwal 23955, Saudi Arabia

Despite approaching 20% efficiency, organic solar cells still lag behind for industrial application. The industrial figure of merit (i-FOM) of OSCs is analyzed, including PCE, photostability, and synthetic complexity (SC) index. Single-component organic solar cells (SCOSCs) employing materials with donor and acceptor moieties chemically bonded within one molecule or polymer exhibit intrinsically high morphological stability. SCOSCs exhibit overall much higher i-FOM values than the corresponding bulk heterojunction OSCs, and the highest value reaches 0.3, which is even higher than the famous PM6:Y6, even though the PCE (8%) is only half of PM6:Y6. Synthetic complexity of SCOSCs is slightly higher than that of the corresponding BHJ OSCs due to extra synthetic step for connecting donor and acceptor moieties. This feature however overcomes the large-scale phase separation and stability issue. SCOSCs based on dyad 1 exhibit surprisingly high photostability under concentrated light (7.5 suns and 30 suns), corresponding to almost unchanged device stability up to 10,000 hours under 1-sun illumination. For realizing industrial application, SCOSCs have to achieve higher efficiencies, while BHJ should be developed with less complicated synthesis.

15 min. break

HL 32.6 Wed 16:30 GÖR 226

Temperature-induced morphology changes at the organic-metal interface: effects on the structure, electronic and thermoelectric performance — •Benedikt Sochor[1], Yusuf Bulut[1,2], Marie Betker[1,3], Anna Lena Oechsle[2], Simon Schraad[1,4], Christopher R. Everett[2], Constantin Harder[1,2], Tzu-Yen Huang[5,6], Anton Le Brun[5], Tim Laarmann[1,4], Peter Müller-Buschbaum[2,7], and Stephan V. Roth[1,3] — [1]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany — [2]TUM School of Natural Sciences, Chair for Functional Materials, James-Franck-Str. 1, 85748 Garching, Germany — [3]KTH Royal Institute of Technology, Teknikringen 56-58, 100 44 Stockholm, Sweden — [4]University Hamburg, Department of Physics, Notkestr. 85, 22607 Hamburg, Germany — [5]ANSTO, New Illawarra Road, Lucas Heights, NSW 2234, Australia — [6]NSRRC, 101 Hsin-Ann Road, Hsinchu Science Park, Hsinchu 30076, Taiwan — [7]MLZ, TUM, Lichtenbergstr. 1,

85748 Garching, Germany

Flexible organic electronics are one of the most sought-after devices in the field of photovoltaics, sensors, or smart wearables. Here, the structure of the organic-metal interface and its modification potential are of utmost interest for future large-scale production. This study focuses on two semiconducting Poly(3-hexylthiophene-2,5-diyl) diblock variants, whose sprayed and doped thin films show excellent potential as thermoelectric generators. Using AFM, ellipsometry, *in situ* GISAXS/GIWAXS, and NR measurements, the structural changes of the polymer-gold interfaces were tracked during thermal annealing.

HL 32.7 Wed 16:45 GÖR 226

Compatible solution-processed interface materials for improving the efficiency of organic solar cells — •Zhuo Xu[1,2], Jose Prince Madalaimuthu[1,2], Josef Bernd Slowik[1,2], Rico Meitzner[1,2], Aman Anand[1,2], Shahidul Alam[1,2,4], Héctor Corte[5], Steffi Stumpf[1,3], Ulrich S. Schubert[1,2,3], and Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry, Friedrich Schiller University Jena, Jena, Germany. — [2]Center for Energy and Environmental Chemistry Jena, Friedrich Schiller University Jena, Jena, Germany. — [3]Jena Center for Soft Matter, Friedrich Schiller University Jena, Jena, Germany. — [4]King Abdullah University of Science and Technology, KAUST Solar Center, Physical Sciences and Engineering Division, Material Science and Engineering Program, Thuwal, Kingdom of Saudi Arabia. — [5]Nanosurf AG, Liestal, Switzerland.

The electron transport layer (ETL) is a key components for better performance and stability in OSCs. Herein, conjugated PDINO, sol-gel derivatized under stoichiometric TiOx, and the same combination as the ETL was used to fabricate solution-processed PBDTTT-C-T:PC71BM-based OSCs. A hybrid of organic-inorganic ETL revealed less bimolecular and trap-assisted recombination than a single ETL of either material. Furthermore, the efficiency of devices using blend ETLs showed better performance in comparison to single ETLs in both fullerene and non-fullerene systems. This blending strategy have demonstrated beneficial consequences in device stability and efficiency, which will play key role for future commercialization of OSCs.

HL 32.8 Wed 17:00 GÖR 226

Influence of dye-doping on the nanostructure of the highly efficient PM6:Y6 solar cells — •Elisabeth Erbes[1,2], Constantin Harder[1,3], Benedikt Sochor[1], Susann Frenzke[1], Naireeta Biswas[1,2], Jan Rubek[1], Matthias Schwartzkopf[1], Volker Körstgens[3], Peter Müller-Buschbaum[3,5], Stephan V. Roth[1,4] und Simone Techert[1,2] — [1]DESY, Hamburg, DE — [2]Institute for X-ray Physics, Goettingen University, Goettingen, DE — [3]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [4]KTH Royal Institute of Technology, Stockholm, SWE. — [5]MLZ, TUM, Garching, DE

Organic solar cells based on the donor polymer PM6 and the acceptor Y6 give power conversion efficiencies (PCE) of 13-16% without any additives. The current study aims to investigate systematically the effect of doping PM6:Y6 with optical-light absorbing, electron transfer (ET) dyes. These pyrene-based dyes (PyxDMA) have inter- and intramolecular charge transfer properties and a very high quantum yield. Also the absorption in the UV regime extends the absorption range of the PM6:Y6 system. The structural and morphological integrity of the dopants within the active layer were studied with grazing incidence X-ray scattering experiments. The analysis showed the intercalation and distribution of the dyes within the PM6:Y6 matrix. The sprayed solar cell architecture Cu/PM6:Y6:PyxDMA/PEDOT:PSS/Au/ITO/Glass was used to measure the PCEs. Correlating these efficiencies with the molecular and nanostructural results allows explaining the changing PCE due to different doping levels of PyxDMA.

HL 32.9 Wed 17:15 GÖR 226

Hydrogenated nanodiamonds as efficient electron extraction layers in organic solar cells — •Aurelien Sokeng Djoumessi[1,2], Anastasia Sichwardt[1,2], Daria Miliaieva[3], Jan Čermák[3], Maximilian Schaal[4], Felix Otto[4], Štěpán Stehlík[3], Vojtech Nádaždy[6], Torsten Fritz[4], Bohuslav Rezek[5], Ulrich S. Schubert[1,2], and Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry, Friedrich Schiller University Jena (IOMC), Jena, Germany — [2]Center for Energy and Environmental Chemistry (CEEC), Friedrich Schiller University Jena, Jena, Germany — [3]Institute of Physics, Czech Academy of Sciences, Prague 6, Czech Republic — [4]Institute of Solid State Physics, Friedrich Schiller University Jena, Jena, Germany — [5]Faculty of Electrical Engineering, Czech Technical University, Prague, Czech Republic — [6]Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovak Republic

Surface tunability is one property of nanodiamonds (NDs), which enables to attachment of a range of functional groups on their surfaces. This may have a significant impact on NDs' electrical and optical characteristics and be helpful for charge extraction in solar cell devices. Herein, the surface chemistries of HPHT NDs modified by hydrogenation in a hydrogen atmosphere exhibit sp2-phases, which may help in improving the material's electrical conductivity and electron extraction when employed as an electron transport layer in PBDB-T:ITIC-based solar cells. The device performance was 7%, which differs only marginally from the outcomes of the state-of-the-art ETLs (ZnO, SnO2).

HL 33: Poster II

Topics:
- 2D semiconductors and van der Waals heterostructures
- Focus Session: Graphene quantum dots
- Materials and devices for quantum technology
- Nitrides: Devices
- Nitrides: Preparation and characterization
- Quantum transport and quantum Hall effects
- Semiconductor lasers
- Spin phenomena in semiconductors
- THz and MIR physics in semiconductors
- Transport properties
- Ultra-fast phenomena

Time: Wednesday 17:00–19:00 Location: P1

HL 33.1 Wed 17:00 P1

Pump-probe spectroscopy on a MoSe2 monolayer — •Max Wegerhoff and Stefan Linden — Physikalisches Institut, Universität Bonn, Nussallee 12, 53115 Bonn, Germany

TMDC monolayers are atomically thin semiconductor materials, which, due to their reduced dimensionality and crystal structure, possess unique optical properties. In particular, they host bound electron-hole pairs, so-called excitons, with binding energies of several 100 meVs.

Here, we report on pump-probe spectroscopy on excitons in a MoSe2 monolayer encapsulated in h-BN. We use spectrally broad probe pulses and a spectrometer to measure the transient differential reflectivity spectra. Based on a mode-locked Ti:Sa laser, a temporal resolution of down to 400fs is achieved. A frequency-doubled OPO can be used

to generate non-resonant pump pulses in the visible wavelength range. Furthermore, probe pulses with a bandwidth of up to 70nm can be generated via supercontinuum generation in a photonic crystal fiber. The experiments are performed at 4K in a helium-flow cryostat.

Within the first few picosecond after the pump pulse, we observe a blueshift of the exciton resonance. This shift depends on the wavelength of the pump pulses as well as the polarization of the pump- and probe pulses. Further experiments with an electrically gated heterostructure to control the doping of the monolayer are in progress.

HL 33.2 Wed 17:00 P1

A Model Study of the Phonon-Impact on Absorption Spectra of Moiré Exciton-Polaritons — •Kevin Jürgens[1], Daniel Wigger[2], and Tilmann Kuhn[1] — [1]Institute of Solid State Theory, University of Münster, Germany — [2]School of Physics, Trinity College Dublin, Ireland

The interaction of multiple quantum emitters coupled to a resonant optical field can produce interesting collective behavior. Twisted bilayers of transition metal dichalcogenides are a class of materials, where localized quantum emitters, in this case moiré excitons, can occur. According to their strong localization at the minima of the moiré potential, these excitons have a relatively flat band structure. If the heterostructure is placed into an optical cavity, all excitons interact with the same mode of the resonator, leading to the formation of exciton-polaritons which can interact with lattice vibrations.

We model the moiré excitons in the limit of small densities as bosonic particles that couple to a single quantized cavity mode, resulting in lower and uper polariton states. In addition, each exciton is coupled to the same acoustic phonon bath. The interaction with phonons leads to inter- and intraband transitions between the two polariton branches that strongly depend on the curvature of the polariton dispersion.

We calculate absorption spectra and discuss the influence of phonons on the spectral shape and peak positions, and systematically study the influence of the band structures curvature.

HL 33.3 Wed 17:00 P1

Nonlinear optical processes in the layered magnetic semiconductor CrSBr — •Minjiang Dan[1], Paul Herrmann[1], Julian Klein[2], Zdenek Sofer[3], and Giancarlo Soavi[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Jena, Germany — [2]Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, USA — [3]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, 166 28 Prague 6, Czech Republic

CrSBr has recently emerged as a new member in the family of layered magnetic materials, with the distinct advantages compared to CrI_3 of being stable in air and having a high Néel temperature in the bulk form. Recently polarization-resolved Second Harmonic Generation (SHG) has been employed to reveal the layer-dependent magnetic order and symmetry in multilayer CrSBr [1]. In this work, we use nonlinear optical spectroscopy, i.e. SHG and Third Harmonic Generation (THG) and two photon absorption, to investigate the electronic and excitonic resonances in few-layer and bulk CrSBr as a function of the lattice temperature which, modulates the magnetic properties of the material. Our results show large enhancement (>100) in the SHG and THG for specific wavelengths and range of temperatures, pointing towards the existence of resonances from the magnetic dipole response of the system. This sheds light on the excited state landscape of this new material and offers viable insights towards its application in spintronic, magnonic and opto-electronic devices.

[1] Lee *et al.*, *Nano Letters* **21**, 8, 3511-3517 (2021)

HL 33.4 Wed 17:00 P1

The Impact of Inert Conditions During the Fabrication Process on the Optical Properties of MoS_2 Monolayers — •Alina Schubert[1], Michael Kempf[1], Rico Schwartz[1], Patricia Gant[2], Felix Carrascoso[2], Carmen Munuera[2], Andres Castellanos-Gomez[2], and Tobias Korn[1] — [1]Institut für Physik, Universität Rostock, Rostock, Germany — [2]Instituto de Ciencia de los Materiales de Madrid, Madrid, Spain

Transition-metal dichalcogenides (TMDCs) are layered materials that can be thinned down to monolayers. The optical properties of these flakes depend strongly on the cleanliness of the surfaces. Transferring TMDCs with PDMS is simple to perform and allows the fabrication of large monolayers [1]. The objective of this work was to improve the methodology so that sample quality is enhanced without reducing the yield or increasing the effort required for production. For this purpose, a statistic of 20 monolayers was set up, which were half transferred to a SiO_2 substrate at ambient conditions and half transferred in a glovebox [2]. All samples were characterised by photoluminescence (PL) spectroscopy at room temperature and ∼4 K. By examining the exciton and trion features in the spectra, it could be shown that only the small difference in the transfer process results in changes of the optical properties that can be attributed to a higher sample quality of the samples produced in the glovebox.

[1] Castellanos-Gomez, A. et al. 2D Mater. 1 (2014)
[2] Gant, P. et al. 2D Mater. 7 (2020)

HL 33.5 Wed 17:00 P1

Stokes shift of twisted bilayer WSe2 — •Zihao Liu[1], Yang Pan[1,2], and Dietrich R. T. Zahn[1,2] — [1]Semiconductor Physics, Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]Center for Materials, Architectures, and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, Chemnitz, Germany

Transition metal dichalcogenides (TMDCs) with a typical layered structure have exceptional optical properties exhibiting a characteristic absorption and emission at excitonic resonances. The weak van der Waals (vdW) interlayer coupling nature enables the possibility of artificial staking, leading to homo- and hetero-structures formation. It was demonstrated in our previous work that the optical properties can be strongly modified by the twisting angle.

Here, WSe2 monolayers (MLs) were obtained by mechanical exfoliation, which were then transferred onto sapphire substrates by a tear-and-stack method to form twisted homo-bilayers with a precision of 0.08°. We then performed optical transmission and photoluminescence (PL) experiments on monolayers, intrinsic bilayers and twisted bilayers to determine the Stokes shift values on a full period (0°-60°) of twisted bilayer WSe2.

HL 33.6 Wed 17:00 P1

Transport and optical characterization of electrically contacted monolayer TMDCs — •Jan-Niklas Heidkamp, Johannes Krause, Swarup Deb, Rico Schwartz, and Tobias Korn — Institute of Physics, University of Rostock, Rostock, Germany

Since Graphene was introduced in 2004, there has been a great interest in other 2D materials as well. Among the most studied is the group of semiconducting transition metal dichalcogenides (TMDCs). The band structure of these crystals changes from an indirect gap in the bulk to a direct gap in the monolayer limit. Herein, a method for contacting monolayer flakes using photolithography and lift-off processes is showcased. Electrical contacts are pre-defined on SiO_2 substrates and thereafter, TMDC flakes are deposited using a deterministic transfer technique. Flakes of the TMDC WS_2 contacted in this way are characterized via gate-dependent photoluminescence measurements and I-V curves.

HL 33.7 Wed 17:00 P1

Enhancing photoluminescence and Raman signals in TMDC monolayers via plasmonic nanostructures — •Johannes Krause, Annika Bergmann, Jan-Niklas Heidkamp, Rico Schwartz, and Tobias Korn — Institute of physics, university of Rostock, Rostock, Germany

Novel 2D thin film materials garnered a great interest in recent years. The family of Transition metal dichalcogenides (TMDCs) among those materials is especially appealing because of the indirect-direct bandgap transition and the possibility to stack different composites of the TMDCs on top of each other to achieve so called heterostructures. Herein, we present a technique to define nanostructures on a SiO_2 wafer using thermal scanning probe lithography. Further, we deposit individual TMDC monolayer flakes on top of the metallized structures via the deterministic transfer technique. We characterize our flakes utilizing photoluminescence and Raman measurements, reporting major enhancements effects (∼10x) in PL and minor enhancement (∼3x) in Raman signals.

HL 33.8 Wed 17:00 P1

investigation of structural and electronic properties of monolayered MoS2 and graphene compared to the MoS2/graphene heterostructure — •Ateeb Shaban[1], Nebahat Bulut[2], Jakob Kraus[2], Franz Selbmann[1], Jens Kortus[2], and Yvonne Joseph[1] — [1]TU Bergakademie Freiberg, Institute of Electronic and Sensor Materials, Germany — [2]TU Bergakademie Freiberg, Institute of Theoretical Physics, Germany

Graphene and other 2D materials have been shown to have interesting structural and electronic properties. Transition metal dichalcogenides such as molybdenum disulfide (MoS2) and tungsten diselenide (WSe2) have tunable bandgaps that change from indirect to direct when decreasing the number of layers. This property allows for applications such as transistors and sensors. On the other hand, graphene is an ideal channel material. It is used as an electronic sensor in field-effect transistors due to the high sensitivity toward the change in the surrounding environment. These remarkable electronic and structural properties of graphene, being highly susceptible and conductive, have reignited the interest in 2D materials. Subsequently, building variable stacks of 2D van-der-Waals (vdW) structures can open the possibility of designing materials with specific properties across various chemistry's and systems.

In this theoretical work, we analyze and review the properties of MoS2 and graphene individually and study their cumulative effect on the electronic and structural properties of the MoS2/graphene vdW heterostructure using density functional theory.

HL 33.9 Wed 17:00 P1

Rapid hyperspectral imaging of transition metal dichalcogenides and their heterostructures — •Marc Schütte, David Tebbe, Christoph Stampfer, Bernd Beschoten, and Lutz Waldecker — 2nd Institute of Physics A, RWTH Aachen University, Aachen, Germany

Transition Metal Dichalcogenides are two-dimensional semiconductors with many interesting properties for optical applications, such as direct bandgaps in the visible spectral region or optically addressable inequivalent valleys. It is well known, however, that their optical properties can vary spatially by local changes of dielectric screening, doping or strain. Here, we present a measurement setup capable of performing photoluminescence and reflection contrast measurements of 2D heterostructures approximately twenty times faster compared to scanning a focal spot over the sample. The setup is based on simultaneously taking spectra along a line with an imaging spectrometer (push-broom technique), which enables the measurement of multiple spectra simultaneously. The speed of the technique allows for taking images in multidimensional sweeps of parameters, such as gate voltages or magnetic fields.

In this way, the measurements can be conducted by imaging sample regions up to the full size of the heterostructure for each sweep. This allows to distinguish inhomogeneities and enhances the statistical relevance of the data.

HL 33.10 Wed 17:00 P1

Black phosphorus field-effect transistors and its application — •Zahra Fekri[1], Himani Arora[1], Victoria Constance köst[2], Jens Zscharschuch[1], Krzysztof Nieweglowski[2], Kenji Watanabe[3], Takashi Taniguchi[4], Manfred Helm[1,2], Karl-heinz Bock[2], and Artur Erbe[1,2] — [1]Helmholtz Zentrum Dresden Rossendorf, Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany — [3]Research Center for Functional Materials, National Institute for Materials Science, Tsukuba, Japan — [4]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Tsukuba, Japan

Black phosphorus (BP) has been known as a more favorable material in many applications compared to other 2D materials due to its exceptional properties. However, its sensitivity to air species has restricted its integration into active devices. In this work, we used a few nm thickness BP for developing field-effect transistors (FETs). Lithography-free via-encapsulation scheme allows us to fabricate fully-encapsulated BP-based field-effect transistors and perform reliable electrical measurements. Based on our results, we find that the electronic properties of the via-encapsulated BP FETs are significantly improved compared to unencapsulated devices. We further demonstrated a gas-sensing performance based on the BP FET. Our Preliminary result shows the promising potential of BP for applications in advanced gas-sensing technology.

HL 33.11 Wed 17:00 P1

Stationary and Time-Resolved Luminescence of Organic-Dye/transition metal dichalcogenide Heterostructures — •Julian Schröer, Tim Völzer, Alina Schubert, Rico Schwartz, Stephan Lochbrunner, and Tobias Korn — University of Rostock, Institute of Physics

Thin layers of organic molecules and layered semiconductors build a new compound material with manifolds of interesting applications. The optoelectronic properties of these heterostructures strongly depend on the chosen compounds. Via stationary and time-resolved photoluminescence experiments, we investigate samples of Perylene-Orange (PO) deposited on top of single-layer tungsten diselenide. This joint material exhibits a type-II band alignment, enabling charge transfer processes between the two material layers. Here, we aim to reveal the temperature dependent dynamics of the charge transfer processes. Our work paves the way for a deeper understanding of organic/inorganic heterointerfaces and the functionalization of organics and TMD's in optoelectronic devices.

HL 33.12 Wed 17:00 P1

Quantum transport in twisted bilayer graphene supermoiré heterostructures — Alexander Rothstein[1], Robin Dolleman[1], Christoph Schattauer[2], •Anthony Achtermann[1], Stefan Trellenkamp[3], Florian Lentz[3], Kenji Watanabe[4], Takashi Taniguchi[5], Dante Kennes[6], Florian Libisch[2], Bernd Beschoten[1], and Christoph Stampfer[1] — [1]2nd Institute of Physics, RWTH Aachen University, Germany — [2]Institute for Theoretical Physics, TU Wien, Austria — [3]Helmholtz Nano Facility, Forschungszentrum Jülich, Germany — [4]Research Center for Functional Materials, National for Material Science, 1-1 Namiki, Japan — [5]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, 1-1 Namiki, Japan — [6]Institute for Theory of Statistical Physics, RWTH Aachen University, and Jara Fundamentals of Future Information Technology, Germany

Twisted bilayer graphene hosts a plethora of correlated quantum phenomena, such as superconductivity, correlated insulators and strange metal phases. The unprecedented in-situ gate-tunability of the system allows the study the underlying physics in detail by means of quantum transport experiments. The microscopic details of the van-der-Waals heterostructure, like the presence of competing moiré lattices, heavily influence the exact characteristics of the device. Here, we investigate different conductance regimes in near-magic angle twisted bilayer graphene devices, focusing on the insulating states. We are able to identify the presence of super-moiré lattices in our devices from magneto-transport experiments and compare our results with theory.

HL 33.13 Wed 17:00 P1

Ultrathin 2D gallium selenide devices for optoelectronics — •Marco N. Dembecki, Simon Bernöcker, Michele Bissolo, Eugenio Zallo, and Jonathan J. Finley — Walter Schottky Institute and TUM School of Natural Sciences, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany

The post-transition metal chalcogenides (PTMC, M = [In, Ga], C = [S, Se, Te]) are a group of semiconducting layered materials with a widely tunable band gap and direct-indirect band gap crossover in the few-layer limit. Type II band alignment of PTMC heterostructures makes them good candidates as photoabsorbers [1].

Among PTMCs, GaSe holds promise for optoelectronics, nonlinear optics, and terahertz (THz) generation but its usefulness for devices is inhibited by strong susceptibility to oxidation. Here, we report on the fabrication of dual gated-FET based on fully hBN-encapsulated GaSe multilayers. To preserve the intrinsic properties of the gallium selenide, the encapsulation process was carried out in a controlled nitrogen atmosphere. The gate electrodes are made from few-layer graphene to allow for an optoelectronic investigation. Electrical transport measurements are carried out and a roadmap for future optoelectronic devices will be discussed.

[1] Arora, H., and Erbe, A. Recent progress in contact, mobility, and encapsulation engineering of InSe and GaSe. InfoMat, 3 (6), 662-693, (2021)

HL 33.14 Wed 17:00 P1

Towards thermoelectric transport measurements in dual-gated bilayer graphene — •Moritz Knaak, Martin Statz, and Thomas Weitz — 1st Physical Institute, Faculty of Physics, University of Göttingen, Friedrich-Hund-Platz 1, Göttingen 37077, Germany

The ratio of the thermal voltage to the corresponding temperature difference is defined as the Seebeck coefficient. As a transport coefficient due to its relation to the density of states (DoS) and its underlying link between entropy and charge transport, the Seebeck coefficient can help to better understand materials with interesting DoS and/or phase transitions. One of these materials is trigonally warped bilayer graphene (BLG), in which Lifshitz transitions can be induced by tuning an out-of plane electric field or the charge carrier density. Near these transitions the DoS is high and electron-electron interaction be-

comes important. To gain further insights into the emerging correlated phases near these Lifshitz transitions [1] and quamtify the changes in the DoS, we measure the thermoelectric voltage and local temperature difference to extract the Seebeck coefficient. For that we combine a hexagonal boron nitride encapsulated, dual-gated BLG device with graphite gates and contacts together with an on-chip heater next to the BLG. The source and drain contacts are simultaneously used as 4-point-probe on-chip resistance thermometers to determine the local temperature differences. The devices are fabricated utilizing the dry transfer method, e-beam lithography, thermal evaporation of contact leads as well as reactive ion etching.

[1] Seiler, A.M. et al. Nature 608, 298-302 (2022)

HL 33.15 Wed 17:00 P1

Niobium-Doping of Atomically Thin Molybdenum Disulfide for Optoelectronic Applications — •Osamah Kharsah, Stephan Sleziona, and Marika Schleberger — Universität Duisburg-Essen, Fakultät für Physik and CENIDE, Germany

Two-dimensional materials are predicted to become a very important disruptive technology, opening the door to a plethora of applications across many fields, especially in the field of optoelectronics. Among these materials, atomically thin molybdenum disulfide (MoS_2) has distinguished itself owing to its electronic properties, good thermal stability, and mechanical durability. However, its intrinsic strong n-type conductivity hinders its implementation. Overcoming this hurdle would allow MoS_2 to be used in structures such as p-n junctions either on its own or in tandem with other 2D materials, with the goal of fabricating the next generation of optoelectronic devices. One approach that could solve this problem is substitutional doping to controllably p-dope MoS_2. We report on the direct growth of niobium-doped monolayer MoS_2, which was characterized by Raman- and photoluminescence spectroscopy. Field-effect transistors, with the as-grown Nb-doped MoS_2, showed n-type transport behavior. After annealing the material in a sulfur atmosphere, this switched to an ambipolar transport behavior, which we attribute to the activation of Nb-doping sites. In addition, the hysteresis of this device exhibited a decrease of 4 orders of magnitude, indicating that the influence of intrinsic defects has been remedied by the annealing process.

HL 33.16 Wed 17:00 P1

Towards strong coupling of confined excitons to a fiber-based microcavity — •Moritz Scharfstädt, Michael Köhl, and Andrea Bergschneider — Physikalisches Institut, Universität Bonn, Wegelerstraße 8, 53115 Bonn, Germany

Excitons in monolayer transition-metal dichalcogenides (TMD) exhibit large oscillator strengths and hence are well-suited for strong light-matter coupling. While for free excitons strong coupling to photonic cavities has been demonstrated in numerous experiments, nonlinearities in those systems are relatively weak. The recently demonstrated quantum confinement of excitons to length scales of about 20nm is a promising route towards enhancing nonlinearities [1].

We want to realize confined excitons with the prospect of embedding them into a high-finesse microcavity and reach the strong coupling regime. To confine the excitons in transverse direction and tune their energy, we develop a specific electric gate configuration. Our microcavity will be fiber-based and tunable at cryogenic temperatures. With this platform we aim for the realization of a quantum emitter in a cavity by harvesting the enhanced nonlinearity combined with a cavity-enabled photon blockade.

[1] Thureja et al., Nature 606, 298-304 (2022)

HL 33.17 Wed 17:00 P1

Photon assisted tunneling in bilayer graphene double quantum dots — •Tobias Deussen[1], K. Hecker[1,2], L. Banszerus[1,2], A. Schäpers[1], A. Peters[1], S. Möller[1,2], E. Icking[1,2], K. Watanabe[3], T. Taniguchi[4], C. Volk[1,2], and C. Stampfer[1,2] — [1]JARA-FIT & 2nd Institute of Physics, RWTH Aachen — [2]Peter Grünberg Institute, Forschungszentrum Jülich — [3]RCFM, NIMS, Japan — [4]MANA, NIMS, Japan

Spin qubits in semiconductor quantum dots (QDs) are attractive candidates for solid state quantum computation. Singlet-triplet qubits, where the logical qubits are encoded in a two-electron spin system in double quantum dots (DQDs), turned out to be of special interest. In such systems, control over the interdot tunnel coupling and, hence, the exchange interaction is essential. Bilayer graphene (BLG) is an attractive host material for spin qubits due to its small spin-orbit and hyperfine interaction and its gate voltage controllable band gap. Only recently, it has become possible to confine single electrons in BLG QDs and to understand their spin and valley texture. However, microwave manipulation has not been demonstrated, so far. Here, we perform photon-assisted tunneling (PAT) spectroscopy, which relies on resonant microwave excitation of electrons across the interdot transition. We extract a lower bound for charge dephasing, T2*, of about 350 ps. In power-dependent measurements, we explore multi-photon processes. We use PAT as a probe for the interdot tunnel coupling in BLG DQDs and can control and measure the interdot tunnel coupling in a range of several GHz which is suitable for qubit operations.

HL 33.18 Wed 17:00 P1

Coherent coupling dynamics between excitonic complexes in a $MoSe_2$ monolayer — •Daniel Wigger[1], Aleksander Rodek[2], Thilo Hahn[3], James Howarth[4], Takashi Taniguchi[5], Kenji Watanabe[5], Marek Potemski[2,6], Piotr Kossacki[2], and Jacek Kasprzak[2,7] — [1]School of Physics, Trinity College Dublin, Ireland — [2]Faculty of Physics, University of Warsaw, Poland — [3]Institute of Solid State Theory, University of Münster, Germany — [4]National Graphene Institute, University of Manchester, UK — [5]National Institute for Materials Science, Tsukuba, Japan — [6]Laboratoire National desChamps Magnétiques Intenses, CNRS-UGA-UPS-INSA-EMFL, Grenoble, France — [7]Université Grenoble Alpes, CNRS, France

In modern heterostructures of layered van der Waals materials that combine graphene, hBN, and TMDCs it is possible to deterministically control the density of free charge carries in a TMDC monolayer. With this approach and the ultrafast nonlinear four-wave mixing (FWM) spectroscopy technique we study the coherent coupling dynamics between neutral and charged excitons in a $MoSe_2$ monolayer. We demonstrate that the so-called Raman coherence between the two exciton species leads to characteristic quantum beats in the FWM signal. By exploiting 2D-FWM spectra, we can conclude that the bias dependent change of dipole strength between the exciton types is not sufficient to explain the experimental findings. Therefore, we conclude that the tuning of the free carrier density directly affects the coherent coupling between neutral and charged excitons.

HL 33.19 Wed 17:00 P1

Resonant Excitation and Resonant Photoluminescence Detection of Silicon Vacancy Centers in 4H Silicon Carbide for Single Photon Emission — •Fedor Hrunski[1], Mike Gerd Georg Köstler[1], Shravan Kumar Parthasarathy[2,1], Maximilian Hollendonner[1], Andre Pointner[1], Christian Gobert[2], Daniel Scheller[1], and Nagy Roland[1] — [1]Chair of Electron Devices (LEB), Friedrich-Alexander-University, Erlangen, Germany — [2]Fraunhofer Institute for Integrated Systems and Device Technology (IISB), Erlangen, Germany

For today, quantum networks deal with the task of entangling several qubits with each other over a larger distance. Therefore, the resonant excitation of the qubits and the resonant detection of emitted photons by them appears to be an essential component of such a network for coherent spin state control. This work hereby deals with the resonant single photon detection of fluorescence, which is emitted by resonantly exited V2 color centers in 4H-SiC. Therefore, a diode laser modulated by an electro-optical modulator performs a pulsed resonant excitation at one of the A_1 or A_2 spin-conservative optical transitions, while the emitted photons are detected by a superconducting single photon detector. However, due to the chromatic equality of the excitation photons and fluorescent photons, they are distinguished by their polarization.

HL 33.20 Wed 17:00 P1

A standalone fiber-bases quantum sensor using ensembles of NV-Centers in diamond — •Benjamin Pohl, Andre Pointner, and Roland Nagy — Chair of Electron Devices, FAU Erlangen-Nuremberg

Though NV-Center magnetometry with diamonds is widely spread in scientific research, it is rarely used in an industrial context. In order to reduce the complexity of the required hardware we fixate the diamond on the tip of a fiber and miniaturize the system so all the required components can be included in a standalone device for magnetic field determination. The measurement is performed with ensembles of NV-Centers used as an optically controlled quantum sensor in a confocal setup. Determination of the magnetic field is achieved through optical detected magnetic resonance (ODMR). In the presence of a local magnetic field, the four orientations of the NV-Centers in the diamond

crystal results in up to four different Zeeman splits, which allows the evaluation of the local magnetic field vector. The resulting sensitivity to magnetic fields is strongly dependent on the number of collected signal photons on the detector. Therefore, to increase the sensitivity, the collection efficiency is crucial. Detection of the collected photons is realized by an integrated photodiode and the signal is evaluated by a field programmable gate array (FPGA) which also controls the measurement hardware. Such a standalone device will enable measurements in various environments and provide a system for users without insight to optics or quantum technology, thus greatly extending the possible applications for NV-Centers as quantum sensors.

HL 33.21 Wed 17:00 P1

Realization of remote entanglement using vacancy-centers in 4H-SiC — •Michael Baron[1], Maximilian Hollendonner[1], Fedor Hrunski[1], Daniel Scheller[1], Andre Pointner[1], Shravan Kumar Parthasarathy[2], and Roland Nagy[1] — [1]Chair of Electron Devices FAU — [2]Fraunhofer Institute for Integrated Systems and Device Technology IISB

The overall performance of quantum applications, such as quantum sensors, quantum tokens and optical quantum computers, can be highly improved by realizing a quantum network in which these constituents are connected. The emerging field of quantum technologies based on color centers in silicon carbide (SiC) will play an important part in the realization of such distributed quantum networks. As a physical platform silicon vacancy centers inside 4H SiC offer numerous advantages, such as low electrical field sensitivity making the system robust against stray fields, high photon yield in the Zero-Phonon-Line, good spin-coherence time and an already well-matured industrial fabrication knowledge for SiC. My research is concerned with the technical implementation and realization of a heralded single-photon entanglement protocol using V2 silicon vacancy centers in 4H-SiC. The experiment employs two such vacancies residing in independently operated cryostats separated by 2 meters, which are connected in an interferometer-like setup. This allows the creation of entanglement between both V2 centers and thus the creation of a quantum network based on these color centers.

HL 33.22 Wed 17:00 P1

Towards an integrated nanophotonic and electronic spin platform in 4H-SiC — •Daniel Scheller[1], Daniel Häupl[2], Lin Jin[3], Christian Gobert[4], Jannik Schwarberg[1], Jörg Schulze[1], Nicolas Joly[2], Wolfram Pernice[3], and Roland Nagy[1] — [1]Chari of Electron Devices, Friedrich-Alexander-University Erlangen-Nuremberg, Erlangen, Germany — [2]Max-Planck-Institue for the science of light, Erlangen, Germany — [3]Responsive Nanosystems, University of Münster, Münster, Germany — [4]Fraunhofer IISB, Erlangen, Germany

The solid state spin system of negatively charged silicon vacancies (V_{Si}) V2 in 4H-SiC shows high spectral stability and excellent spin coherence times required for efficient quantum processing. Moreover, silicon carbide provides standardized semiconductor processes enabling the implementation of integrated quantum photonics. However, high-fidelity spin photon coupling and low-loss chip-to-fiber interfaces are necessary to improve experimental rates and, thus, the performance of quantum devices. Recently, high coupling efficiencies of emitted photons from the VSi color center into angle-etched SiC waveguides have been predicted which can be further enhanced by photonic crystal cavities. Further, a low-loss optical interface from on-chip diamond tapered waveguides to tapered optical fibers was shown. Our goal is to combine these properties and implement single VSi color centers into nanophotonic SiC waveguides coupled to tapered fibers for realizing the on-chip entanglement of color centers and two locally separated quantum registers.

HL 33.23 Wed 17:00 P1

Towards Silicon Vacancy centers based quantum repeaters for a distributed quantum computing network in 4H-SiC — •Maximilian Hollendonner[1], Fedor Hrunski[1], Andre Pointner[1], Shravan Kumar Parthasarathy[2,1], Christian Gobert[2], Daniel Scheller[1], and Roland Nagy[1] — [1]Chair of Electron Devices, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Fraunhofer Institute for Integrated Systems and Device Technology IISB, Schottkystraße 10, Erlangen, Germany

For the successful integration of quantum technological systems, like for instance optical quantum computers and quantum sensors [1] into a quantum internet of things it is vital to have quantum repeaters which mediate the exchange of information between various quantum nodes. Due to its excellent optical and spin properties [2], the V_2 silicon vacancy center in 4H-SiC is a promising platform for this task. Within this project we aim at building an interferometer in which after a first 50/50 beam splitter, two single V_2 centers separated by 2 meters are excited by 916nm photons. The single photon emitted by one of the two color centers then enters a second beam splitter, which effectively removes the which-path information and therefore creates a maximally entangled Bell state [3]. Successful demonstration of this entanglement between these two V_2 centers will be a vital step towards realization of a quantum internet of things.

Sources: [1] J. R. Maze *et al.*, *Nature* **455**, 644-647 (2008) [2] R. Nagy *et al.*, *Nat Commun* **10**, 1954 (2019) [3] P. C. Humphreys *et al.*, *Nature* **558**, 268-273 (2018)

HL 33.24 Wed 17:00 P1

On the positioning accuracy of single quantum emitters in photonic nano-structures embedded through in-situ electron beam lithography — •Jan Donges, Johannes Schall, Imad Limame, Ching-Wen Shih, Sven Rodt, and Stephan Reitzenstein — Technische Universitaet Berlin, Hardenbergstr. 36, 10623 Berlin

The precise integration of single quantum emitters at the target position inside of photonic nano-structures is of upmost importance for their optimum performance. Differences between simulated photon extraction efficiencies and experimentally determined values are often at least partially contributed to a spatial misalignment of the emitter. This is a reasonable assumption considering that for instance in the case of Bullseye cavities simulations yield that the efficiency can drop more than 50% just in case of a 50nm misplacement between structure and emitter. The main problem with this approach so far has been that there is no direct way of determining the emitter position inside the structure. Therefore, all statements about the position were based indirectly on results of photoluminescence (PL) experiments. Here, we present a solution for this issue. Through the simultaneous measurement of the structure via cathodoluminescence and electron microscopy we can directly determine the emitter position inside a photonic structure with. Furthermore, this approach enables us to make a clear statement about the positioning accuracy of in-situ electron beam lithography.

HL 33.25 Wed 17:00 P1

Quantum Polyspectra for an uncompromising and universal evaluation of quantum measurements — •Markus Sifft and Daniel Hägele — Ruhr University Bochum, Faculty of Physics and Astronomy, Experimental Physics VI (AG), Germany

The analysis of a continuous measurement record $z(t)$ poses a fundamental challenge in quantum measurement theory. Different approaches have been used in the past as records can, e.g., exhibit predominantly Gaussian noise, telegraph noise, or clicks at random times. This poster summarizes our latest findings that show that quantum measurements from all cases above can be analyzed in terms of higher-order temporal correlations of the detector output $z(t)$ and be related to the Liouvillian of the measured quantum system. The comparison of temporal correlations via so called quantum polyspectra is based on expressions derived without approximation from the stochastic master equation [1] and automatized without the need for manual post-processing of the detector output. This allows for fitting of system parameters like e.g., tunneling rates in a quantum transport experiment [2]. The very general stochastic master equation approach includes coherent quantum dynamics, environmental damping, and measurement backaction at arbitrary measurement strength. This enables a systematic evaluation of quantum measurements from the realms of conventional spin noise spectroscopy, quantum transport experiments, and, as our newest finding, ultra-weak measurements with stochastically arriving single photons [3]. [1] Hägele et al., PRB 98, 205143 (2018), [2] Sifft et al., PRR 3, 033123 (2021), [3] Sifft et al., arXiv:2109.05862

HL 33.26 Wed 17:00 P1

Detection of half-vortices in confined polariton condensates — •Yannik Brune, Bernd Berger, and Marc Assmann — Department of Physics, TU Dortmund, Germany

A half-vortex describes a rotating quantum fluid carrying a spin dependent topological charge. Theory predicts half-vortices as solutions of the spin dependent GPE. We experimentally demonstrate the existence of half-vortices in an all optical circular confined polariton condensate. Therefore we excite a polariton microcavity across the treshhold using a ringlike excitation profile and observe the polariton emission. Finally,

we measure the topological charge of the condensate state, using spin filtered OAM sorting [1], and thereby confirm its half vortex character.

[1]Berger et al., Optics Express 26(24):32248 (2018)

HL 33.27 Wed 17:00 P1

Adaptive Bayesian estimation of an Overhauser field gradient — •Jacob Benestad[1], Jan Krzywda[2], Evert van Nieuwenburg[2,3], Fabrizio Berritta[3], Torbjørn Rasmussen[3], Anasua Chatterjee[3], Ferdinand Kuemmeth[3], and Jeroen Danon[1] — [1]Center for Quantum Spintronics, Norwegian University of Science and Technology, Norway — [2]Leiden Institute of Advanced Computer Science, Leiden University, The Netherlands — [3]Center for Quantum Devices, University of Copenhagen, Denmark

Slow fluctuations of the Overhauser field gradient are an important source for decoherence in singlet-triplet spin qubits hosted in type III-V semiconductors. Single-shot Ramsey experiments are well suited for Bayesian inference of the Overhauser gradient, where smart experiment design and prior knowledge can be leveraged to increase the information gain of a new measurement. This has led to the development of adaptive schemes, where between each measurement one attempts to determine the optimal next experiment in order to gain the most possible information about an Overhauser field gradient before the qubit decoheres. A real-time exact treatment of this problem at each step is difficult to achieve in an experimental setting. However an approximate treatment using only Gaussian distributions has been shown to give an exponential reduction of the distribution variance and would require only tracking two parameters. We propose a modification of this scheme that should make it more robust for gradients distributed around a mean of zero by evaluating the squared values and performing the Bayesian update scheme on the resulting chi-square distribution.

HL 33.28 Wed 17:00 P1

Zero-phonon line and electron-phonon coupling of the NV center in cubic silicon carbide: first-principles calculations — •Timur Biktagirov[1], Hans Jürgen von Bardeleben[2], Jean-Louis Cantin[2], Wolf Gero Schmidt[1], and Uwe Gerstmann[1] — [1]Universität Paderborn, Paderborn, Germany — [2]Sorbonne Université, Paris, France

The nitrogen-vacancy (NV) center in cubic silicon carbide (3C polytype), the analog of the NV center in diamond, has recently emerged as a solid-state qubit with competitive properties and significant technological advantages [1, 2]. Most applications of NV centers are based on optical spectroscopy of the zero-phonon line (ZPL) and the analysis of the spin states. Thus, we use density functional theory (DFT) calculations to provide thorough insight into the ZPL and the related magneto-optical properties of this center. In the case of NV in diamond, the ZPL is known to be in the visible spectral range [3]. In contrast, we identify the ZPL of the NV center in 3C-SiC at 1289 nm (within the telecom O-band), which is more suitable for device applications due to low transmission losses in optical waveguides. An analysis of the measured phonon sideband reveals the Huang-Rhys factor of 2.85 and the Debye-Waller factor of 5.8 %. Along with exceptionally long low-temperature spin-lattice relaxation times [2], these properties make NV in 3C-SiC a strong competitor for qubit applications.

1. S. A. Zargaleh et al., Phys. Rev. B 98, 165203 (2018).
2. H. J. Von Bardeleben et al., Nano Lett. 21, 8119-8125 (2021).
3. M. W. Doherty et al., Phys. Rep. 528, 1-45 (2013).

HL 33.29 Wed 17:00 P1

Design of a microwave resonator for coherent nuclear spin control of ^{13}C and ^{29}Si isotopes near V_2 color centers in 4H-SiC at cryogenic temperatures — •Jan Philipp Ahnfeldt[1], Fedor Hrunski[1], Shravan Kumar Parthasarathy[1,2], Maximilian Hollendonner[1], Daniel Scheller[1], Andre Pointner[1], and Roland Nagy[1] — [1]Chair of Electron Devices, FAU Erlangen-Nürnberg, Erlangen, Germany — [2]Fraunhofer Institute for Integrated Systems and Device Technology (IISB), Erlangen, Germany

One step to meaningful quantum technologies is to scale up the currently developed ones. This can be done by parallelizing several quantum systems through a quantum network. Therefore it is crucial that the network contains quantum memory nodes in which the quantum system used has a long coherence time. This can be ensured by the nuclear spin of the ^{13}C or ^{29}Si isotopes surrounding a silicon vacancy in 4H-SiC. However, due to the low gyromagnetic ratio of a nuclear spin a large magnetic flux is needed for the spin control. Accordingly, a large RF power with a frequency in the upper kHz domain is required. Because the power dissipation causes problems when upscaling these systems, it is important to improve the spin control's efficiency. Hence, a resonator creating a standing magnetic wave polarized perpendicular to the quantization axis of the vacancy seems to be a promising approach. Since it must operate at room and cryogenic temperatures, the resonator must be mechanically stable and needs a wide bandwidth. Therefore, several resonators are investigated which could meet these requirements in a small package of a few cubic centimeters.

HL 33.30 Wed 17:00 P1

Optical Beamsplitter for Orbital Angular Momentum Modes — •Rebecca Aschwanden[1], Bernhard Reineke[2], Lingling Huang[3], Klaus D. Jöns[1], Tim Bartley[1], and Thomas Zentgraf[1] — [1]Department of Physics, Paderborn University, Paderborn, Germany — [2]Institute for Photonic Quantum Systems PhoQS, Paderborn University, Paderborn, Germany — [3]Beijing Institute of Technology, Beijing, China

Metasurfaces consist of periodically arranged antennas of subwavelength dimensions that allow for specifically engineered functionalities and interaction with the incident light beam. They cannot only be used to replace conventional bulk optical elements but also to provide new functionalities. Here, we present the design and fabrication of a dielectric metasurface acting as a beamplitter with multiple output ports for orbital angular momentum (OAM) states. The dielectric metasurface consists of silicon nanofins which are fabricated by electron beam lithography and etching. We show that the metasurface splits the beam containing a superposition of OAM states into four spatially separated output directions.

HL 33.31 Wed 17:00 P1

Integration of free-standing GaAs nanobeam cavities hosting InAs/GaAs QD with LNOI waveguides — •Oscar Camacho Ibarra, Ioannis Caltzidis, Marc Sartison, and Klaus D. Jöns — Paderborn University, Paderborn, Germany

Monolithic integration is the most straightforward approach to incorporate single photon emitters and photonic integrated circuits (PICs). However, this approach limits you to the optical properties of the chosen material platform. Furthermore, the current best emitters on monolithic integration are randomly positioned [1]. Based on this context, hybrid integration, despite also requiring localization, stands out, in this approach different materials are integrated into one PIC, allowing one to exploit the advantages of each different material system (whether they are optical properties of the material or the emitters properties). In our work, we seek to hybridly integrate InAs/GaAs quantum dots embedded in nanobeam cavities with LNOI waveguides. To achieve this, we chose a transfer printing method [2] to place the nanobeam cavities (hosting the emitters) on top of the LNOI waveguides. Therefore, we report on the current progress and challenges for localization and nanofabrication of the free-standing nanobeam cavities.

[1] Marc Sartison et al, Scalable integration of quantum emitters into photonic integrated circuits, Mater. Quantum. Technol. 2 023002, 2022.

[2] Ryota Katsumi et al, Transfer-printed single-photon sources coupled to wire waveguides, Optica Vol. 5, No. 6, 2022.

HL 33.32 Wed 17:00 P1

Observation of quantum Zeno effects for localized spins — •Vitalie Nedelea — Experimentelle Physik 2, Technische Universität Dortmund, 44221 Dortmund, Germany

One of the main dephasing mechanisms for the localized carrier spins in semiconductors is the coupling to the fluctuating nuclear spin environment. Here we present an experimental observation on the effects of the quantum back action under pulsed optical measurements of spin ensemble and demonstrate that the nuclei-induced spin relaxation can be influenced. We show that the fast measurements freeze the spin dynamics and increase the effective spin relaxation time, the so-called quantum Zeno effect. Furthermore, we demonstrate that if the measurement rate is comparable with the spin precession frequency in the effective magnetic field, the spin relaxation rate increases and becomes faster than in the absence of the measurements, an effect known as the quantum antiZeno effect. A theory describing both regimes allows us to extract the system parameters and the strength of the quantum back action.

HL 33.33 Wed 17:00 P1

On-demand strain-induced recombination dynamics in semiconductor quantum wells — Daniel Hensel[1], Daniel Schmidt[3],

Fariba Hatami[2], and •Peter Gaal[1,3] — [1]Leibniz-Institut für Kristallzüchtung, 12489 Berlin — [2]Humboldt Universität zu Berlin, 12489 Berlin — [3]TXproducts UG, 22547 Hamburg

Todays technology enables the fabrication of semiconductor structures with a high control over the electronic states. New technologies emerged from the manipulation of these states. To gain full control over the quantum state encrypted in a particle one must control both its lifetime and its coherence. Tailored transient strain pulses provide a new tool for the manipulation of nanoscale quantum objects. The strain-induced deformation of the crystal lattice manipulates the electronic bandstructure via deformation potential coupling. A convenient method to administer strain pulses to a sample are so-called surface acoustic waves (SAW). They are generated electronically by interdigitated circuits (IDT). The experimental control is limited by the ability to generate arbitrary lattice deformations on timescales short compared to the quantum decoherence. The photoacoustic method allows controlling the spatial and temporal shape of the optical excitation and thus shapes the strain pulse. In consequence, arbitrary SAWs can be generated on ultrafast timescales. Time-resolved photoluminescence (TRPL) spectroscopy is used to monitor the strain-induced change in electronic bandstructure. The control of the efficiency of radiative transitions of excitons through the applied strain could be the missing step for the realization of a fast on-demand single photon source.

HL 33.34 Wed 17:00 P1

Fiber-based Open Cavity: a tailored solution for Solid-state Quantum Emitters and their characterization. — •Francesco Salusti[1], Lukas Hanschke[1], Eva Schöll[1], Jonathan Noe[2], Manuel Nutz[2], Michael Förg[2], Thomas Hümmer[2], and Klaus D. Jöns[1] — [1]PhoQS, CeOPP, and Department of Physics, Paderborn University, 33098 Paderborn, Germany — [2]Qlibri GmbH, 80337 Munich, Germany and Fakultät für Physik, Ludwig-Maximilians-Universität, 80799 Munich, Germany

For the realization of bright and reliable quantum light emitters, the integration of these emitters into cavity structures represents an elegant solution. However, in many cases, the fabrication of such photonic structure requires remarkable efforts to precisely match the position and the emission wavelength of the emitter with respect to the cavity mode. The required level of control of the materials, size, and positioning makes the realization of a practical cavity resource intensive. Recent works have demonstrated the possibility to take advance of open cavities to easily tailor the cavity around the specifications of individual emitters, such as 2D flakes and quantum dots. In our collaboration between industry and academia, we show that it is possible to take advantage of a fiber-based device to realize a tunable cavity at room and cryogenic temperature. In addition to the advantages of in-situ tuning of an optical resonator to specific emitter resonances, the high finesse of the system enables spatially resolved measurements of the absorption coefficient from oxidized 2D material.

HL 33.35 Wed 17:00 P1

Monolithic, heterogeneous and hybrid Integration of quantum emitters — •Marc Sartison, Oscar Camacho Ibarra, Ioannis Caltzidis, Dirk Reuter, and Klaus D Jöns — Institute for Photonic Quantum Systems, Center for Optoelectronics and Photonics Paderborn, and Department of Physics, Paderborn University, 33098 Paderborn, Germany

Modern integrated quantum photonic devices can be built out of a variety of material platforms like Lithium-Niobate on insulator (LNOI), Silicon-Nitride or Silicon with different kinds of quantum emitters like quantum dots, NV centres or emitters hosted in 2D materials. Exploiting the unique material properties several integration approaches were realized that can coarsely be categorized and belong to one of the following types: Monolithic, heterogeneous, and hybrid integration. In our work we give an overview of the different integration methods and compare them in terms of yield and scalability. We discuss the advantages and disadvantages of monolithic, heterogeneous and hybrid integration methods and provide a perspective on the upcoming challenges to realize scalable systems with high yield.

[M. Sartison et al, Mater. Quantum. Technol. 2 023002 (2022)]

HL 33.36 Wed 17:00 P1

Electrical Stark tuning of multiple waveguides with integrated quantum dots — •Yuhui Yang[1], Shulun Li[1,2], Johannes Schall[1], Chirag Palekar[1], Léo Roche[1], Hanqing Liu[2], Sven Rodt[1], Haiqiao Ni[2], Zhichuan Niu[2], and Stephen Reitzenstein[1] — [1]Institut für Festkörperphysik, TU Berlin, 10623 Germany — [2]Institute of Semiconductors, CAS, 100083, China

Self-assembled quantum dots (QDs) are promising candidates for future photonic quantum technologies owing to their close-to-ideal quantum properties. However, the random spectral and spatial distribution of single QD complicates the controlled integration of single QD into photonic structures using standard nano-processing technologies such as standard electron beam lithography and makes upscaling to complex quantum circuits practically impossible. We overcome these technical issues by combining cryogenic cathodoluminescence (CL) mapping for spectrally selected integration of QDs and the quantum-confined Stark effect for spectral fine-tuning. Two spectrally similar self-assembled QDs in a p-i-n diode membrane are pre-selected and are deterministically integrated into the hybrid structure waveguides using marker-based electron beam lithography. Moreover, the gate voltage-dependent micro photoluminescence spectra reveal the achievement for tuning individual QD in waveguide systems and spectrally overlying them together. Our work demonstrates the high potential of deterministic quantum device processing for the scalable fabrication of complex quantum integrated circuits with multiple single-photon emitters as an attractive platform for future quantum technologies.

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Electrical Stark tuning of multiple waveguides with integrated quantum dots — •Yuhui Yang[1], Shulun Li[1,2], Johannes Schall[1], Chirag Palekar[1], Léo Roche[1], Hanqing Liu[2], Sven Rodt[1], Haiqiao Ni[2], Zhichuan Niu[2], and Stephen Reitzenstein[1] — [1]Institut für Festkörperphysik, TU Berlin, 10623 Germany — [2]Institute of Semiconductors, CAS, 100083, China

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Donor Spins in Compressively Strained Silicon — •Basak Cigdem Özcan, David Vogl, and Martin S. Brandt — Walter Schottky Institut and School of Natural Sciences, Technische Universität München, 85748 Garching, Germany

Silicon doped with donors is a promising system for quantum computing applications due to long coherence times, fast spin control and the possibility of scaling as well as integration with conventional microelectronics. In order to achieve long coherence times, coupling to other nuclear spins should be avoided. This is achieved by using isotopically purified Si-28 samples, which is the naturally more abundant isotope without nuclear spin. The conventional architecture to conduct measurements on doped Si-28 involves the placement of control and read-out gate structures on top of the sample. Such additional structures cause strain near the donors, which makes it important to understand the effect of strain on their spin properties. To study this under controlled strain conditions, we utilize a no-contact capacitive read-out scheme, where optical excitation of donor-bound excitons (DBE) followed by an Auger recombination facilitates spin-dependent excitation, spin polarization and spin-state read-out. Combining infrared optical excitation and microwave pulses, we perform electron nuclear double resonance (ENDOR) experiments, with which we achieve coherent control of nuclear spins of the donors. Here, we investigate the strain-dependent shift of DBE resonance frequencies under uniaxial compressive stress. We acknowledge the financial support of MCQST.

HL 33.39 Wed 17:00 P1

Application of low-cost visible light LEDs in avalanche mode as sensitive photoreceivers in a plastic optical fiber data

transmission system — •Heinz-Christoph Neitzert — Dept. of Industrial Engineering (DIIN) Salerno University Fisciano, Italy

Commercial low-cost light emitting diodes have been tested as photoreceivers without and with applied reverse bias voltage. In particular the possibility to operate the devices in the breakdown regime as sensitive avalanche photodiodes has been succesfully tested. High photogain amplification at relatively low breakdown voltage values has been observed. Based on this possibility to operate the LEDs efficiently not only as emitters but also as photoreceivers, a simple half-duplex bidirectional optical transmission scheme, which is based on the plastic-optical-fiber (POF) as transmission medium and green LEDs as receiving/emitting elements has been developed. The choice of the green wavelength range gives the possibility to operate the system at the minimum absorption of the plastic optical fiber

HL 33.40 Wed 17:00 P1

High Resolution Spectroscopy for (Al,In)GaN Laser Diodes — •Dominic J. Kunzmann, Raphael Kohlstedt, and Ulrich T. Schwarz — TU Chemnitz, 09126 Chemnitz, Germany

We investigate laser diodes based on the (Al,In)GaN material system with the help of high-resolution spectroscopy. Therefore, we use two setups, one with a grating spectrometer and a Fabry-Pérot-Interferometer. The grating spectrometer is used to measure the longitudinal mode spectra above and below the threshold current. Below the threshold we perform Hakki-Paoli gain spectroscopy to obtain the internal losses of laser diodes which is getting even more challenging, when the diodes get better and the losses smaller. Above the threshold wavelength shifts with current and temperature can be observed and with these shifts the thermal resistance is available. Additionally for broad ridge high power laser diodes the interplay of different longitudinal mode combs is investigated with the high-resolution spectrometer. The Fabry-Pérot-Interferometer enables us to go to even higher resolutions and to verify single mode behavior of laser sources and to observe much smaller wavelength shifts.

HL 33.41 Wed 17:00 P1

Indium incorporation in thin c-plane GaInN/GaN quantum wells grown via plasma-assisted molecular beam epitaxy — •Farouk Aljasem, Heiko Bremers, Uwe Rossow, and Andreas Hangleiter — Institut für Angewandte Physik & Laboratory for Emerging Nanometrology, Technische Universität Braunschweig, Germany

This work aims to investigate the physical mechanisms of the incorporation of indium atoms in GaInN QW structures with an emphasis on interface properties by growing thin GaInN multiple quantum wells. A comparison of the obtained results using MBE with the results from the previous work using MOVPE offers more information about indium incorporation mechanisms. As well known, the flux of the activated nitrogen in the plasma-assisted molecular beam epitaxy (PAMBE) is independent of the growth temperature. This feature enables the growth of GaInN MQWs at low temperatures and in different growth regimes compared to MOVPE. Fivefold thin GaInN/GaN MQWs are grown via PAMBE in the c-direction using MOVPE-grown GaN templates on sapphire as substrates. The GaInN/GaN MQW samples were grown at different growth temperatures with various III/V ratios and QW thicknesses. MQW thickness ranged between less than half a c-lattice constant and 2 nm with no significant relaxation. To provide a precise understanding of the physical processes during the growth process of GaInN monolayers, the samples were characterized using HR-XRD, AFM, HR-TEM and CW-PL.

HL 33.42 Wed 17:00 P1

Temperature dependent Raman spectroscopy on GaN:Si — •Christina Harms, Jona Grümbel, Martin Feneberg, and Rüdiger Goldhahn — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Germany

GaN structures are of high interest for optical and electronic applications in current research projects. We investigate the Raman excitations of hexagonal bulk GaN:Si under temperature variation from 80 K up to 300 K. Seven samples with carrier concentrations ranging between 10^{12} - 10^{19} cm^{-3} were measured using laser excitation of 532 nm. It is shown, that within room temperature measurements both coupled phonon-plasmon-modes ($LPP_{\pm}$) are visible and follow the prediction of polaritonic excitations. Under variation of temperature the LPP_{+} mode shows a weak frequency shift with elevated temperature or remains unaffected for low carrier concentrations. Surprisingly, the LPP_{-} mode shifts towards lower frequencies with increasing temperatures for all samples, which contradicts previous assumptions. A qualitative description of the results and possible interpretations will be presented. Additionally, we also investigated the temperature dependent FWHM of the $LPP_{\pm}$ mode and the E_2 phonon mode. Here, both behaviours match the theoretical and experimental previous research.

HL 33.43 Wed 17:00 P1

Indium incorporation during GaInN quantum well growth: role of underlayer surface morphology — •Rodrigo de Vasconcellos Lourenço[1,2], Uwe Rossow[1], Philipp Horenburg[1], Heiko Bremers[1,2], and Andreas Hangleiter[1,2] — [1]Institute of Applied Physics, Technische Universität Braunschweig, Germany — [2]Laboratory for Emerging Nanometrology, Technische Universität Braunschweig, Germany

The control of Indium incorporation is a key factor for the optoelectronic devices in the visible and near UV spectral region. The luminescence efficiency of such devices has been improved by the so-called underlayer, i.e the layer grown just before the active region. We investigate the surface morphology as function of the underlayer (UL) composed of GaN or InAlN. For GaN UL, we find extended, very smooth terraces separated by macrosteps in a range of growth temperature from 770 to 950 °C. Additionally, morphologies associated to the Ehrlich-Schwöbel barrier are not observed. On the other hand, for InAlN UL lattice matched to GaN, evidence for nuclei forming at step edges is observed, which may be due to lower surface mobility of Al compared to Ga or In. In the next step, we want to understand how the underlayer morphology affects the Indium incorporation of GaInN quantum wells.

HL 33.44 Wed 17:00 P1

The impact of laser lift-off on the optical properties of InGaN/GaN LEDs — •Stefan Wolter, Steffen Bornemann, Hendrik Spende, and Andreas Waag — Institut für Halbleitertechnik, Technische Universität Braunschweig, 38106 Braunschweig

InGaN/GaN LEDs are typically grown on sapphire, but sapphire is a disadvantageous material when it comes to electrical or thermal conductivity. This limits the performance, when the LED structure is processed into a device. For this reason, it is useful to transfer the LED structure to another carrier after growth, which can be achieved by laser lift-off (LLO). In this process, a pulsed laser beam is focused on the sapphire/GaN interface, leading to absorption of the laser photons in the GaN layer and subsequent decomposition of GaN near the interface resulting in detachment of the GaN film from sapphire. The usage of ultra short laser pulses can reduce the required laser fluence compared to nanosecond pulses, but has the disadvantage of penetrating deep into the LED structure and possibly even reaching the active region. This leads to a change in the characteristic properties of the LED, which is investigated in this study. For this purpose, in-house grown blue InGaN/GaN LEDs are investigated before and after LLO, which was conducted with sub-bandgap (520 nm) and above-bandgap (347 nm) laser light at a pulse width of 0.4 ps. Temperature-dependent photoluminescence experiments in the temperature range of 6 K to 295 K indicate that the maximum internal quantum efficiency decreases by at least 10 % after LLO. Furthermore, LLO can have an impact on the localization strength of the carriers inside the active region.

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haracterization of a semiconductor microstructure analogous to a Venturi pump — •Severin Krüger, Fabian Liedtke, Peter Zajac, Andreas Wieck, Arne Ludwig, and Ulrich Kunze — Ruhr-Universität Bochum, Universitätsstraße 150, 44801 Bochum, Germany

Micro-structuring a high-mobility two-dimensional electron gas allows investigation of the ballistic transport regime for electrons. The electrons in the examined channel structures show edge effects like a minimal resistance at finite currents [1]. Furthermore, the electrons show hydrodynamical behavior and can create a rectifing voltage at the narrow channel, similar to the Venturi-effect [2]. Here, first results of measurements regarding the Venturi analogon with different channel sizes, gate voltages and source-drain currents are presented.

[1] Gurzhi, R.N.: "Minimum of Resistance in Impurity-free conductors" *Soviet Phys. JETP 17*, 521-522 (1963).
[2] Szelong, M.: "Ballistische und hdydrodynamische Vollwellengleichrichtung in nanoskaligen elektronischen GaAs/AlGaAs-Kreuzstrukturen" Disseration, Ruhr-Universität Bochum (2017).

HL 33.46 Wed 17:00 P1

Novel approach to real-space renormalization group analysis of the quantum Hall effect — •Nathan Shaw and Rudolf A. Römer — Department of Physics, University of Warwick, Coventry, CV4 7AL, UK

Consensus on the value of the critical exponent ν of the plateau-to-plateau transitions in the quantum Hall effect has not yet been achieved. Recent work has highlighted a discrepancy between field theory based predictions and numerical high-precision estimates. A necessarily approximate real-space renormalization group (RG) approach to the Chalker-Coddington model has previously been shown to suggest a critical exponent of $\nu \approx 2.3$. However, most recent numerical estimations suggest that $\nu = 2.58(3)$. In this study, we experiment with varying the analytical form of the scattering matrix elements with the goal of increasing the numerical stability of the fixed point distribution constructed by the RG flow. Using this improved distribution, we recalculate the critical exponent with higher accuracy.

HL 33.47 Wed 17:00 P1

Epitaxial growth of high-density short wavelength InGaAs QDs for low-threshold VCSELs — •Sarthak Tripathi, Kartik Gaur, Ching-Wen Shih, Imad Limame, Sven Rodt, and Stephan Reitzenstein — Inst. for Solid State Phys., Technical Univ. of Berlin, Germany

Self-assembled growth of InGaAs quantum dots by MOCVD is used to form the active region of low-threshold vertical-cavity surface-emitting lasers (VCSELs). In our work, we optimize the QD gain medium for room-temperature lasing at 935-955 nm which is attractive for gas sensing applications. Multiple layers of high-density InGaAs quantum dots are stacked in order to maximize the modal gain. The density of dislocations and point defects in QD heterostructures is strongly reduced by annealing which enables a significant reduction of the spacer thickness (thinner active region) between stacked QD layers without forfeiting their crystalline quality. Surface characterization is performed using atomic force microscopy AFM to determine the QD density. Moreover, during growth optimization photoluminescence studies are conducted to evaluate the optical properties of single and stacked layers of QD emitting in the target wavelength range. In future, the resulting QDs will be integrated in an active region embedded VCSELs with monolithically integrated high contrast grating (MHCG) hybrid structure.

HL 33.48 Wed 17:00 P1

Simulation and fabrication of a WS_2-nanobeam cavity with a $MoSe_2$ monolayer as active material — •Aris Koulas-Simos[1], Bárbara Rosa[1], Chirag Palekar[1], Léo Roche[1], Yang Yuhui[1], Felix Binkowski[2], Sven Burger[2,3], Battulga Munkhbat[4], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany — [2]Zuse Institute Berlin (ZIB), 14195 Berlin, Germany — [3]JCMwave GmbH, D-14050 Berlin, Germany — [4]Department of Electrical and Photonics Engineering, Technical University of Denmark, 2800 Kongens Lyngby, Denmark

Transition metal dichalcogenides (TMDCs) exhibit extraordinary optical, electrical, and mechanical properties that can be easily tailored for novel integrated photonic applications. Different TMDCs can be combined to form novel nanostructures with highly interesting complex dynamics. Here, we report on the simulation and fabrication of a WS_2-nanobeam cavity with a $MoSe_2$ monolayer (ML) as active material. Utilizing a FEM eigenfrequency solver, cavity simulations are performed on a 3D stripe of WS_2 with a finite periodic air hole arrangement. The calculated eigenmodes exhibit high Q-factors and tight mode confinement with mode volumes near the fundamental diffraction limit after parameter optimization. The final parameter set is employed in the fabrication process of WS_2-nanobeam cavities with a $MoSe_2$ ML embedded in them. This work paves further the way toward the realization of novel nanolaser devices consisting purely of TMDC materials.

HL 33.49 Wed 17:00 P1

Design and optimization of Monolithic High Contrast Grating for tuneable quantum dot VCSEL arrays — •Floriana Laudani[1], Mikołaj Janczak[2], Bartosz Kamiński[3], Niels Heermeier[1], Anna Musiał[3], Grzegorz Sek[3], Tomasz Czyszanowski[2], Sven Rodt[1], and Stephan Reitzenstein[1] — [1]Institute of Solid State Physics, Technische Universität Berlin, 10623 Berlin, Germany — [2]Institute of Physics, Lodz University of Technology, 90-924 Łódź, Poland — [3]Department of Experimental Physics, Wroclaw University of Science and Technology, 50-370 Wrocław, Poland

Water vapor measurements are essential for industrial applications to ensure a qualitative processing and control chain and require gas sensors with short response times in a broad wavelength range. In contrast to standard vertical-cavity surface-emitting lasers (VCSELs), devices with monolithically integrated high contrast gratings (MHCGs) can provide a high flexibility with respect to the emission wavelength. We compare reflectivity measurements and theoretical results on GaAs-based MHCGs for a target wavelength around 940 nm. A numerical model based on Plane-Wave Admittance Method solving set of Maxwell equations was used to search for optimal geometric parameters for effective device optimization, allowing a controlled parameter tuning throughout the fabrication process based on high-resolution electron-beam lithography. Since MHCGs can be custom designed before fabrication, they offer great potential for realizing on-chip tuneable VCSEL arrays, e.g. in a variety of short-range communication systems.

HL 33.50 Wed 17:00 P1

In-plane coupling between a WGM micropillar laser and a ridge waveguide — •Léo Roche[1], Imad Limame[1], Ching-Wen Shih[1], Aris Koulas-Simos[1], Yuhui Yang[1], Sven Burger[2], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik (TUB), Berlin, Germany — [2]JCMwave GmbH, Berlin, Germany

Integrated quantum photonic circuits (IQPCs) are very promising candidates for scalable and flexible on-chip quantum computation and quantum communication hardware. One critical requirement for their realization is the scalable integration of on-demand indistinguishable single-photon emitters. This is potentially possible through the resonant excitation of an integrated QD in a waveguide by means of an on-chip integrated coherent light microlaser. Towards this goal, we investigate the coupling and lasing properties of coherent light laterally emitted from a whispering gallery mode (WGM) type micropillar laser evanescently coupled to a single mode ridge waveguide. Using finite element method (FEM) simulations, we predict the pillar dimensions allowing for lasing modes in the typical emission wavelength of InGaAs QD (930nm) and investigate the coupling efficiency and the Q-factor of the pillar-waveguide system for different angular mode number, pillar-waveguide air gap distances and interface types (point-like or pulley coupling). The III-V semiconductor type nanostructures composed of a GaAs cavity with InGaAs QDs and distributed Bragg reflectors are processed using high-resolution electron beam lithography. Simulation predictions and micro-photoluminescence spectroscopy performed on the nanoprocessed devices are compared and discussed.

HL 33.51 Wed 17:00 P1

Relativistic calculation of hyperfine splittings of hydrogen-like atoms with finite-size nuclei — •Katharina Lorena Franzke, Wolf Gero Schmidt, and Uwe Gerstmann — Paderborn University, Warburger Str. 100, 33098 Paderborn

The hyperfine splittings of spin qubits play an important role in quantum information and spintronics application. They allow for readout of the spin qubits, while simultaneously being the dominant mechanism for the detrimental spin decoherence. Their exact knowledge is thus of prior relevance. In this work we show that the formula of Blügel et al. [1] also holds in the full relativistic regime even if finite-size structure of the nuclei are taken into account. For this purpose, different models for the nuclear charge and spin distributions are compared analytically. The calculated hyperfine splittings of H-like alkali atoms up to ^{133}Cs show a good agreement for all nuclei models. For the real one-electron systems ^{1}H, ^{2}H, ^{3}H, ^{3}He^{+} they are also in very good agreement with available experimental data. Deviations of DFT-predicted hyperfine splittings from experiment are thus actually due to the use of the frozen-core approximation and limitations of the exchange-correlation (XC) functional.

[1] S. Blügel et al., *Hyperfine fields of 3d and 4d impurities in nickel.* Physical Review B **35**, 3271 (1987).

HL 33.52 Wed 17:00 P1

Calculation of zero-field splitting in high-spin defects in semiconductors — •Timur Biktagirov, Wolf Gero Schmidt, and Uwe Gerstmann — Universität Paderborn, Paderborn, Germany

High-spin defects in semiconductors represent an attractive class of potential solid-state qubits [1]. One of their key spectroscopic fingerprints is the splitting of their spin sublevels in the absence of external magnetic fields. Here we discuss recent progress and open challenges

in the theoretical prediction of this zero-field splitting [2, 3].

1. J. R. Weber et al., PNAS 107, 8513-8518 (2010).
2. T. B. Biktagirov and U. Gerstmann, Phys. Rev. Research 2, 023071 (2020).
3. T. B. Biktagirov et al., Phys. Rev. Research 2, 022024 (2020).

HL 33.53 Wed 17:00 P1

Electro-optic response function of thin Quartz for sampling of high-field THz pulses — •Maximilian Frenzel, Michael S. Spencer, and Sebastian F. Maehrlein — Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany

As high-field THz sources are currently getting more broadly employed, it becomes increasingly important to characterize intense single-cycle THz fields (> 1 MV/cm) in amplitude and phase without saturation or nonlinearities in the electro-optic detection. After previous attempts of spectrally neutral attenuation, z-cut α-Quartz has been recently found as a suitable electro-optic sampling (EOS) crystal. Nevertheless, its accurate response function, which allows the THz electric field to be exactly determined from the measured EOS signal, is still missing. Here, we employ intense THz fields (0.5 - 4 THz) generated via optical rectification in $LiNbO_3$ to measure EOS in Quartz of various thicknesses between 30 and 150 μm. We find that both EOS peak amplitude and signal shape are significantly thickness-dependent. By modeling the Quartz EOS detector response function, we find good agreement between parameter free theory and experiment, thus explaining the measured thickness dependence. Our work will therefore allow accurate measurement of intense THz electric fields wherever conventional EOS materials are facing saturation effects.

HL 33.54 Wed 17:00 P1

Fourier Transform Infrared Spectroscopy of Quantum Dot and Bragg Mirror Layers in Semiconductor Heterostructures — •Nikolaj Lehl, Andreas Wieck, Nathan Jukam, and Amar Alok — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Deutschland

A purposefully designed distributed Bragg reflector (DBR) in a semiconductor heterostructure improves this device's photon yield gathered from its quantum dot (QD) layer. In this master thesis the transmission spectra of such semiconductor heterostructure samples are taken using Fourier-transform infrared spectroscopy (FTIR). The molecular beam epitaxy (MBE) grown gallium arsenide (GaAs) based samples include indium arsenide (InAs) QDs, and DBRs made of sequences of GaAs layers and aluminium arsenide (AlAs) layers. The DBR stopband measurements are taken in the near-infrared (NIR) and mid-infrared (MIR) region, in vacuum, under room temperature. Furthermore, it is planned to investigate the QD intersubband transitions implied in the far-infrared (FIR) transmission spectra as a function of applied voltage at liquid nitrogen and liquid helium temperatures. All acquired spectra are compared to the devices' simulated spectra, in order to make a conclusion on the initially expected growth rates and the growth rates resulting from the measurements.

HL 33.55 Wed 17:00 P1

MIR Time-Domain Ellipsometry via 2D Electrooptic Sampling — •Leona Nest, Michael Scott Spencer, Martin Wolf, and Sebastian Maehrlein — Fritz Haber Institute of the Max Planck Society, Department of Physical Chemistry, Faradayweg 4-6, 14195 Berlin, Germany

Terahertz time-domain spectroscopy (THz-TDS) has been established as a powerful tool in fundamental material science as it allows to measure conductivities, dielectric functions, and related phase transitions in e.g. semiconductors, topological insulators, and high-temperature super-conductors. Moreover, THz-TDS is well suited to investigate ultrafast, and thus non-equilibrium, quasi-particle dynamics in such solid- state systems. The time-resolved detection of the electric field provides direct access to complex-valued static and transient material properties. Here, we extend this technique to additionally measure the temporal evolution of the field's polarization for direct determination of complex tensorial material responses. Operating our time-domain ellipsometer in the mid-Infrared (MIR, 15-40 THz) enables anisotropic transmittivity or reflectivity studies in a spectral region where fundamental resonances such as phonons can be found. As a benchmark system, we extract the complex-valued dielectric tensor components of y-cut α-quartz in the vicinity of its anisotropic 21 THz and 24 THz phonon resonances. Good agreement with free-electron-laser-based studies shows that we developed a versatile table-top time-domain ellipsometer that will be used to also measure non-equilibrium tensorial properties in the near future.

HL 33.56 Wed 17:00 P1

Comprehensive model for the thermoelectric properties of two-dimensional carbon nanotube networks — •Aditya Dash, Dorothea Scheunemann, and Martijn Kemerink — Institute for Molecular Systems Engineering and Advanced Materials, Heidelberg University, Im Neuenheimer Feld 225, 69120 Heidelberg, Germany.

Networks of semiconducting single-walled carbon nanotubes (SWCNTs) are interesting thermoelectric materials due to the interplay between CNT and network properties. Here we present a unified model to explain the charge and energy transport in SWCNT networks. We used the steady-state master equation for the random resistor network containing both the intra- and inter-tube resistances, as defined through their 1D density of states that is modulated by static Gaussian disorder. The tube resistance dependence on the carrier density and disorder is described through the Landauer formalism. Electrical and thermoelectric properties of the network were obtained by solving Kirchhoffs laws through a modified nodal analysis, where we used the Boltzmann transport formalism to obtain the conductivity, Seebeck coefficient, and electronic contribution to the thermal conductivity. The model provides a consistent description of previously published experimental data for temperature and carrier density-dependent conductivities and Seebeck coefficients, with energetic disorder being the main factor explaining observed mobility upswing with carrier concentration. For lower disorder, the Lorentz factor obtained from simulation is in accordance with the Wiedemann-Franz law. Suppressed disorder and lattice thermal conductivity can be a key to higher zT.

HL 33.57 Wed 17:00 P1

Electric field assisted transport in photodiodes studied by EBIC and STEM — •Lennart Nolte[1], Christoph Flathmann[1], Tobias Meyer[2], and Michael Seibt[1] — [1]IV. Physical Institute, University of Goettingen, Göttingen, Germany — [2]Institute for Materials Physics, University of Goettingen, Göttingen, Germany

P-i-n diodes consist of an intrinsic layer sandwiched between an n- and p-doped layer. Due to lack of carriers in the intrinsic layer, it shows a high Ohmic resistance and realizes more extended depletion zones compared to a typical p-n junction. This makes p-i-n-diodes particularly interesting for high frequency and high voltage electronic applications in addition to photo detection. In this study, we perform electron beam induced current (EBIC) investigations in cross-section geometry combined with scanning transmission electron microscopy (STEM) in order to study electric field assisted diffusion of excess carriers on a nanometer scale under well-defined experimental conditions. Special focus will be on carrier recombination at surfaces produced by focused ion beam (FIB) preparation.

HL 33.58 Wed 17:00 P1

Investigating the influence of stoichiometry-fluctuations on the electronic properties of ultra-scaled HBTs — •Daniel Dick[1,3], Jörg Schuster[1,2,3], Florian Fuchs[2,3], and Sibylle Gemming[3,4] — [1]Center for Microtechnologies, Chemnitz University of Technology, Chemnitz, Germany — [2]Fraunhofer Insitute for Electronic Nano Systems (ENAS), Chemnitz, Germany — [3]Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, Chemnitz, Germany — [4]Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany

Silicon-germanium (SiGe) heterojunction bipolar transistors (HBTs) have found widespread use in high-frequency applications. Scaling of the HBT base layer thickness to 5 nm and below makes an atomistic treatment indispensable as fluctuations of dopant concentrations play a bigger role.

We investigate the effect of scaling on properties such as band gap and carrier effective mass and obtain effective material parameters for use in simulations at a larger scale. The use of semi-empirical methods such as extended Hückel theory enables us to simulate a large number of permutations of the atomic structure and study statistical variation of its properties while first-principles methods such as density functional theory allow us to verify the results. Finaly, using the non-equilibrium Green's function method we investigate the effect of alloy and phonon scattering on transport through such a layer.

HL 33.59 Wed 17:00 P1

Investigation of Transport Phenomena Through Functionalized Single Molecules Using Liquid Mechanically Controllable Break Junctions — •Harpreet Sondhi — FWIO-T, Helmholtz-

Zentrum Dresden-Rossendorf, Dresden, Germany

The creation of molecular components for use as electronic devices has made enormous progress. In order to advance the field further toward realistic electronic concepts, methods for the controlled modification of the conducting properties of the molecules contacted by metallic electrodes need to be further developed. Here a comprehensive study of charge transport in a class of molecules that allows modifications by introducing metal center/side chain groups into organic structures is presented. Single molecules are electrically contacted and characterized in order to understand the role of the metal center/side chain groups in the conductance mechanism through the molecular junctions. It is shown that the presence of single metal ions/side chain groups modifies the energy levels and the coupling of the molecules to the electrical contacts, and that these modifications lead to systematic variations in the statistical behavior of transport properties of the molecular junctions.

HL 33.60 Wed 17:00 P1

Time-gated coherent two-dimensional spectroscopy on the nanoscale — •Luisa Brenneis, Julian Lüttig, Matthias Hensen, and Tobias Brixner — Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg

The observation of the temporal dynamics of excitons, i.e., electron-hole pairs, is essential for the understanding of fundamental phenomena in nature, e.g., photosynthesis [1]. The method of optical two-dimensional (2D) spectroscopy has proven to be particularly suitable for this purpose. For example, electronic couplings and energy transport phenomena can be directly revealed as cross peaks in a 2D spectrum, i.e., a correlation spectrum of excitation and probe frequency as a function of time. To additionally decipher the spatial dynamics of a system in a nanostructured environment beyond the optical diffraction limit, we have combined 2D spectroscopy with photoemission electron microscopy to realize coherent "2D nanoscopy" [2,3]. Here, using coupled molecular dimers in numerical simulations, we investigate the potential of 2D nanoscopy. In particular, we show how the exciton and biexciton dynamics can be disentangled by resolving the kinetic energy spectrum of photoemitted electrons and by realizing a time gate using an additional ionization pulse.

[1] T. Brixner et al., Nature **434**, 625-628 (2005).
[2] M. Aeschlimann et al., Science **333**, 1724 (2011).
[3] S. Pres et al., Nat. Phys. (2022) (accepted).

HL 33.61 Wed 17:00 P1

Negative thermal expansion in HgTe/CdTe heterostructures on ultrafast timescales — •Marc Herzog[1], Matthias Rössle[2], Jan-Etienne Pudell[3], Maximilian Mattern[1], Lukas Lunczer[4], Claus Schumacher[1], Hartmut Buhmann[1], Laurenz Molenkamp[1], and Matias Bargheer[2,3] — [1]Institut für Physik und Astronomie, Universität Potsdam, Germany — [2]Helmholtz-Zentrum Berlin, Germany — [3]European XFEL, Germany — [4]Physikalisches Institut EP3, Universität Würzburg, Germany

Materials that would exhibit an ultrafast negative thermal expansion (NTE) are desirable to generate ultrashort and high-amplitude acoustic waves as unconventional stimulus e.g. in the context of nonlinear acoustics or magnetoelastic effects. Both semimetallic HgTe and semiconducting CdTe exhibt pronounced NTE behaviour in thermal equilibrium below their Debye temperatures $\Theta_D \approx 150\,K$ owing to a negative Grüneisen parameter and correspondingly negative stress by transverse acoustic (TA) phonons.

Using ultrafast x-ray diffraction we investigate the coherent (sound) and incoherent (heat) lattice response in HgTe thin films on a CdTe substrate to ultrashort laser pulse excitation. While above Θ_D both materials exclusively expand upon excitation, below Θ_D a pronounced NTE is observed. However, the time scale for this NTE to develop is a few 100 ps suggesting a slow excitation of the TA modes. At few-ps time scales, however, a strong expansion of HgTe prevails at all measured excitation densities indicating a fast and dominant positive stress due to non-TA phonon modes and/or hot carriers.

HL 33.62 Wed 17:00 P1

h-BN as a protective encapsulation layer for monolayer graphene — •V. Calvi[1], M. Barnes[1], M. Buscema[1], D. Wehenkel[1], I.M.N. Groot[2], and R. van Rijn[1] — [1]Applied Nanolayers B.V., Feldmannweg 17, 2628 CD Delft, The Netherlands — [2]Leiden Institute of Chemistry, Leiden University, P.O. Box 9502, 2300 RA Leiden, The Netherlands

Graphene surface contamination by polymer residues used in the graphene processing is a key problem for certain device applications. PMMA is used for graphene transfer from a growth substrate to a target substrate. Transfer process leaves polymer residues on the graphene monolayer which causes p-doping. Technique used for the removal of polymer residue is annealing in different gas or vacuum atmospheres. Annealing in oxygen rich environment effectively removes polymer residue, but at the same time also causes damage to the graphene monolayer.

We have investigated stacking a monolayer of h-BN on top of a monolayer of graphene prior to transfer of the graphene. In this way the polymer necessary for the transfer only has direct contact with the surface of the h-BN and graphene would be protected in this way. We compared the damage and cleanliness to both bare graphene and stacked h-BN/graphene by Raman spectroscopy and AFM. We tested different annealing temperatures between 100°C and 500°C and found that the graphene is indeed protected from damage from the annealing process by covering it with a layer of h-BN. At the same time, we were able to show that polymer residue is effectively removed at the higher annealing temperatures.

HL 34: 2D Materials V (joint session HL/CPP)

Time: Thursday 9:30–12:00 Location: POT 81

HL 34.1 Thu 9:30 POT 81

Negative differential resistance with ultra-high peak-to-valley current ratio in tunnel diodes based on two-dimensional cold metals — •Ersoy Sasioglu and Ingrid Mertig — Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, 06120 Halle (Saale)

The negative differential resistance (NDR) effect is of great interest for future memory and logic circuit applications. We propose a novel semiconductor-free NDR tunnel diode concept with ultra-high peak-to-valley current ratio (PVCR) [1]. Our proposed NDR diode consists of two cold metal electrodes separated by a thin insulating tunnel barrier. The NDR effect stems from the unique electronic band structure of the cold metal electrodes, i.e., the width of the isolated metallic bands around the Fermi level as well as the energy gaps separating higher- and lower-lying bands determine the current-voltage characteristics and PVCR value of the tunnel diode. By proper choice of the cold metal electrodes either Λ-type or N-type NDR effect can be obtained. We employ the nonequilibrium Green's function method combined with density functional theory to demonstrate the NDR characteristics of the proposed diode based on two-dimensional NbS_2/h-BN/NbS_2 vertical and AlI_2/MgI_2/AlI_2 planar heterojunctions. For the lateral tunnel diode, we obtain a Λ-type NDR effect with an ultra-high PVCR value of 10^{16} at room temperature, while the vertical tunnel diode exhibits a conventional N-type NDR effect with a smaller PVCR value of about 10^4. The proposed concept provides a semiconductor-free solution for NDR devices to achieve desired I-V characteristics.

[1] Ersoy Şaşıoğlu and Ingrid Mertig, arXiv:2207.02593 (2022).

HL 34.2 Thu 9:45 POT 81

Electrical contact engineering on 2D material through ion implantation and flash lamp annealing — •kaiman lin[1,2], yi li[2], manfred helm[2], shengqiang zhou[2], yaping dan[1], and slawomir prucnal[2] — [1]University of Michigan-Shanghai Jiao Tong University Joint Institute, Shanghai Jiao Tong University, 20024 Shanghai, P. R. China — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

In recent years, 2D material-based nanodevices have been extensively studied and exhibit highly competitive performance compared with conventional bulk semiconductors. Before they can be fully integrated with existing Si-based technology or offer new platform for novel nanoelectronics, some challenges must be solved. One of the key challenges in 2D devices is the large Schottky barrier at the 2D/metal interface, which limits the charge carrier injection from metal to 2D channel. In

this paper, we propose a novel method, which exploits the top metal electrode as the capping layer during the ion implantation process, followed by ms-range flash lamp annealing to repair the defects caused by ion implantation and to activate dopants. Our approach allows to realize effective doping at the interface between multilayer 2D materials and metal electrodes and simultaneously minimize the defect concentration created during the ion implantation process. As a result, the ohmic contact between 2D material and metal electrodes will be realized.

HL 34.3 Thu 10:00 POT 81

Impact of free carriers on exciton and trion diffusion in monolayer WSe2 — •Marzia Cuccu[1], Koloman Wagner[1], Zakhar A. Iakovlev[2], Jonas D. Ziegler[1], Takashi Taniguchi[3], Kenji Watanabe[3], Mikhail M. Glazov[2], and Alexey Chernikov[1] — [1]TU Dresden, Dresden, Germany — [2]St. Petersburg, Russia — [3]National Institute for Materials Science, Tsukuba, Japan

In monolayer transition metal dichalcogenides excitons are tightly bound, mobile at room and cryogenic temperatures, and interact strongly with free charge carriers. However, the role of the exciton-electron interaction in the context of exciton propagation remains unclear. Here, we address this question by demonstrating diffusion of excitons in hBN-encapsulated WSe2 in the presence of a continuously tunable Fermi sea. Using ultrafast microscopy, we reveal a non-monotonic dependence of the exciton diffusion coefficient on the charge carrier density in both electron- and hole-doped regimes. We identify distinct regimes of elastic scattering and quasiparticle formation determining exciton diffusion and highlight the importance of treating exciton-electron scattering in the presence of additional energy and momentum dissipation via phonons. We further show that trions remain mobile even at low temperatures down to 5 K, with an effective trion mobility up to 3000 cm2/(Vs).

HL 34.4 Thu 10:15 POT 81

Electrical Characterization of Thin $ZrSe_3$ 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

Two dimensional materials have been of great interest in the past years, because of their huge potential for new applications [1]. While graphene has been extensively researched, a lot of other materials have emerged. One of the most notable groups are the transition metal chalcogenides because of their variety of different compounds. Among these the lesser known transition metal trichalcogenides show unique properties [2].

Here, we have researched the transition metal trichalcogenide $ZrSe_3$ [3]. Its bulk material was produced by a chemical vapor transport method and was then exfoliated to obtain thin films. Electrical measurements show a band gap of 0.6 eV which increases for thinner samples. The material is shown to be an n-type semiconductor by transistor measurements and a mean free path of about 103 nm was determined by looking at different samples with varying thicknesses.

[1] A. K. Geim, I. V. Grigorieva, Nature, 499, 419-425 (2013).
[2] J. O. Island et al., 2D Materials, 4, 0220033 (2017).
[3] L. Thole et al., ACS Omega, 7, 39913 (2022).

HL 34.5 Thu 10:30 POT 81

Electrically active deep defects in 2D vdW semiconductors — •Michele Bissolo[1], Rongxin Li[1], Masako Ogura[2], Svitlana Polesya[2], Hubert Ebert[2], Eugenio Zallo[1], Gregor Koblmüller[1], and Jonathan J. Finley[1] — [1]Walter Schottky Institute and TUM School of Natural Sciences, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany — [2]Department of Chemistry/Phys. Chemistry, LMU Munich, Butenandtstrasse 11, 81377 Munich, Germany

Mid-gap defect states in semiconductors can both potentially degrade the performance of (opto)electronic devices and simultaneously act as a platform for technologies such as (photo)catalysis and quantum computing. Characterizing the electrically active mid-gap defects in the emerging class of 2D van-der-Waals materials is thus a necessary step in the development of future 2D-based devices. Here, we employ Deep Level Transient Spectroscopy (DLTS) techniques to directly probe deep defects in transition metal dichalcogenides (TMDCs) and group-III monochalcogenides (III-MCs), which have recently gained traction in "more-than-Moore", low-power and renewable energy device applications. Unlike transmission electron or scanning tunneling microscopies, DLTS is both a non-destructive and bulk sensitive technique that provides multiple information on the electronically active defect states, such as concentration, energy and capture cross section. DLTS spectra are collected from few-layer MoS_2, $MoSe_2$ and GaSe Schottky diodes in the 10-300 K temperature range with 10 mK stability, and the properties and role of the observed defects are discussed.

15 min. break

HL 34.6 Thu 11:00 POT 81

Ionic based gate control of insulator-to-metal phase transitions on ZrS_2 — •Jose Guimaraes[1,2], Dorsa Fartab[1], Marcus Schmidt[1], and Haijing Zhang[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]School of Physics and Astronomy, University of St Andrews, St Andrews KY16 9SS, UK

The possibility of tuning the properties of solids, such as their carrier density, allows for the amplification of their potential: In the context of 2D materials, ionic liquid gating provides a highly efficient doping alternative to traditional chemical doping.

Transitional metal dichalcogenides (TMDCs) have emerged as a potential 2D replacement for silicon in many technological applications, however their carrier mobility needs to be vastly increased. Ionic liquid gating enables carrier concentrations of the order of 10^{14} carriers per cm^2 in certain TMDCs, moreover, it allows for the emergence of unique physical phenomena, such as ambipolar behaviour. To realize transistor applications, materials that can be easily switched between p-type and n-type by applying an electric field are essential to minimize circuit size.

Here, an overview of the ionic liquid gating technique is given, including device fabrication and characterization methods, focusing on the TMDCs: ZrS_2 and $ZrSe_2$. Being $ZrSe_2$ an oxygen sensitive material, a method of estimating its thickness by its optical image is discussed. Furthermore, experimental efforts reporting ambipolar behaviour in ZrS_2 for the first time are presented.

HL 34.7 Thu 11:15 POT 81

Lattice reconstruction in twisted transition metal dichalcogenide heterobilayers — •Wei Li, Thomas Brumme, and Thomas Heine — TU Dresden, Dresden, Germany

Twisted heterostructures of 2D crystals have resulted in a series of high-impact contributions to condensed matter physics, most prominently flat bands and superconductivity in twisted bilayer graphene. But also two-dimensional crystals beyond graphene, such as transition metal dichalcogenides, show strong proximity effects that are affected by twisting. Here, we systematically investigate the structural impact of twist angles on transition metal dichalcogenide van der Waals heterobilayers consisting of MoS_2, WS_2, $MoSe_2$ and WSe_2 monolayers. We find that the significant lattice reconstruction involving in- and out-of-plane displacements strongly depends on the twist angle: from a continuous variation of local stacking alignment at large twist angles to a soliton-domain structure at small twist angles. Especially, starting from either 2H or 3R stacking, two different critical twist angles exist, above which the two constituting layers show dramatically asymmetrical corrugation, in contrast to the symmetry-preserving out-of-plane deformation in twisted homobilayers. We reveal that the development of either the corrugation or the soliton-domain results from the competition between strain energy cost and van der Waals energy gain. Our calculations show that van der Waals heterobilayers develop, besides the well-investigated moiré structures, also systems with large areas of special local stackings arranged in a superlattice, suggesting intriguing electronic properties of these systems.

HL 34.8 Thu 11:30 POT 81

Pump Probe Signatures of Interlayer Excitons in TMDC Heterostructures — •Henry Mittenzwey[1], Manuel Katzer[1], Benjamin Kaiser[2], Veronica Policht[3], Oleg Dogadov[3], Stefano Dal Conte[3], Giulio Cerullo[3], Andreas Knorr[1], and Malte Selig[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Zuse Institute Berlin, Takustraße 7, 14195 Berlin, Germany — [3]Dipartimento di Fisica, Politecnico di Milano, I-20133 Milano, Italy

TMDC heterobilayers are promising candidates for novel optoelectronic applications, since they exhibit long-lived excitonic states with spatially separated electrons and holes located in different layers. The

relaxation dynamics of these interlayer excitons and their interplay with intralayer excitons are still under investigation.

Here, we present a microscopic description for the phonon and tunneling induced formation and relaxation of intra- and interlayer excitons in a $MoSe_2/WSe_2$ stack. Based on the microscopic dynamics we calculate the pump probe signal for intra- and interlayer transition and their population dynamics including hot exciton bottleneck effects and unbound interlayer occupations.

HL 34.9 Thu 11:45 POT 81

Microscopic picture of interlayer exciton-phonon coupling — Muralidhar Nalabothula, Ludger Wirtz, and •Sven Reichardt — University of Luxembourg, Luxembourg

Excitons play a key role for opto-electronic applications of 2D heterostructures. They also can strongly couple to phonons as evidenced by their imprint on resonant Raman scattering intensities [1,2]. In 2D heterostructures, this sort of strong coupling and its signature Raman scattering offers an ideal setting to learn about exciton-phonon coupling both within and across material layers. Here we focus on the example of monolayer WSe2 and hBN. Its Raman spectrum features the norminally silent out-of-plane optical phonon mode of hBN that becomes active due to symmetry breaking and - most curiously - very strongly enhanced due to resonant exciton-phonon scattering [1]. While the resonant scattering pathways have been identified as involving excitons in WSe2 that couple to the phonons in hBN [1], a microscopic understanding of this interlayer exciton-phonon coupling is still missing. We provide such understanding using the state-of-the-art method for the computation for resonant Raman scattering intensities [2,3], which allows a detailed atomistic and quantum mechanical dissection of the Raman scattering process. Supplemented by a classical picture, our work sheds light on the microscopic mechanism behind exciton-phonon coupling in 2D heterostructures.

[1] C. Jin, et al. Nat. Phys., 13, 127-131, (2017).
[2] S. Reichardt and L. Wirtz. Sci. Adv. 6, eabb5915, (2020).
[3] S. Reichardt and L. Wirtz. Phys. Rev. B 99, 174312, (2019).

HL 35: Focus Session: Transient multi-wave mixing on excitonic resonances

Coherent nonlinear optical spectroscopy and, in particular, transient multi-wave mixing processes provide valuable information for basic research in material science and applications in photonics and quantum technology. It allows one to obtain detailed information about the energy structure and dynamic evolution of quantum systems including excited states which is not possible via linear optical spectroscopy and gives direct access to higher-order correlations among the elementary optical excitations. In addition, multi-wave mixing processes can be used as a powerful tool to coherently control the electronic states of the system and to generate non-classical states of light, which is appealing for the implementation in quantum information devices. Importantly for these studies is that excitons possess high oscillator strength which leads to a significant increase of higher-order mixing under resonant excitation with ultrashort optical pulses. This session will focus on multi-wave mixing processes as a unique tool to uncover the fascinating physics of excitons and many-body correlations in emerging materials such as transition metal dichalcogenides and perovskites and establish novel approaches for the coherent control of excitonic quantum systems with classical and quantum light.

Organized by I.A. Akimov and T. Meier

Time: Thursday 9:30–13:30 Location: POT 361

Invited Talk HL 35.1 Thu 9:30 POT 361

Quantum Dynamics of Polarons in Doped Semiconductor Monolayers — •Xiaoqin Elaine Li[1] and Di Huang[2] — [1]Physics Department, University of Texas at Austin, Austin, TX, U.S.A. — [2]Physic Department, TongJi University, Shanghai, China

When mobile impurities are introduced and coupled to a Fermi sea, new quasiparticles known as Fermi polarons are formed. We study Fermi polarons in two dimensional systems, where many questions and debates regarding their nature persist. The model systems we investigate are doped MoSe2 and WSe2 monolayers. In MoSe2, we find the observed attractive and repulsive polaron energy splitting and the quantum dynamics of attractive polarons agree with the predictions of a simple theory. As the doping density increases, the quantum dephasing of the attractive polarons remains constant, indicative of stable quasiparticles, while the repulsive polaron dephasing rate increases nearly quadratically. In WSe2, two distinct species of attractive polarons exist, singlet and triplet polarons. The singlet (triplet) dynamics are mediated by the Fermi seas in the same (opposite) valley. A long-lived valley polarization component is found and likely related to a reservoir of dark states.

Invited Talk HL 35.2 Thu 10:00 POT 361

Impact of phonons on time-resolved optical signals from excitons — •Doris E. Reiter — Condensed Matter Theory, TU Dortmund, 44221 Dortmund

A major difference between optical manipulation of atoms and excitons in semiconductors is the interaction of the latter with the vibrational modes of the solid, i.e., the phonons. In particular in nanostructures like quantum dots, the interaction with acoustic phonons is non-monotonous as function of energy, yielding interesting phenomena like phonon sidebands, reappearance of Rabi rotations or phonon-assisted state preparation. When a quantum dot is optically driven exhibiting Rabi oscillations of the exciton, the pure dephasing-type electron-phonon interaction results in polaron formation accompanied by the emission of phonon wave packets. While for the occupation, the phonon influence leads to an exponential damping, optical multi-wave mixing experiments are more sensitive to the quantum dot polarization. Here, the phonons cannot be described by a simple damping, but their interaction can be understood as a relaxation into the lower dressed state. In this talk, we use a simple model of phonons [1] to discuss their impact on time-resolved optical signals in semiconductor quantum dots. We consider the impact of phonon on continuous wave excitation in a pump-probe configuration [1] and on optical photon echo signals, where the model is in excellent agreement with experiments [2]. Ref: [1] Ann. Phys. 533, 2100086 (2021) [2] PRB 106, 205408 (2022).

Invited Talk HL 35.3 Thu 10:30 POT 361

Hot-Exciton Quantum Dynamics in Zero-Dimensional Structures — •Alfred Leitenstorfer — Department of Physics and Center for Applied Photonics, University of Konstanz, Germany

Electronic quantum processes in intrinsic dimensions of time and space are investigated with femtosecond transient transmission spectroscopy of individual II-VI quantum dots. With our experiments, we are aiming at single-photon amplification for the ultimate control of the quantum statistics of ultrashort light pulses [1]. In these systems, the elementary dynamics of charges and spins is dominated by fundamental aspects such as Coulomb correlations and the Pauli principle [2]. Harnessing a pump-probe microscope optimized for single-electron sensitivity at cryogenic temperatures and high magnetic fields [3], we find extremely asymmetric relaxation characteristics in valence and conduction bands where e.g. femtosecond quantum kinetics of hole-phonon coupling is compatible with persistent spin coherence of hot excitons [4].

[1] F. Sotier et al., Nature Phys. 5, 352 (2009)
[2] C. Hinz et al., Phys. Rev. B97, 045302 (2018)
[3] C. Traum et al., Rev. Sci. Instr. 90, 123003 (2019)

[4] P. Henzler et al., Phys. Rev. Lett. 126, 067402 (2021)

HL 35.4 Thu 11:00 POT 361

Multi-wave mixing applied to explore and control the coherent dynamics of ensembles of semiconductor quantum dots — •Hendrik Rose[1], Stefan Grisard[2], Artur V. Trifonov[2], Rilana Reichhardt[2], Doris E. Reiter[3], Matthias Reichelt[1], Christian Schneider[4,5], Martin Kamp[4], Sven Höfling[4], Manfred Bayer[2], Ilya A. Akimov[2], and Torsten Meier[1] — [1]Paderborn University, Department of Physics & Institute for Photonic Quantum Systems (PhoQS), 33098 Paderborn, Germany — [2]Experimentelle Physik 2, Technische Universität Dortmund, 44221 Dortmund, Germany — [3]Condensed Matter Theory, Technische Universität Dortmund, 44221 Dortmund, Germany — [4]Technische Physik, Universität Würzburg, 97074 Würzburg, Germany — [5]Institute of Physics, University of Oldenburg, 26129 Oldenburg, Germany

Multi-wave mixing provides various possibilities to investigate the ultrafast dynamics of semiconductors. Here, we focus on ensembles of quantum dots where the nonlinear dynamics leads to emission in the form of photon echoes. We show that photon echoes can be temporally controlled by the application of multi-wave mixing [1] and furthermore demonstrate that a damping mechanism based on the spatial shape of the applied laser pulses can be circumvented by pulse shaping [2].

[1] A. N. Kosarev, H. Rose, et al., Commun. Phys. **3**, 228 (2020).
[2] S. Grisard, H. Rose, et al., Phys. Rev. B **106**, 205408 (2022).

HL 35.5 Thu 11:15 POT 361

Four-wave mixing at excitonic resonances in the telecom spectral range — •Sebastian Klimmer[1], Artem Sinelnik[1,2], Muhammad Hussain[1], Isabelle Staude[1,2], Habib Rostami[3], and Giancarlo Soavi[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Germany — [2]Institute of Applied Physics, Friedrich Schiller University Jena, Germany — [3]Nordita, KTH Royal Institute of Technology and Stockholm University, Sweden

Over the last few decades, nonlinear optical (NLO) processes have become a pillar for novel photonic devices. In particular, four-wave mixing (FWM) effects can be used to generate quantum optical states of light, such as entangled photons. Transition metal dichalcogenides (TMDs) offer significant advantages compared to conventional nonlinear materials, as their strong light-matter interaction and ease of integration into existing photonic platforms[1] make them perfect for enhancing the performance of integrated NLO devices. In addition, their atomic thickness softens phase matching limits, providing a virtually unlimited bandwidth for FWM[2]. This could be exploited to entangle photons from various spectral regions, making them an ideal source for quantum imaging applications[3]. In this work, we study broadband and exciton enhanced FWM in the telecom spectral range in MoS_2, highlighting the capability of TMDs for integrated photonics and communication applications.

[1] He, J. *et al.*, Nano Lett. **21**, 7, 2709-2718 (2021)
[2] Trovatello, C. *et al.*, Nat. Photonics. **15**, 6-10 (2021)
[3] Gilaberte Basset, M. *et al.*, Laser Photonics Rev. **13**, 10 (2019)

30 min. break

Invited Talk HL 35.6 Thu 12:00 POT 361

Ultrafast dynamics and wave mixing at excitonic resonances in atomically thin semiconductors — •Andreas Knorr, Dominik Christiansen, Florian Katsch, Manuel Katzer, and Malte Selig — Technische Universität Berlin

Atomically thin semiconductors constitute an ideal playground for exciton physics in two dimensions. This involves optically accessible (bright) as well as spin- or momentum-forbidden (dark) excitonic states including intravalley and intervalley excitations. The nonlinear, coherent exciton and wave mixing dynamics induced by short light pulses result from the interplay of strong intrinsic exciton-exciton and exciton-phonon interactions and can be described in a many body Heisenberg equation of motion formalism. Here, we present applications of the theory to:

-exciton-exciton scattering and biexcitons in wave mixing,
-exciton wave function dynamics in time resolved ARPES,
-control of nonlinear excitonic Rabi-oscillations, and
-limits of the boson description of excitons.

Invited Talk HL 35.7 Thu 12:30 POT 361

Spontaneous parametric down-conversion in semiconductor metasurfaces — •Maria Chekhova — Max-Planck Institute for the Science of Light, Erlangen, Germany — Friedrich-Alexander Universität Erlangen-Nürnberg

Spontaneous parametric down-conversion (SPDC) is the most efficient way to generate pairs of entangled photons for quantum photonics applications such as quantum communication, quantum imaging and sensing, and quantum metrology. Today, several groups are trying to implement SPDC on nanoscale quasi-2D platforms, such as subwavelength crystalline layers and metasurfaces. These ultrathin sources have numerous advantages. They are integrable, ultrafast, ultrabroadband and, most importantly, multifunctional. Metasurfaces, in addition, can enhance the rate of photon pair generation due to their *geometric* resonances.

In my talk I will show our recent results on the generation of photon pairs in metasurfaces made of gallium arsenide and gallium phosphide. The metasurfaces are structured to support bound states in the continuum (also known as Fano) resonances, with the quality factors Q reaching several hundred. The resonances enhance the spontaneous emission of pairs by a factor on the order of Q if the frequency of one of the photons coincides with the resonance. Due to the ultrasmall thickness of such sources, SPDC can be pumped slightly above their bandgap without considerable effect of absorption. The inevitably high level of photoluminescence can be overcome by time-resolved registration of photon pairs.

HL 35.8 Thu 13:00 POT 361

Time-resolved four-wave mixing spectroscopy of excitons in a $FA_{0.9}Cs_{0.1}PbI_{2.8}Br_{0.2}$ perovskite crystal — •Stefan Grisard[1], Artur V. Trifonov[1], Dmitry N. Dirin[2,3], Maksym V. Kovalenko[2,3], Ilya A. Akimov[1], Dmitri R. Yakovlev[1], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund — [2]Institute of Inorganic Chemistry, Department of Chemistry and Applied Bioscience, ETH Zürich — [3]Laboratory for Thin Films and Photovoltaics, Empa-Swiss Federal Laboratories for Materials Science and Technology

Formamidinium lead triiodide ($FAPbI_3$) shows outstanding characteristics for future photovoltaic or light emitting devices, suffers however from poor phase stability. Additives such as cesium and bromine help to improve the phase stability, but possibly increase the localization of the charge carriers. In this work, we present time resolved four-wave mixing spectroscopy as a versatile tool to investigate the coherent optical properties of a $FA_{0.9}Cs_{0.1}PbI_{2.8}Br_{0.2}$ crystal. At low temperatures of 1.5K, the coherent optical response is represented by photon echoes due to the strong inhomogeneous broadening of exciton resonances. We find that the coherence time T_2 is surprisingly long (≈100ps), comparable with the lifetime T_1. The spectral dependence of T_2 and T_1 indicate the importance of carrier localization.

HL 35.9 Thu 13:15 POT 361

Multi-photon pump probe of magnetic-field-induced quantum beats in Cu_2O — •Nikita V. Siverin, Andreas Farenbruch, Dietmar Fröhlich, Dmitri R. Yakovlev und Manfred Bayer — TU Dortmund, Dortmund, Germany

Multi-photon processes such as second harmonic generation are suitable for the investigation of exciton symmetries by analyzing the linear polarization angles of the incoming and the outgoing light. We use difference frequency generation (DFG) with two-photon as the optical technique. The initial laser pulse excites an exciton population by a two-photon excitation process. Probe pulse stimulates a DFG photon. Delaying the second pulse in time enables us the measurement of exciton coherence times and quantum beats between several states. There is also an additional degree of freedom compared to the SHG technique in the polarization of the emission channel. We measure the coherence time of yellow series in Cu_2O. By applying a magnetic field up to 10T in Voigt geometry the $1S$ orthoexciton splits into three states denoted by the quantum number M = -1,0,1. We observe a beating between these three states. By a selection of the linear polarization setting in the emission channel one can deliberately choose to detect single-frequency beats between the M=+1 and M=-1, triple-frequency beats between all three states or only the M=0 state without beats. Beat frequencies scale with magnetic field strength.

HL 36: Transport properties

Time: Thursday 9:30–11:45 Location: POT 151

HL 36.1 Thu 9:30 POT 151

Charge carrier mobilities in 2D covalent organic frameworks — •Elif Unsal[1], Alexander Croy[2], Alessandro Pecchia[3], Arezoo Dianat[1], Rafael Gutierrez[1], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Nanotechnology, TU Dresden, Dresden, Germany. — [2]Institute of Physical Chemistry, FSU Jena, Germany. — [3]CNR-ISMN, Rome, Italy

2D COFs are functional porous crystalline structures, which have high chemical and thermal stabilities. Having tunable chemistry and structures are their major properties which make 2D COFs attractive for wide range of applications, such as electro-catalysis, gas storage, and optoelectronic applications[Xiao Feng, 2012, Chem. Soc. Rev.]. Despite the intensive studies on 2D COFs, charge transport properties of most of these materials are still unknown. Here, we present a new approach based on DFTB calculations of the phonon-limited mobility in 2D COFs. We are modelling charge transport properties by combining state-of-the-art electron-phonon coupling calculations and semiclassical Boltzmann transport theory. We are using our own code DFTBephy whose implementation is based on DFTB+ [Marcus Elstner et al. 1998, Phys. Rev. B: Condens. Matter Mater. Phys.; Marcus Elstner, 2007, J. Phys. Chem. A] and phonopy [Atsushi Togo, 2015, Scr. Mater.] and it interfaces with BoltzTrap2 [Georg K. H. Madsen, 2018, Comput. Phys. Commun.] to calculate transport properties. Our results are benchmarked against state-of-the-art EPW [Samuel Ponce, 2016, Comput. Phys. Comm.] calculations.

HL 36.2 Thu 9:45 POT 151

Active Dopant Sites in Hyperdoped Si and Ge Investigated by Photoemission — •Moritz Hoesch[1], Mao Wang[2], Slawomir Prucnal[2], Shengqiang Zhou[2], Olena Fedchenko[3], Christoph Schlüter[1], Katya Medjanik[3], Sergey Babenkov[3], Anca Ciobanu[1], Dmitrii Potorochin[1,4], Sanjoy Mahatha[1,5], Markus Scholz[1], Quynh Nguyen[6], Aimo Winkelmann[7], H.-J. Elmers[3], and Gerd Schönhense[3] — [1]DESY Photon Science, Hamburg, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [3]JGU, Institut für Physik, Mainz, Germany — [4]TU Bergakademie Freiberg, Germany — [5]UGC-DAE, Indore, India — [6]SLAC, Menlo Park, USA — [7]AGH University of Kraków, Poland

Hyperdoping of silicon and germanium, with dopant concentration well above the thermal solubility limit, is achieved by ion implantation followed by pulsed laser or flash lamp annealing. Here, we probe the materials by photoemission spectroscopy thus revealing the metallic carriers in the valence region as well as core level shifts of the dopant species. The samples are p-doped Ge:Ga and n-doped Si:Te, both well into the metallic regime. The latter shows non-saturating growth of the free carrier concentration with increasing doping [1]. We present experimental determinations of the Fermi surfaces of these materials by soft x-ray ARPES as well as geometrical structure measurements by photoelectron diffraction [2,3].

[1] M. Wang et al. Phys. Rev. Appl. 11 054039 (2019). [2] O. Fedchenko et al NJP 21, 113031 (2019); [3] O. Fedchenko et al NJP 22, 103002 (2020).

HL 36.3 Thu 10:00 POT 151

Rapid Electronic Transport Predictions via the Kubo-Greenwood Formalism — •Florian Fiebig, Matthias Scheffler, and Christian Carbogno — The NOMAD Laboratory at the FHI of the Max-Planck-Gesellschaft and IRIS-Adlershof of the Humboldt-Universität zu Berlin

For the first-principles evaluation of electronic heat and charge transport coefficients, the Kubo-Greenwood (KG) formalism [1] represents a more general and accurate alternative to perturbative approaches, [2] since it naturally incorporates all orders of anharmonic and vibronic effects. In practice, however, KG calculations come with a prohibitive computational cost, since ordered crystalline materials typically require both dense reciprocal-space **k**-grids for the electronic degrees of freedom and large real-space supercells for the vibrational ones. In this work, we propose an adaptive, KG-specific scheme for the **k**-space sampling that alleviates this issue. It enables the use of very coarse **k**-grids during the self-concistency cycle, whereas very dense **k**-grids are used for the evaluation of the KG formula, but only for those Brillouin-zone regions that contribute to the conductivities. As demonstrated for Silicon, this massively reduces the involved computational cost, and hence paves the way towards affordable, fully anharmonic predictions of electronic heat and charge transport coefficients.

[1] B. Holst, M. French, and R. Redmer, *Phys. Rev. B* **83**, 235120 (2011).
[2] S. Poncé, E. R. Margine, and F. Giustino, *Phys. Rev. B* **97**, 121201 (2018).

HL 36.4 Thu 10:15 POT 151

Semiconductor to Semimetall Transition in Bi-based Core-Shell Nanowires — Maximilian Kockert[1], Rüdiger Mitdank[1], Mahni Müller[1], Hongjae Moon[2], Jongmin Kim[2], Wooyoung Lee[2], and •Saskia Fischer[1] — [1]Humboldt-Univ. zu Berlin, Germany — [2]Yonsei Univ., Seoul, Korea

The full-thermoelectric characterization of individual core/shell Bi-based nanowires is presented. Compressive strain induced by a TiO_2 shell can lead to a band opening increasing the absolute Seebeck coefficient by up to 30 percent compared to bulk at room temperature [1]. If the strain exceeds the elastic limit the semimetallic state is recovered due to the lattice relaxation. The influence of strain on the temperature dependence of the electrical conductivity, the absolute Seebeck coefficient and the thermal conductivity of bismuth/titanium dioxide (Bi/TiO_2) nanowires with different diameters was measured and compared to bismuth (Bi) and bismuth/tellurium (Bi/Te) nanowires and bismuth bulk. Different nano-contacting methods are discussed.

[1] M. Kockert, *et al.*, Nanoscale Advances **3** (2021) 263

30 min. break

HL 36.5 Thu 11:00 POT 151

Comprehensive model for the thermoelectric properties of two-dimensional carbon nanotube networks — •Aditya Dash, Dorothea Scheunemann, and Martijn Kemerink — Institute for Molecular Systems Engineering and Advanced Materials, Heidelberg University, Im Neuenheimer Feld 225, 69120 Heidelberg, Germany.

Networks of semiconducting single-walled carbon nanotubes (SWCNTs) are interesting thermoelectric materials due to the interplay between CNT and network properties. Here we present a unified model to explain the charge and energy transport in SWCNT networks. We used the steady-state master equation for the random resistor network containing both the intra- and inter-tube resistances, as defined through their 1D density of states that is modulated by static Gaussian disorder. The tube resistance dependence on the carrier density and disorder is described through the Landauer formalism. Electrical and thermoelectric properties of the network were obtained by solving Kirchhoffs laws through a modified nodal analysis, where we used the Boltzmann transport formalism to obtain the conductivity, Seebeck coefficient, and electronic contribution to the thermal conductivity. The model provides a consistent description of previously published experimental data for temperature and carrier density-dependent conductivities and Seebeck coefficients, with energetic disorder being the main factor explaining observed mobility upswing with carrier concentration. For lower disorder, the Lorentz factor obtained from simulation is in accordance with the Wiedemann-Franz law. Suppressed disorder and lattice thermal conductivity can be a key to higher zT.

HL 36.6 Thu 11:15 POT 151

Thermal mapping of a c-plane oriented GaN membrane — •Mahmoud Elhajhasan[1], Isabell Hüllen[1], Wilken Seemann[1], Jean-François Carlin[2], Ian Rousseau[2], Nicolas Grandjean[2], and Gordon Callsen[1] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]Institute of Solid State Physics, École Polytechnique Fédérale de Lausanne (EPFL), Switzerland

The thermal characterization of modern semiconductor membranes commonly employed for photonic devices like nanobeam lasers (1D) or photonic crystals (2D), often lacks spatial resolution and appropriate quantification of local temperatures. However exactly these two points are relevant for the detection of e.g., thermal anisotropies, heat leakage, and interfaces providing thermal resistance.

In this contribution, Raman thermometry employing one laser beam (1LRT) is used to quantify the thermal conductivity κ of 250-nm-thick, state-of-the-art, c-plane wurtzite GaN membranes. The same mem-

branes are then probed by two laser Raman thermometry (2LRT) to map the temperature distribution caused by a heating laser via a second probe laser. From such a map, κ is extracted for all in-plane crystal directions, yielding a thermal anisotropy in the c-plane of GaN. Comparing this direct, sub-μm spatially resolved imaging technique to classical Fourier simulations reveals a significant divergence at the heating laser spot pointing to non-diffusive phonon transport.

In conclusion, our comparison of 1LRT and 2LRT measurements provides insight into the applicability of each technique to determine the thermal conductivity of photonic membranes.

HL 36.7 Thu 11:30 POT 151

Tunable preferable orientation of α-FeSi2 crystallites on silicon surfaces — •Tatiana Smoliarova, Ivan Tarasov, and Ulf Wiedwald — Faculty of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, 47057, Duisburg, Germany

Nowadays, one of the most important applications of silicon (Si) and Si-based functional materials is microelectronics. Silicon forms compounds in the form of solid solutions or intermetallic compounds * silicides. Metallic α-FeSi2 phase can be used as a contact material to silicon or to the semiconducting β FeSi2 phase with good ohmic characteristics.

In this work, we discuss the growth of α-FeSi2 submicron-size crystallites on gold-activated and gold-free p-Si(001), p-Si(110) and p-Si(111) surfaces via molecular beam and reactive epitaxy. The study reveals that the surfactant-assisted mediated epitaxy regulates morphology and the preferable orientation relationship (OR) of the crystallites to Si. According to the X-ray diffraction, strongly preferable ORs are α-FeSi2(001)//Si(001), α-FeSi2(001)//Si(111), α-FeSi2(001)//Si(110) for gold-activated and α-FeSi2(111)//Si(001), α-FeSi2(211)//Si(110), α-FeSi2(112)//Si(111) for gold-free Si substrates. Thus, the orientation control of fabricated α-FeSi2 crystallites can be used for tuning electron transport across the metal/semiconductor interface.

We acknowledge Ivan Yakovlev and Ivan Nemtcev (Krasnoyarsk, Russia) for assistance in sample preparation.

HL 37: Materials and devices for quantum technology II

Time: Thursday 9:30–12:15 Location: POT 251

HL 37.1 Thu 9:30 POT 251

Long-range shuttling of single electron by Si/SiGe conveyor — •Ran Xue[1], Max Beer[1], Jhih-Sian Tu[2], Simon Humpohl[1], Inga Seidler[1], Tom Struck[1], Tobias Hangleiter[1], Hendrik Bluhm[1], and Lars. R Schreiber[1] — [1]JARA-FIT Institute for Quantum Information, Forschungszentrum Jülich GmbH and RWTH Aachen University, Aachen, Germany — [2]Helmholtz Nano Facility (HNF), Forschungszentrum Jülich, Jülich, Germany

Electrostatically confined electrons are promising candidates for spin-qubits due to their long coherence in ^{28}Si/SiGe. To scale up qubit numbers and integrate control electronics, we propose to use a 10 μm long quantum bus (QuBus), which requires four control lines independent of the shuttle distance. Providing a propagating sinusoidal potential in a gate-defined 1D channel, adiabatic movement of a quantum dot filled by a single electron representing the qubit has achieved a shuttling fidelity of $99.4 \pm 0.02\%$ in a 420 nm long QuBus [1]. Here, we propose and demonstrate the tomography of a single electron shuttling process on a scaled-up 10 μm long QuBus. The electron is shuttled forth and back over micrometer-scale by a time-reversible pulse composed by only four sine-waves. Our tomography measures the shuttling fidelity and detects shuttling failures such as electron tunneling across pockets of the sinusoidal shuttling potential due to local potential disorder [2].

[1] Seidler, I. *et al.*, npj Quantum Inf. 8: 100 (2022).
[2] Langrock, V. *et al.*, arXiv: 2202.11793 (2022).

Work funded by the DFG under project number EXC 2004/1-390534769.

HL 37.2 Thu 9:45 POT 251

Telecom C-band photon emission from (In,Ga)As quantum dots generated by filling nanoholes in In0.52Al0.48As layers — •Dennis Deutsch, Christopher Henrik Buchholz, Klaus Jöns, and Dirk Reuter — Universität Paderborn, Warburger Str. 100, 33098 Paderborn

Quantum communication technology requires sources for the on-demand generation of entangled photon pairs, preferably in the optical C-band for long-haul fiber-based communication. Quantum dots grown on InP substrates seem to be an ideal candidate: Here photon pairs can be generated from the biexciton-exciton cascade with emission wavelengths around 1.55 μm. However, the conventional approach of Stranski-Krastanov grown InAs quantum dots leads to several challenges related to the strain driven growth. In this study we report on an alternative approach allowing for unstrained quantum dots by filling of local droplet etched (LDE) nanoholes. The quantum dots are embedded in an $In_{0.52}Al_{0.48}As$ matrix lattice-matched to the InP substrate and grown by molecular beam epitaxy. We show detailed investigations of the hole morphology measured by atomic force microscopy. Statistical analysis of nanoholes shows promising symmetry for a good number of them when etched at optimized temperatures. Furthermore, we see that filling of the holes with $In_{0.53}Ga_{0.48}As$ works under the right growth conditions. By capping the filled holes and performing photoluminescence measurements we observe emission in the O-band up into the C-band depending on the filling height of the nanoholes.

HL 37.3 Thu 10:00 POT 251

Scalable Quantum Memory Nodes using nuclear spins in Silicon Carbide — •Shravan Kumar Parthasarathy[1,2], Birgit Kallinger[1], Florian Kaiser[3,4], Patrick Berwian[1], Durga Dasari[3,4], Jochen Friedrich[1], and Roland Nagy[2] — [1]Fraunhofer Institute for Integrated Systems and Device Technology (IISB), Erlangen, Germany — [2]Chair of Electron Devices, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen, Germany — [3]3rd Institute of Physics and Stuttgart Research Center of Photonic Engineering (SCoPE), University of Stuttgart,70569 Stuttgart, Germany — [4]Center for Integrated Quantum Science and Technology (IQST), Germany

The ultimate motivation of my project is to address the possibility of building a quantum analogue of Internet of Things in order to improve the standards of quantum information processing. A distributed quantum computing network which is capable of achieving this goal, would require large sets of memory nodes. The challenge in this field has been in realizing such memory nodes with features for scalable quantum computing. Solid state spins in 4H-Silicon Carbide (4H-SiC) provides a suitable platform in achieving this goal wherein a controlled generation of highly coherent qubit registers using nuclear spins (^{13}C or ^{29}Si) and silicon vacancy color centers (V_Si^- center) are possible. A numerical model is hence established in order to investigate the influence of material or experimental parameters on number of such controllable nuclear spins. This study would be helpful in finding the optimal parameters to maximize qubits in Quantum Memory Nodes.

HL 37.4 Thu 10:15 POT 251

Coherent Conveyor Mode Shuttling of Electrons and their Spin — •Tobias Offermann, Tom Struck, Lino Visser, Mats Volmer, Ran Xue, Hendrik Bluhm, and Lars R. Schreiber — JARA-FIT Institute for Quantum Information, Forschungszentrum Jülich GmbH and RWTH Aachen University, Aachen, Germany

A missing key technology for scaling up electron spin qubits in ^{28}Si/SiGe is a coherent medium-range coupling between two qubits. It would enable a sparse-qubit architecture and makes space for signal-line fan-out and cryogenic electronics tiles integrated on the qubit chip. We present an approach named *conveyor-mode shuttling*, which relies on physically transporting the electron by a propagating wave-potential with simple input signals across an electrostatically defined quantum-channel [1,2]. We will introduce high fidelity single electron shuttling at a velocity high enough to reduce the shuttling time well below the typical spin-dephasing time of natural silicon. We show initialisation of the shuttle device on one end by two electrons in a spin-singlet. Shuttling only one of these electrons, we generate a separated Einstein-Podolsky-Rosen spin-pair. Combining the electrons by shuttling again, we detect their spin-singlet fraction by Pauli-spin blockade and explore the spin-coherence of the shuttling process.

[1] Seidler, I. *et al.*, npj Quantum Inf. 8: 100 (2022).

[2] Langrock, V. *et al.*, arXiv: 2202.11793 (2022).
Work funded by the DFG under project number EXC 2004/1-390534769.

HL 37.5 Thu 10:30 POT 251

Prospects for electrically controlled, directly fiber-coupled circular Bragg gratings as high performance quantum light sources — •Lucas Rickert[1], Fridtjof Betz[2], Matthias Plock[2], Sven Burger[2,3], and Tobias Heindel[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany — [2]Zuse Institute Berlin, Takustraße 7, 14195 Berlin, Germany — [3]JCMwave GmbH, Bolivarallee 22, 14050 Berlin, Germany

Semiconductor quantum dots in (hybrid) circular Bragg gratings (hCBGs) have shown seminal performances as bright sources of indistinguishable entangled photons at wavelengths below 900 nm and have also shown significant boosts in performances for telecom wavelength single photons sources. To fully harness their potential for photonic quantum technologies, a direct coupling to single mode fibers (SMFs) for robust quantum light sources as well as designs with gate-contacts allowing for electrical control of the embedded emitters charge environment and spectral Stark-tuning is desirable. In this contribution, we present hCBG-based designs enabling electrical control, which are numerically optimized to show >85% direct fiber coupling efficiencies to SMFs, and Purcell enhancements >20 at operation wavelengths for 930 nm, 1310 nm and 1550 nm respectively. We investigated extensively the impact on performance of deviations in the fabrication using machine-learning algorithms, and show our recent progress in the experimental realization of directly fiber-coupled hCBG single photon sources.

30 min. break

HL 37.6 Thu 11:15 POT 251

X-ray nanobeam measurements of nanoscale elastic strain in electron shuttling devices — •Cedric Corley-Wiciak[1], Marvin H. Zoellner[1], Ignatii Zaitsev[1], Costanza L. Manganelli[1], Edoardo Zatterin[2], Ketan Anand[1], Agnieszka A. Corley-Wiciak[1], Felix Reichmann[1], Yuji Yamamoto[1], Michele Virgilio[3], Lars Schreiber[4], Wolfram Langheinrich[5], Carsten Richter[6], and Giovanni Capellini[1,7] — [1]IHP, Frankfurt(Oder), Germany — [2]ESRF, Grenoble, France — [3]Department of Physics, Università di Pisa, Italy — [4]JARA Institute, RWTH Aachen University, Germany — [5]Infineon Technologies Dresden GmbH und Co.KG, Germany — [6]IKZ, Berlin, Germany — [7]Dipartimento di Scienze, Universita Roma Tre, Italy

Recently, spin qubits housed in electrostatic quantum dots in epitaxial Si/SiGe heterostructures have evolved by the demonstration of multi-qubit algorithms. One key requirement for realizing arrays of qubits with shared gate control is highly homogenous lattice strain in the Si quantum well (QW) hosting the qubits. We leverage Scanning Xray Diffraction Microscopy (SXDM), performed at the beamline ID01/ESRF, to map the strain tensor around several fully CMOS compatible electron shuttling devices for qubit interconnection (QuBus). We observe local modulations of the lattice strain by several 10^{-4}, which are translated into spatially resolved profiles for the energy of the conduction band valley state, showing local fluctuations > 1meV. Thus, our results demonstrate that material inhomogeneities must be considered in the design for scaled quantum processors.

HL 37.7 Thu 11:30 POT 251

Quantum optimal control for conveyor-mode single-electron shuttling in Si/SiGe — •Alessandro David[1], Veit Langrock[2], Julian D. Teske[3], Lars R. Schreiber[3], Hendrik Bluhm[3], Tommaso Calarco[1], and Felix Motzoi[1] — [1]Institute of Quantum Control (PGI-8), Forschungszentrum Jülich GmbH, Jülich, Germany — [2]Institute of Theoretical Nanoelectronics (PGI-2), JARA-FIT Institute for Quantum Information, Forschungszentrum Jülich GmbH, Jülich, Germany — [3]JARA-FIT Institute for Quantum Information, Forschungszentrum Jülich GmbH and RWTH Aachen University, Aachen, Germany

A quantum bus (QuBus) is a promising candidate for the scalability of spin-qubits quantum computers. We consider a gated Si/SiGe quantum well capable of shuttling electrons smoothly by a translating confining potential (conveyor-mode). Dephasing coupling with valley degree of freedom and geometry of the quantum well dictate a maximum shuttling speed to keep the electron state adiabatically in the ground state and avoid excitation of the valley state. In this work we use the position of the electron as a control parameter and we optimise the trajectory of the electron to show how the electron can be shuttled faster and with lower infidelity compared to the adiabatic regime.

HL 37.8 Thu 11:45 POT 251

Determination of optical dipole orientation of quantum emitters in monolayer MoS_2 — •Anna Herrmann, Katja Barthelmi, Lukas Sigl, Mirco Troue, Thomas Klokkers, Jonathan Finley, Christoph Kastl, and Alexander Holleitner — Walter Schottky Institut and Physics Department, Technische Universität München, Am Coulombwall 4a, Garching bei München, Germany

Single photon emitters in 2D materials are interesting for applications in quantum science and technology. Recently, we demonstrated that defect-based single photon emitters can be site-selectively generated in monolayer MoS_2 van der Waals heterostacks by a focused beam of helium ions with an overall positioning accuracy below 10 nm. The emitters show a luminescence with narrow emission lines around 1.75 eV. To determine the optical dipole orientation of the emitters we discuss the far-field photoluminescence intensity distribution of the defect emission in a back-focal plane geometry. The data is compared to simulations by an analytical model, which describes the dipolar emission pattern in the dielectric environment of the heterostructure. The demonstrated approach allows determining the relative contributions for in- and out-of-plane transition dipole moments of quantum emitters.

HL 37.9 Thu 12:00 POT 251

Interface control of valley splitting in Si-based heterostructures — •Jonas R F Lima[1,2] and Guido Burkard[1] — [1]Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — [2]Departamento de Física, Universidade Federal Rural de Pernambuco, 52171-900, Recife, PE, Brazil

The spin of electrons is a natural two-level system that works as an excellent qubit. The control of the spin of isolated electrons in silicon-based heterostructures is very promising for high performance and scalable qubits. To achieve this, it is very important to predict and control the valley splitting in this system, since a very fast qubit relaxation is obtained, for instance, when the valley splitting becomes equal to the qubit Zeeman splitting. For this reason, different works have investigated the valley splitting in silicon spin qubits, both experimentally and theoretically. In this work we used the effective mass theory, which enables us to obtain the electron envelope function, to predict the valley splitting of silicon-based heterostructures, where we consider fluctuations in the interfaces of the heterostructure. We obtain how the valley splitting can be tuned by the width of the interfaces and compare our results with results obtained by other methods.

HL 38: Functional semiconductors for renewable energy solutions I

Time: Thursday 9:30–11:45 Location: POT 6

HL 38.1 Thu 9:30 POT 6

Energy landscape of B–Si defects calculated by DFT for modelling light-induced degradation in silicon — •Aaron Flötotto[1], Wichard J.D. Beenken[1], Kevin Lauer[1,2], and Erich Runge[1] — [1]Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany — [2]CiS Forschungsinstitut für Mikrosensorik GmbH, Erfurt, Germany

Boron is a technologically highly relevant p-dopant of silicon. Often, boron does not simply replace a silicon atom, but forms a B-Si pair that shares one lattice site. Several metastable pair configurations exist, with boron being closer to either a more substitutional or a more interstitial position. Using DFT, we calculated all neutral and charged metastable configurations of these defects and – using the Nudged Elastic Band algorithm – the minimal-energy paths between them. The resulting energy minima, barrier heights, and conversion rates will be discussed within the A_{Si}–Si_i model for light-induced degradation (LiD) as suggested by K. Lauer et al. [1].

[1] for a recent review, see: K. Lauer, K. Peh, D. Schulze, T. Ortlepp, E. Runge, and S. Krischok, "The A_{Si}–Si_i Defect Model of Light-Induced Degradation (LID) in Silicon", phys. status solidi A 219, 2200099 (2022), https://doi.org/10.1002/pssa.202200099

HL 38.2 Thu 9:45 POT 6

Nanoscale characterization for understanding performance limitations in water splitting photoelectrodes — Lukas Wolz[1], Harishankar Balakrishnan[2], Guanda Zhou[1], Ian Sharp[1], Achim Hartschuh[2], and •Johanna Eichhorn[1] — [1]Walter Schottky Institute, TU München, Am Coulombwall 4, 85748 Garching, Germany — [2]Department of Chemistry, LMU München, Butenandtstr. 5-13, 81377 Munich, Germany

Economically viable systems for photoelectrochemical water splitting are often based of polycrystalline or nanostructured semiconductor thin films. Their nano- to micrometer properties often control critical processes, such as efficiency and stability, of the macroscale system.

Here, we aim at resolving local heterogeneities and at elucidating their effect on light-driven processes of BiVO4 thin films using a correlative nanoscale approach. Scanning nearfield infrared microscopy shows varying absorption from VO4 stretching modes across the film which correlates with local photoconductivity heterogeneities revealed by photoconductive atomic force microscopy. Furthermore, local temperature-dependent current-voltage spectroscopy in controlled gas environment shows that the low intrinsic bulk conductivity limits the electron transport [1], and that adsorbed oxygen acts as surface trap states for electrons [2]. Overall, combining insights from different nanoscale techniques generates a comprehensive picture of charge transport and transfer at the nanoscale, which provides the foundation for the rational design of durable and efficient solar fuel devices.

[1] Nat. Commun. 2597 (2018) [2] ACS Interfaces, 10, 35129 (2018)

HL 38.3 Thu 10:00 POT 6

Calibration of low temperature photoluminescence of boron doped silicon with increased temperature precision — •Katharina Peh[1], Aaron Flötotto[1], Kevin Lauer[1,2], Dirk Schulze[1], and Stefan Krischok[1] — [1]TU Ilmenau, Institut für Physik und Institut für Mikro- und Nanotechnologien, 98693 Ilmenau, Germany — [2]CiS Forschungsinstitut für Mikrosensorik GmbH, Konrad-Zuse-Str. 14, 99099 Erfurt, Germany

Low-temperature photoluminescence spectroscopy (LTPL) enables the determination of the dopant concentration of shallow impurities in silicon. We present a method which allows the determination of the boron concentration in silicon in a range from $10^{11}cm^{-3}$ to $10^{17}cm^{-3}$ at temperatures from 4.2 to 20 K with increased temperature accuracy. This method requires only one calibration function for the photoluminescence intensity ratio $I_{B_{TO(BE)}}/I_{I_{TO(FE)}}$. We obtain the measurement temperature from the intrinsic silicon photoluminescence line of free excitons ($I_{TO(FE)}$) using a fitting method, which distinguish the TO and LO components of the free exciton peak. The determined calibration function is
$I_{B_{TO(BE)}}/I_{I_{TO(FE)}} = (5.8 \pm 0.08) \cdot 10^{-18} cm^3 \cdot c_{boron} \cdot e^{(56.7 \pm 0.7K)/T}$.
The obtained exciton binding energy to boron, $E_b = 4.9 \pm 0.1meV$, agrees well with literature data.

HL 38.4 Thu 10:15 POT 6

Coaxial Nanowire-in-Nanopore Arrays Enabling Anti-Agglomeration and Reliable Length Retention — •Chengzhan Yan, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany.

Nanowire arrays, a typical one-dimensional (1D) nanostructure used in energy storage systems, have significantly improved the electrochemical performance by optimizing the active material distribution and promoting the charge transport kinetics in energy storage systems. Notably, nanowire arrays with well-defined arrangements and high aspect ratios are of particular interest. To this end, one prevailing strategy is to combine ordered templates with wet chemical techniques. However, nanowires with high aspect ratios have a more severe tendency to agglomerate because of uneven capillary forces, which leads to poor arrangement reliability and degrades the electrochemical performance. Herein, the ultra-thin honeycomb alumina nanopores are constructed to ensure the structural stability of nanowire arrays, achieving a reliable quadrupling of the length. Based on the integrated nanowire-in-nanopore architecture, MnO2 and polypyrrole are further electrodeposited on these free-standing nanowires to form vertically aligned core-shell 1D nanostructure arrays as cathodes and anodes for micro-supercapacitors (MSCs). Attributed to the high specific surface area and low charge diffusion resistance, these MSCs attain remarkably improved energy density, rate performance and lifespan.

30 min. break

HL 38.5 Thu 11:00 POT 6

Tails states, Voc loss and semiconductor compensation — •Susanne Siebentritt and Omar Ramirez — University of Luxembourg, Laboratory for Photovoltaics

It has been shown for many solar cell absorbers that Voc loss correlates with the Urbach energy, which describes the decay of tail states into the band gap. In chalcopyrites it was furthermore observed that heavy alkali postdeposition treatments reduce both: Urbach energy and Voc loss. This behaviour has been attributed to passivation of grain boundaries. However, recently we have shown, that alkali treatment in single crystalline films without grain boundaries also leads to a reduction of Voc loss and Urbach energies. This behaviour can be traced back to a reduced compensation by increasing the doping level. It is to be expected that a similar mechanism plays a role in polycrystalline films. Part of the dependence of the Voc loss on Urbach energy can be attributed to radiative and non-radiative recombination in and through tail states. However, the dependence is stronger than would be expected from the increased recombination. We now understand that this is due to a simultaneous effect: increasing doping increases Voc and decreases tail states. Thus we propose, that one effect of heavy alkali treatment is due to the observed increase of Na doping inside the grains, because it increases the net-doping, reduces tail states and thereby reduces radiative and non-radiative recombination. All this increases Voc.

HL 38.6 Thu 11:15 POT 6

Dependence of the activation energy of light-induced degradation (LID) in silicon on the illumination intensity — •Kevin Lauer[1,2], Katharina Peh[1], Dirk Schulze[1], and Stefan Krischok[1] — [1]Technische Universität Ilmenau, Institut für Physik und Institut für Mikro- und Nanotechnologien, Ilmenau, Germany — [2]CiS Forschungsinstitut für Mikrosensorik GmbH, Erfurt, Germany

It was found that the activation energy of the dissociation process of the acceptor-iron defects (A_{Si}-Fe_i) in silicon depends on the illumination intensity.[1] This implies that besides the thermal energy an additional supply of energy due to e.g. carrier recombination is possible in that defect reaction. To check whether this is also the case for the slow process of the light-induced degradation (LID) in silicon,[2] which can be explained by acceptor-silicon defects (A_{Si}-Si_i),[3] we measured the activation energy for the slow LID process for different illumination intensities. No impact of the illumination intensity on the activation energy of the slow LID process could be found indicating a pure thermally activated process.

[1] K. Lauer, C. Möller, D. Debbih, M. Auge, and D. Schulze, Solid

State Phenom. 242, 230 (2015).

[2] J. Lindroos and H. Savin, Sol. Energy Mater. Sol. Cells 147, 115 (2016).

[3] K. Lauer, K. Peh, D. Schulze, T. Ortlepp, E. Runge, and S. Krischok, Phys. Status Solidi A 219, 2200099 (2022).

HL 38.7 Thu 11:30 POT 6

Photoelectrochemical Catalyst Deposition on III-V Semiconductor Surfaces for Direct Solar Water Splitting — •Erica Schmitt, Moritz Kölbach, Margot Guidat, Marco Flieg, Max Nusshör, Anna-Lena Renz, and Matthias May — Universität Tübingen, Institute of Physical and Theoretical Chemistry, Tübingen, Germany

The conversion of solar electrical energy to chemical energy by the generation of hydrogen is believed to play a key role in the transition towards a sustainable energy system. One approach to generate sustainable hydrogen is the use of III-V photoelectrodes in a highly efficient photoelectrochemical water splitting device. Such fully integrated, monolithic systems have a potentially lower balance of system cost compared to more conventional decoupled PV-electrolysis approaches and have already shown to be highly efficient [1].

The III-V semiconductor-electrolyte interface plays a crucial role in the performance of a photoelectrochemical device. Our work focuses on the photoelectrochemical modification of the semiconductor surface with a suitable catalyst and its stabilization in the harsh environment of an acidic electrolyte under operating conditions while also understanding the underlying physicochemical processes. We present an optimized functionalization process to increase the solar-to-hydrogen efficiency and stability of a photoelectrochemical cell, as well as the electrochemical and spectroscopical characterization using, among other methods, reflection anisotropy spectroscopy. [1] May, M., Lewerenz, HJ., Lackner, D. et al., Nat. Commun. 6, 8286 (2015).

HL 39: Organic Electronics and Photovoltaics III (joint session CPP/HL)

Time: Thursday 9:30–12:30 Location: GÖR 226

HL 39.1 Thu 9:30 GÖR 226

Determining exciton diffusion lengths in organic non-fullerene acceptors with Kinetic Monte Carlo Simulation — •Wenchao Yang, Safakath Karuthedath, Catherine Castro, Julien Gorenflot, and Frederic Laquai — KAUST Solar Center, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

Optimal exciton diffusion length (L_D) is a key parameter for reducing losses during exciton to charge carrier conversion in organic solar cells (OSC). However, different research groups report contradicting numbers for the same non-fullerene acceptors (NFA) using different lifetimes to calculate L_D. In this work, in order to verify the measured L_D's in NFAs (ITIC, IT4F, ITM and IT2Cl) using transient absorption (TA) spectroscopy, we employed the Kinetic Monte Carlo (KMC) method to simulate the exciton dynamics and calculate the corresponding L_D. With the assumption of Förster resonant energy transfer type exciton hopping rate in a cubic lattice, the TA decay kinetics under different fluences are reproduced by the KMC simulation, and the only free parameter: the energetic disorder σ is extracted. The use of the lifetime τ measured by time-resolved photoluminescence in neat NFA enables to reproduce the transients using more realistic σ values. The L_D's in the NFAs are further calculated with the τ's and found to be consistent with the experimental values. This work provides microscopic descriptions of exciton diffusion and more insight into the determination of L_D in organic semiconductors.

HL 39.2 Thu 9:45 GÖR 226

A thorough analysis of conformational locking and related electrical properties in fluorinated thieno-quinoxalines — •Md Moidul Islam[1,2], Arthur Markus Anton[1,2,5], Shahidul Alam[6], Rico Meitzner[1,2], Christos L. Chochos[3,4], Ulrich S. Schubert[1,2], and Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry (IOMC),Friedrich Schiller University Jena, Jena, Germany — [2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Jena, Germany — [3]Institute of Chemical Biology, National Hellenic Research Foundation, Athens 11635, Greece — [4]Advent Technologies SA, Patra, Greece — [5]Peter Debye Institute for Soft Matter Physics, Universität Leipzig, Leipzig, Germany — [6]King Abdullah University of Science and Technology (KAUST), KAUST Solar Center (KSC), Physical Sciences and Engineering Division (PSE), Material Science and Engineering Program (MSE), Kingdom of Saudi Arabia

Thieno-quinoxaline derivatives with low band gaps are promising donor materials for organic solar cells. Therefore, investigations have been conducted on thieno-quinoxaline polymers with systematically varied fluorination sites. Cyclic voltammetry revealed that fluorination lowers both the HOMO as well as LUMO energy levels, whereas the size of photochromic units is affected through the particular kind of fluorination demonstrated by UV-Vis absorption spectra. Furthermore, excitation-emission mapping exposed excitation-independent and excitation-selective PL pathways.

HL 39.3 Thu 10:00 GÖR 226

Orientation and Order of Molecular Subunits and Excited State Dynamics in a P3HT Bottlebrush Copolymer — •Arthur Markus Anton[1,2], Friedrich Kremer[1], Jenny Clark[2], and Frank Cichos[1] — [1]Leipzig University, Peter Debye Institute for Soft Matter Physics, Linnéstr. 5, 04103 Leipzig, Germany — [2]The University of Sheffield, Department of Physics and Astronomy, Hounsfield Rd, Sheffield S37RH, United Kingdom

Orientation and order at different length scales are believed to play a crucial role for the performance of organic semiconductor devices. Taking advantage of the material properties of *bottlebrush copolymers* and gain control of structure formation, a poly-(3-hexylthiophene) grafted copolymer has been studied [1]. In order to investigate the structure on the molecular scale the technique of *Infrared Transition Moment Orientational Analysis* (IR-TMOA) has been employed [2,3]. The absorbance of structure-related bands is evaluated depending on the inclination of the sample film (ϑ) and polarization of the IR light (φ). This combination then allows to determine the tensor of absorption separately for the respective molecular moieties and to deduce their orientation (Θ,Φ) relative to a sample-fixed coordinate system. In addition *transient absorption* measurements have been conducted. The dynamics of exciton and polaron formation and decay has been investigated and the derived results on the basis of the bottlebrush copolymer are compared with results from linear P3HT. [1] Heinrich and Thelakkat, *J. Mater. Chem. C* **4** (2016) 5370 [2] Anton et al, *J. Am. Chem .Soc.* **137** (2015), 6434 [3] Anton et al, *Macromolecules* **49** (2016) 1798

HL 39.4 Thu 10:15 GÖR 226

Utilizing High Gain and Spectral Narrowing for Near-Infrared Organic Photodetectors — •Louis Conrad Winkler[1], Jonas Kublitski[2], Johannes Benduhn[1], and Karl Leo[1] — [1]TU Dresden, Germany — [2]Federal University of Technology Paraná UTFPR, Curitiba, Brazil

There is a multitude of applications for infrared photodetectors that demand high-volume fabrication, including blood oxygen determination, continued monitoring of food quality, control of industrial processes, and many more. Organic photodetectors (OPDs) have great potential to enrich today*s photodetector marked with their low-cost fabrication, flexible devices and tunable response. However, most studied organic semiconducting materials have neglectable absorption above 1000 nm. This contribution presents a donor-acceptor blend with a low-energy and broad charge-transfer (CT) feature. To overcome the inherent increase of charge carrier recombination of such low-energy systems, we introduce two photocurrent multiplication (PM) mechanisms. By embedding this OPD into an optical micro-cavity, a spectral response (SR) of 15 AW-1 at 1095 nm is achieved. Furthermore, a very narrow response of only 18 nm makes this architecture ideal for spectroscopic resolved measurements that could be easily integrated into CMOS readout circuitry due to the optimization for operation under reverse bias.

HL 39.5 Thu 10:30 GÖR 226

Realizing a high-performance, fully thermal-evaporated, blue narrowband organic photodetector — •Tianyi Zhang, Johannes Benduhn, and Karl Leo — Dresden Integrated Center for

Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, Dresden, Germany

Organic photodetector (OPD) boasts of its tunable absorption window, mechanical flexibility, transparency, non-toxicity, facile processing, and cheaper cost. Recent development of high-performing polymers and small molecules further reveals its potential in numerous communication and biomedical applications. To realize visible light communication, commercially available inorganic photodetector usually incorporates additional optical filters, which further increases the complexity and cost of the sensing system. Therein, we demonstrate a blue absorbing organic photodetector with ultrahigh specific detectivity (D^*) approaching 10^{14} Jones. By employing a wide bandgap hole transporting layer BF-DPB with Rubrene:C_{60} active layer, the absorption peaks at 450nm with an external quantum efficiency (EQE) of 50% at zero bias. The parasitic absorption renders the narrowband characteristic of the blends to span merely over the blue wavelength region. Upon BF-DPB incorporation, ultrafast responses are also observed at sub-microseconds. We conclude that the judicious choice of transporting layer is critical for achieving application-tailored properties, namely high speed or high D^*. To date, those values are among the best-reported blue OPDs.

HL 39.6 Thu 10:45 GÖR 226

Investigation of high performance organic photodetectors based on single component photoactive layer — •Jakob Wolansky[1], Cedric Hoffmann[2], Felix Talnack[3], Michel Panhans[4], Donato Spoltore[5], Stefan C.B. Mannsfeld[3], Frank Ortmann[4], Natalie Banerji[2], Johannes Benduhn[1], and Karl Leo[1] — [1]IAPP, TU Dresden — [2]University of Bern — [3]Cfaed, TU Dresden — [4]TU Munich — [5]University of Parma

In organic semiconductor applications such as organic photovoltaics and photodetectors, an intermolecular interface with an energetic gradient between electron donating and accepting materials is usually required for efficiently generating charges. This driving force facilitates the dissociation of the photogenerated excitons. At the same time, this energy offset reduces the maximum possible open-circuit voltage, and the additional interface can act as a recombination site and increases the dark current. Therefore, single-component devices are extensively researched to overcome these drawbacks.

Here, we report on single-component devices that perform very well as organic photodetectors. By utilizing different device processing parameters and employing different interface layers, we optimized the device characteristics such as external quantum efficiency, dark current, and specific detectivities of more than 1e13 Jones. Investigations of the morphology, combined with ultrafast transient absorption measurements, give insight into the charge generation mechanism in our material system.

HL 39.7 Thu 11:00 GÖR 226

Reduced defect density in crystalline halide perovskite films via methylamine treatment for the application in photodetectors — •Emilia Rosa Schütz[1], Azhar Fakharuddin[1], Yenal Yalcinkaya[2,3], Efrain Ochoa-Martinez[4], Shanti Bijani[5], Abd. Rashid bin Mohd Yusoff[6], Maria Vasilopoulou[7], Tobias Seewald[1], Ullrich Steiner[4], Stefan Weber[2,3], and Lukas Schmidt-Mende[1] — [1]University of Konstanz, Konstanz, Germany — [2]Max Planck Institute for Polymer Research, Mainz, Germany — [3]Johannes Gutenberg University Mainz, Mainz, Germany — [4]Adolphe Merkle Institute, University of Fribourg, Fribourg, Switzerland — [5]Unidad de Nanotecnología, Centro de Supercomputador y Bioinnovación SCBI, Universidad de Málaga, Málaga, Spain — [6]Pohang University of Science and Technology, Pohang, Republic of Korea — [7]National Center for Scientific Research Demokritos, Attica, Greece

The quality of a perovskite layer strongly depends on the processing conditions. Consequently, the fabrication process is often complex, and reproducibility is a challenge. Our methylamine gas-based method is able to recrystallize perovskite layers of any given quality in a controlled way, leading to millimeter-sized domains. Crystallinity significantly increases upon methylamine treatment, and crystal growth follows a preferred orientation. Photoluminescence- and space-charge limited current measurements imply that the trap density decreases after recrystallization. When applied in photodetectors, the improved film quality of the recrystallized films leads to increased detectivities and shorter response times.

15 min. break

HL 39.8 Thu 11:30 GÖR 226

Reducing Dark Current in Highly Ordered Rubrene:C_{60} Heterojunctions for Organic Photodetectors — •Anna-Lena Hofmann[1], Jakob Wolansky[1], Lucy Winkler[1], Max Herzog[1], Felix Talnack[2], Eva Bittrich[3], Johannes Benduhn[1], and Karl Leo[1] — [1]IAPP, TU Dresden, Dresden, Germany — [2]Cfaed, Dresden, Germany — [3]Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany

Vacuum-deposited rubrene can form highly ordered phases, demonstrating an exceptionally high charge carrier mobility for holes ($> 10\,\mathrm{cm^2\,V^{-1}\,s^{-1}}$) even in thin films. Depending on the post-treatment of our films, we can control different crystalline phases. For fast-response OPDs, the triclinic phase is very promising since it exhibits high hole mobility in the vertical direction. However, the high surface roughness is a key reason why these devices fall short in specific detectivity. In this work, we employ different strategies to reduce the impact of Ohmic shunts within the device to minimize the noise current of our devices. We characterize the morphology of our films and investigate the performance parameters of fully working devices. Finally, these characteristics are compared to rubrene's other two crystalline phases.

HL 39.9 Thu 11:45 GÖR 226

Utilizing charge-transfer states for narrowband and highly sensitive photodetection — •Johannes Benduhn, Louis Conrad Winkler, Awais Sawar, Jonas Kublitski, and Karl Leo — IAPP, TU Dresden, Germany

Near-infrared (NIR) spectroscopic material sensing has the potential to revolutionize many aspects of life, ranging from food control to material determination. However, currently available products are either too bulky or too expensive to be used in mobile customer applications. In this regard, organic photodetectors (ODPs) can open new perspectives due their cheap and versatile processing techniques. Nevertheless, the external quantum efficiency (EQE) as well as the specific detectivity of those devices in the NIR wavelength range are still lacking behind. In this contribution, we explore photomultiplication (PM) in fully vacuum deposited OPDs. Broadband devices achieve a maximum EQE of almost 2000 % at -10 V. Employing very sensitive measurement techniques as well as optical modelling of our devices, we are able to proof that the photomultiplication can take place even if weakly absorbing charge-transfer states are responsible for the photon harvesting. Employing a suitable donor-acceptor system as well as an optimized device architecture for photomultiplication and constructive interference in the NIR wavelength range, we achieve narrowband OPDs with the spectral response of more than $10\,\mathrm{A\,W^{-1}}$ at a wavelength of 1100 nm with full width at half maximum even below 20 nm. These results demonstrate the versatility of OPDs and their potential for spectroscopic material sensing.

HL 39.10 Thu 12:00 GÖR 226

Design of Integrated All-Organic Oxygen Sensors — •Toni Bärschneider and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Technische Universität Dresden

Organic electronic devices, such as light-emitting diodes (OLEDs) and photodetectors (OPDs), are ideal for sensor applications because of their versatility and flexibility. Additionally, they can be easily fabricated on any substrate, making integrated sensor applications possible. This allows for easy miniaturization and cheap fabrication. Organic room temperature phosphorescence (RTP) materials are well suited for optical oxygen sensing because of their strong oxygen dependency.

In this work, we developed a monolithic all-organic oxygen sensor composed of a RTP sensing layer, an ultraviolet OLED as an excitation source, and a narrow bandwidth OPD for detection. The RTP sensing layer simultaneously shows fluorescence and phosphorescence at room temperature, which enables self-referencing to avoid photodegradation-caused distortion. Due to the long phosphorescence lifetime, sensing within the ultra-trace range is possible.

The presented sensors overcome drawbacks of current optical oxygen sensors, such as complexity, expensive read-out electronics, and a lack of possible miniaturization.

HL 39.11 Thu 12:15 GÖR 226

Atomistic insights on the electrode material CuDEPP — •Christoph Jung[1,2] and Timo Jacob[1,2] — [1]Universität Ulm, Institut für Elektrochemie, Ulm, Germany — [2]HIU, Ulm, Germany

Devices for electrical energy storage need to provide high energy yields

as well as output power while at the same time guaranteeing safety, low costs and long operation times. The porphyrin CuDEPP [5,15-bis(ethynyl)-10,20-diphenylporphinato]copper(II) is a promising electrode material for various battery systems both as anode or cathode. CuDEPP combines the positive properties of lithium ion batteries (high energy density) with those of a supercapacitor (fast electron release and absorption). While its functionality has been demonstrated experimentally, there had been no atomistic information as to why CuDEPP expresses these interesting properties or how the incorporation of ions affects its structure. Starting with the smallest possible unit (i.e. a single molecule) we successively increased the spatial dimensionality of the structure by studying: a) di- and trimers, b) molecular stacking in a 1D chain, c) extending these chains to planar CuDEPP sheets and finally c) a three-dimensional extended polymer structure. Combining the individual results of the molecule, the chain, the plane and the extended polymer lead to a comprehensive and consecutive understanding of the CuDEPP system. Afterwards the insertion (or intercalation) of different ions (including Li, Mg and Na) has been studied. Based on the optimal ion intercalation structure, discharge voltage curves have been calculated and compared to experimental measurements.

HL 40: Focus Session: Frontiers of Electronic-Structure Theory VI (joint session O/HL)

Time: Thursday 10:30–12:45 Location: TRE Ma

HL 40.1 Thu 10:30 TRE Ma

Nailing down charge-density-wave phase-transition temperatures with downfolding approaches — •Arne Schobert[1], Jan Berges[2], Michael Sentef[3], Erik van Loon[4], Sergey Brener[1], Mariana Rossi[3], and Tim Wehling[1] — [1]University of Hamburg, Germany — [2]University of Bremen, Germany — [3]MPSD, Hamburg, Germany — [4]Lund University, Sweden

The coupled dynamics of electrons and nuclei is an extremely complex problem of relevance to multiple branches of sciences. *Ab initio* molecular dynamics (AIMD) simulations are often challenging — especially in large systems, on long time scales, in non-equilibrium or in presence of strong correlation. We can overcome these problems by mapping the full *ab initio* density functional theory (DFT) Hamiltonian onto a low-energy lattice model through downfolding. Three different downfolding strategies based on constraining, unscreening and combinations thereof are compared. The best performing model, which properly accounts for anharmonicity, is combined with path integral molecular dynamics (PIMD). This allows us to nail down the transition temperatures of charge-density waves — for instance in 1H-TaS_2.

HL 40.2 Thu 10:45 TRE Ma

Structural and electronic properties of the $Ba_8Au_xGe_{46-x}$ clathrate: an ab-initio study with cluster expansion — •Peter Weber, Santiago Rigamonti, and Claudia Draxl — Humboldt-Universität zu Berlin, Berlin, Germany

Intermetallic clathrate materials are promising candidates for high-efficiency thermoelectric applications as they can reach very low thermal conductivity. These materials possess a cage-like structure containing guest atoms. Their electronic properties can be tailored by exploiting the idea of the phonon-glass–electron-crystal which allows for reaching a large figure of merit. We study the compound $Ba_8Au_xGe_{46-x}$ ($0 \leq x \leq 8$), which has raised interest due to its glass-like thermal conductivity [1]. Using the Zintl concept, a semiconducting state is expected to occur at the charge-balanced composition corresponding to x=5.33. This composition requires a supercell of at least 3 unit cells (162 atoms) which makes a direct *ab initio* study challenging. We tackle this problem by using the cluster expansion method combined with density-functional theory calculations. In this way, we are able to find the atomic ground-state configurations, together with various properties at different temperatures and gold content. These include lattice constants, bond lengths, site occupancies, as well as band gaps and band structures which are compared with available experimental data.

[1] P.-F. Lory, *et al.* Nature Communications **8**, 491 (2017).

Topical Talk HL 40.3 Thu 11:00 TRE Ma

New Opportunities for First Principles Simulations of Thousands of Atoms Using Linear Scaling Density Functional Theory — •Laura Ratcliff — University of Bristol, Bristol, United Kingdom

Density-functional theory (DFT) is routinely used to simulate a wide variety of materials and properties, however, standard implementations are cubic scaling with the number of atoms, limiting the system sizes which can be treated. This motivated the development of alternative implementations of DFT, which exploit the nearsightedness principle by using a localised description of the system, leading to algorithms with linear scaling (LS) cost which can treat large systems containing tens of thousands of atoms. One approach, which is implemented in the wavelet-based BigDFT code, uses localised orbitals, also known as support functions, which are optimised to reflect their local chemical environment, and thus constitute an accurate minimal basis set. Beyond reduced computational cost, the localised support function description also facilitates additional developments, such as the ability to automate a fragment-based description. In this talk we will present the formalism behind LS-BigDFT, including some examples of the new types of systems and analyses which are opened up by the ability to treat such large systems. We will also describe recent developments in PyBigDFT, a python-based interface which aims to simplify the usage of LS-BigDFT for complex systems and workflows.

15 min. break

HL 40.4 Thu 11:45 TRE Ma

Fully Anharmonic Electronic Transport Coefficients from Temperature-dependent Spectral Functions — •Jingkai Quan, Matthias Scheffler, and Christian Carbogno — The NOMAD Laboratory at the FHI of the Max-Planck-Gesellschaft and IRIS-Adlershof of the Humboldt-Universität zu Berlin

The combination of *ab initio* molecular dynamics (aiMD) and band-structure unfolding techniques provides a non-perturbative route to obtain temperature-dependent spectral functions. [1] In contrast to commonly employed perturbative approaches [2], this technique accounts for all orders of anharmonic and vibronic couplings. Building on this non-perturbative formalisms, we here present an approach to obtain electronic transport coefficient such as the electrical conductivity using Kubo's formulation of the fluctuation-dissipation theorem. By this means, all relevant quantities, including electron lifetimes, are obtained from the unfolded, self-consistent wave functions computed during the aiMD runs. We critically benchmark the approach against existing perturbative data for harmonic systems, carefully analyzing to which extent short- and long-range couplings are captured with increasing supercell size. Furthermore, we demonstrate the advantages of the proposed approach for strongly anharmonic systems, for which perturbative approaches become unreliable.

[1] M. Zacharias, M. Scheffler, and C. Carbogno, *Phys. Rev. B* **102**, 045126 (2020).
[2] F. Giustino, *Rev. Mod. Phys.* **89**, 015003 (2017).

HL 40.5 Thu 12:00 TRE Ma

Accurate prediction of vibrational spectra for solid state systems from ab initio molecular dynamics — •Ekin Esme Bas, Thomas Heine, and Dorothea Golze — Chair of Theoretical Chemistry, Technische Universität Dresden, 01062 Dresden, Germany

We present a highly accurate computational method to calculate vibrational spectra for solid state materials, primarily for covalent-organic frameworks (COFs). IR and Raman spectra are important tools that are frequently used for material characterization. However, the experimental spectra are often difficult to interpret without aid from theory. The computation of IR and Raman spectra is usually based on the harmonic approximation where molecular vibrations can be determined as normal modes from the second derivatives of the electronic energy with respect to the coordinates. Although this method is more straightforward and computationally less expensive, anharmonic modes cannot be captured. Thus, we employ an AIMD (ab initio molecular dynamics) based approach to include vibrational anharmonicities. Power, IR and Raman spectra can then be calculated via a Fourier transformation of the time correlation functions of velocities, dipole moments and polar-

izability tensors, respectively [1]. We discuss different approaches to compute dipole moments and polarizabilities. We present the power, IR and Raman spectra we calculated for COF-1, and we compare our AIMD based approach to the spectra obtained via harmonic approximation and experiment.
[1] M. Thomas, M. Brehm, R. Fligg, P. Vöhringer, B. Kirchner. Phys. Chem. Chem. Phys., 6608-6622, 5, 2013.

HL 40.6 Thu 12:15 TRE Ma

Anharmonic Fingerprints from THz Modes of Polyacene Crystals — •Paolo Lazzaroni, Shubham Sharma, and Mariana Rossi — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

Organic molecular crystals exhibit strong lattice anharmonicity, especially in the collective motions that are governed by intermolecular interactions and lie in the low-frequency THz range [1]. Inspired by recent observations that the polarization-orientation (PO) Raman spectra can give exquisite insight into the anharmonic couplings between modes [2], we devise a first-principles framework that can reproduce, explain and give quantitative insight into the type and strengths of mode coupling. This framework is based on machine-learned potentials and polarizability tensors trained on *ab initio* molecular dynamics trajectories [3]. We obtain results through the time-correlation formalism for PO Raman signals, retaining the full anharmonic nature of the potential, and perform a novel analysis of effective temperature-dependent mode couplings from our trajectories. [1] M. Asher *et al.*, Adv. Mater. **32**, 1908028 (2020) [2] N. Benshalom *et al.*, arXiv:2204.12528 (2022) [3] N. Raimbault *et al.*, *New J. Phys.* **21** 105001 (2019)

HL 40.7 Thu 12:30 TRE Ma

A first-principles Newns-Anderson chemisorption function applied to ultrafast electron transfer — •Simiam Ghan[1], Elias Diesen[1], Christian Kunkel[1], Karsten Reuter[1], and Harald Oberhofer[2] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany. — [2]University of Bayreuth, Bayreuth, Germany

We offer a method to calculate the electronic couplings H_{ad} between an adsorbate and substrate in an ab-initio fashion. The couplings are acquired by projection of the Kohn-Sham Hamiltonian onto a diabatic basis[1]. By averaging over the Brillouin Zone, it becomes possible to calculate a convergent chemisorption function of Newns and Anderson[2], which gives the energetic broadening of an adsorbate frontier orbital upon adsorption. This broadening corresponds to the experimentally-observable lifetime of an electron in the state, which we confirm for the case of core-excited $Ar^*(2p_{3/2}^{-1}4s)$ atoms on a number of transition metal surfaces[3].

We find that the (tunneling) model captures and elucidates aspects of energy-dependence, spin, phase cancellation and k-space in the electron transfer process, in particular suggesting a significant role played by the surface d-bands. Given the prevalence of electronic couplings - and the chemisorption function - in theoretical models, we discuss potential for further applications.
[1] S. Ghan et al., J. Chem. Theory Comput. **16**, 7431 (2020).
[2] D. Newns, Phys. Rev. **178**, 3, 1123 (1969).
[3] F. Blobner et al., Phys. Rev. Lett. **112**, 086801 (2014).

HL 41: Oxide Semiconductors I: Ga_2O_3

Time: Thursday 15:00–17:00 Location: POT 81

HL 41.1 Thu 15:00 POT 81

Thermal Conductivities of Ga_2O_3 Polymorphs: Analysis of Anharmonicity and Anisotropy — •Shuo Zhao, Matthias Scheffler, and Christian Carbogno — The NOMAD Laboratory at the FHI of the Max-Planck-Gesellschaft and IRIS-Adlershof of the Humboldt-Universität zu Berlin

Gallium oxide (Ga_2O_3) is an ultra-wide bandgap material with substantial potential for electronics, e.g., in field effect transistors [1]. In this context, an atomistic understanding of its heat transport characteristics is essential for thermal management. For this purpose, we compute the lattice thermal conductivity of the α-, β-, and κ-polymorphs of Ga_2O_3 using the *ab initio* Green-Kubo formalism [2,3] that incorporates all orders of anharmonic effects via first-principle molecular dynamics. We discuss the role of anharmonic effects for the different polymorphs and investigate their influence on the anisotropy of the conductivity tensor. Our results provide guiding rules for maximizing and minimizing thermal transport in thin Ga_2O_3 films.
[1] M. Higashiwaki, *et al.*, *Appl. Phys. Lett.* **100**, 013504 (2012).
[2] C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901 (2017).
[3] F. Knoop, M. Scheffler, and C. Carbogno, *arXiv:*2209.01139 (2022).

HL 41.2 Thu 15:15 POT 81

Strain-induced polymorph conversion in gallium oxide via focused ion beam irradiation — •Umutcan Bektas, Paul Chekhonin, and Gregor Hlawacek — Insitute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Monoclinic β-Ga_2O_3 is chemically and thermally the most stable compound compared to its other polymorphs. It is a promising semiconductor material for power electronics, optoelectronics, and batteries. However, controlling the metastable polymorph phases is challenging, and the fabrication technology at the nanoscale is immature. Our goal is to understand and control the polymorph conversion, so we can establish new fabrication methods of single-phase polymorph coatings, buried layers, multilayers, and different nanostructures in gallium oxide.

Under ion beam irradiation, most semiconductors show transformation from crystalline to amorphous structure due to ion beam induced damage. However, it is observed that, this transformation is suppressed in gallium oxide, and a polymorph conversion is observed instead. Here, we use Gallium and Neon focused ion beams (FIB) from different sources (GFIS, LMIS) to create local strain and induce the polymorph transition. After irradiation, characterization of the exposed areas was conducted by electron backscatter diffraction (EBSD) and atomic force microscopy (AFM). First results indicate that the strain created by the FIB irradiation leads to a local transformation of beta gallium oxide to another polymorph.

HL 41.3 Thu 15:30 POT 81

Comparative Study of Temperature-dependent Bandgap Transitions in Ga2O3 Polymorphs — •Benjamin Moritz Janzen[1], Marcella Naomi Marggraf[1], Moritz Meissner[1], Nils Bernhardt[1], Conrad Valentin Hartung[1], Nima Hajizadeh[1], Felix Nippert[1], and Markus Raphael Wagner[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Germany

We employ a combined experimental-theoretical study to investigate the electronic bandgap transitions in Ga2O3 polymorphs as a function of the sample temperature. For this purpose, we apply temperature-dependent UV photoluminescence excitation (PLE) spectroscopy for the β-, κ-, α- and γ-polymorphs in the temperature range between 5 and 300 K and compare the obtained bandgap values with room temperature measurements of the dielectric function as determined by spectroscopic ellipsometry. The obtained temperature dependencies are discussed in conjunction with DFT calculations regarding the effects of electron-phonon coupling.

HL 41.4 Thu 15:45 POT 81

Anisotropic IR active phonon modes and fundamental direct band-to-band transitions in α-$(Al_xGa_{1-x})_2O_3$ alloys grown by MOCVD — •Elias Kluth[1], A F M Anhar Uddin Bhuiyan[2], Lingyu Meng[2], Hongping Zhao[2], Rüdiger Goldhahn[1], and Martin Feneberg[1] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Germany — [2]Department of Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio, USA

The corundum-like Ga_2O_3 polymorph α-Ga_2O_3 is of high research interest as it allows bandgap-engineering by alloying e.g. with α-Al_2O_3, α-In_2O_3, α-Ti_2O_3 and similar materials. Since the corundum-like crystal structure is anisotropic, a direction dependent investigation of the material properties is crucial. m-plane α-$(Al_xGa_{1-x})_2O_3$

thin film samples up to x=0.76, grown on m-plane sapphire substrate by MOCVD have been investigated by infrared (IR) and visible-ultraviolet (UV) spectroscopic ellipsometry. IR ellipsometry yields the anisotropic IR active phonons and their shift to higher wavenumbers with increasing x. Furthermore, with UV ellipsometry, we find the anisotropic dielectric functions up to 6.6eV and the shift of the fundamental direct band-to-band transitions with increasing x. We report an anisotropic bowing parameter for α-$(Al_xGa_{1-x})_2O_3$ of b_{ord}=2.7eV and b_{extra}=2.5eV.

15 min. break

HL 41.5 Thu 16:15 POT 81

Adsorption enhanced photocatalytic degradation of Rhodamine B using GdxBi1-xFeO3@SBA-15 (x= 0, 0.05, 0.10, 0.15) nanocomposites under visible light irradiation — •Thomas Cadenbach[1] and Maria Jose Benitez[2] — [1]Universidad San Francisco de Quito, Quito, Ecuador — [2]Escuela Politecnica Nacional, Quito, Ecuador

In the present work show that very high removal efficiency of a variety of organic pollutants by GdxBi1-xFeO3@SBA-15 nanocomposites (x = 0, 0.05. 0.10, 0.15) under visible light irradiation. Specifically, we study the photocatalytic degradation of dyes using the above nanocomposite materials, with pore volume loadings of 5-25%. We compare the obtained catalytic results for the nanocomposite materials to monodisperse BiFeO3 nanoparticles with a particle diameter of 5.5 nm. We find that the best removal performance is achieved by a 10 vol% Gd0.05Bi0.95FeO3@SBA-15 sample, shown by a complete dye degradation in approximately 3h using extremely low concentrations of the actural active photocatalyst. The superior efficiencies of the nanocomposites, which outperformed their parent compounds, i.e. GdxBi1-xFeO3 nanoparticles as well as unfilled SBA-15, are attributable to a synergistic adsorption enhanced photocatalytic degradation process. The possible mechanism in the photodegradation process was investigated and discussed on the basis of trapping experiments.

HL 41.6 Thu 16:30 POT 81

Electrical and thermal transport properties of $ZnGa_2O_4$ — Johannes Boy[1], Rüdiger Mitdank[1], Zbigniew Galazka[2], and •Saskia Fischer[1] — [1]Novel Materials Group, Humboldt-Univ. zu Berlin, Germany — [2]Leibniz-Institute of Crystal Growth, Berlin, Germany

The first full experimental determination of the low-temperature electrical, thermo-electrical [1] and thermal properties [2] of novel highly pure single crystalline $ZnGa_2O_4$ is reported. The temperature-dependences of the charge carrier density, mobility, and Seebeck coefficient including phonon drag are discussed between 10 K and 310 K. The thermal conductivity and diffusivity were determined by the so-called 2ω-method. At room temperature the electrical conductivity is 286 S/cm, the mobility 55 cm^2/Vs, the Seebeck coefficient 125$\mu V/K$ and the thermal conductivity is 22.9 W/mK. For temperatures above 100 K the phonon transport is limited by phonon Umklapp scattering. At lower temperatures boundary scattering at lattice defects limits the thermal conductivity to 95 W/mK. Therefore, if the cause of boundary scattering is reduced or eliminated, the thermal conductivity of $ZnGa_2O_4$ may be increased at low temperatures.

[1] J. Boy, *et al.*, AIP Advances 10, 055005 (2020) [2] J. Boy, *et al.*, Materials Research Express 9, 065902 (2022).

HL 41.7 Thu 16:45 POT 81

Temperature- and Polarisation- Dependant Photoluminescence Excitation Spectroscopy of $\beta - Ga_2O_3$. — •Moritz Meissner[1], Nils Bernhard[1], Felix Nippert[1], Benjamin M. Janzen[1], Conrad V. Hartung[1], Zbigniew Galazka[2], and Markus R. Wagner[1,3] — [1]Technische Universität Berlin, Institute of Solid State Physics, Berlin, Germany — [2]Leibniz-Initut für Kristallzüchtung, Berlin, Germany — [3]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

The anisotropic, ultra-wide bandgap semiconductor $\beta - Ga_2O_3$ represents a promising candidate for applications in high power electronics. The high anisotropy of the monoclinic crystal structure and the formation of self-trapped excitons has made a precise determination of the bandgap parameters a challenging endeavor. In this work, we apply polarization- and temperature-dependent photoluminescence excitation spectroscopy (PLE) measurements to study the anisotropy of the optical bandgap transitions. The temperature dependence of the PLE spectra between 5K and 300K provides information on the strength of the electron-phonon coupling and zero temperature bandgap energies along the principal axes of the material. The measurements were performed on the three crystal planes (100), (010) and (001) prepared and polished from the same single bulk crystal grown by the Czochralski method. Our results are discussed in comparison with absorption, transmission, and reflectance spectroscopy data in the literature.

HL 42: Quantum dots: Growth

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

HL 42.1 Thu 15:00 POT 151

Cone-shell quantum structures with tunable wave functions — •Christian Heyn, Ahmed Alshaikh, Kristian Deneke, and Robert Blick — Center for Hybrid Nanostructures (CHyN), University of Hamburg

We discuss the tailoring of the wave functions (WF) in strain-free GaAs quantum structures (QS) fabricated using self-assembled local droplet etching (LDE) during molecular beam epitaxy (MBE). Here, Al droplets are deposited on an AlGaAs surface and drill nanoholes with tunable shape and size. Subsequently, the holes are filled with GaAs to form strain-free QS. Dependent on the process parameters, the QS have the shape of a cone or of a cone-shell. In particular the low-density (about 1x10^7 cm^{-2}) cone-shell QS (CSQS) demonstrate sharp exitonic lines with linewidth down to 25 μeV, a precise control of the emission wavelength from 680...810 nm by the nanohole filling level, a neutral exiton fine-structure splitting below 5 μeV, and nearly perfect single photon emission. To tune the WF in CSQS, a vertical electric field is applied which causes a strong charge-carrier separation. The resulting Stark shift is measured using micro-photoluminescence (PL). In combination with simulation results the optical data allow the determination of the QS size and shape. In addition, simulations indicate the transformation of either the electron or the hole WF into a quantum ring. As a further consequence of the field-induced charge-carrier separation, simulations of the exciton-recombination lifetimes predict a variability from nanoseconds up to milliseconds. This suggests CSQS for applications in the field of light storage

HL 42.2 Thu 15:15 POT 151

DNA Origami for low-dimensional electronics — •Borja Rodriguez-Barea[1], Shima Jazavandi-Ghamsari[1], Madhuri Chennur[1], Archa Jain[1], Turkan Bayrak[1], Jingjing Ye[2], Ralf Seidel[2], and Artur Erbe[1] — [1]Institute of Ion Beam Physics und Material Science, Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Peter Debye Institute for Soft Matter Physics, Universität Leipzig, Germany

The increasing demand for energy-efficient products gave rise to electronic fabs looking for new green manufacturing processes. Bottom-up techniques have the potential to reduce economic and environmental costs due to implementing low-dimensional materials with unique properties.

We demonstrated the formation of low-dimensional metallic nanostructures based on the DNA origami technique, which can be considered as building blocks for electronic circuits. DNA templates are used as molds to guide the placement and growth of the metallic 1D nanowires. This solution-based and high-resolution nanofabrication technique complements other nanolithography techniques such as electron-beam lithography and thermal scanning probe lithography. Thus, the shape of the nanostructures can be controlled and measured.

Electronic transport on these assemblies is non-ohmic and deteriorates at low temperatures. Temperature-dependent charge transport measurements reveal the dominating mechanisms along these wires.

HL 42.3 Thu 15:30 POT 151

1D Nanowires on DNA mold-based template — •Madhuri

Chennur[1], Borja Rodriguez-Barea[1], Jazavandi-Ghamsari Shima[1], Archa Jain[1], Türkan Bayrak[1], Ulrich Kemper[2], Jingjing Ye[2], Christoph Hadlich[2], Ralf Seidel[2], and Artur Erbe[1] — [1]Institute of Ion Beam PhysicsundMaterial Science, HZDR — [2]Peter Debye Institute for Soft MatterPhysics, Universität Leipzig, Germany

Sensors have a fundamental role in improving the world around us. For increasing sensitivity and faster response, new bottom-up approaches are required. DNA nanotechnology allows the creation of nanostructure arrays that can serve the purpose.

We study the controlled growth of 1D metallic nanostructures using DNA origami templates. The DNA nanomolds are folded via staples to obtain the desired conformation. The functionalized template provides the active site for a localized seed nanoparticle attachment, thus allowing metallization by electroless plating. We report continuous Pd and Au 1D nanowires based on this method.

The conductance of the assembled nanostructures through two-probe measurements was investigated. Different origami templates lead to diverse metal morphologies, which influence electronic properties. Temperature-dependent measurements determined the transport mechanism of these nanowires, proving the first step toward an electronic nanosensor.

HL 42.4 Thu 15:45 POT 151

Maximizing Homogeneity of GaAs LDE-QDs on Full Wafer Scale — •Hans-Georg Babin, Timo Kruck, Andreas D. Wieck, and Arne Ludwig — Lehrstuhl für angewandte Festkörperphysik, Ruhr-Universität Bochum, Deutschland

Local droplet etched GaAs quantum dots (LDE-QDs) are a promising candidate for excellent single and entangled photon sources. [1] Taking further steps towards application, this requires structures of increasing complexity, engineering the electronic and photonic environments of the QDs. [2] In previous studies, we showed how properties of GaAs LDE-QDs can be modulate, containing both 737 nm and 795 nm QDs on a single wafer. [3]

However, in device mass production, for example for creating larger quantum networks, it can also be intriguing to maximize the useable area of the produced wafer. This means for the QDs, that the ensemble should be of high homogeneity locally, but also on global wafer scale. Due to the short deposition times of material during LDE this can be challenging due to intrinsic inhomogeneities. We overcome these problems by matching the substrate rotation time with the material deposition time. With this method we receive light emitting QDs on over 96 % of the wafer, with 86 % of the wafer emitting between 792 nm and 802 nm (peak-center). The mean ensemble FWHM of the QD emission is as low as (11.3+-0.4) meV.

[1] Huber, Daniel et al., Nat. Commun. 8 (1), S. 15506 (2017).
[2] Zhai, Liang et al. Nat. Commun. 11 (1), S. 4745 (2020).
[3] Babin et al.; J. Cryst. Growth 591, S. 126713 (2022)

30 min. break

HL 42.5 Thu 16:30 POT 151

Wafer-Scale Epitaxial Modulation of Quantum Dot Densitiy — •Nikolai Bart[1,2], Christian Dangel[2], Peter Zajac[1], Nikolai Spitzer[1], Marcel Schmidt[1], Kai Mueller[2,3], Andreas D. Wieck[1], Jonathan Finley[2], and Arne Ludwig[1] — [1]Ruhr-Universitaet Bochum, Lehrstuhl fuer Angewandte Festkoerperphysik, Universitaetsstraße 150, 44801 Bochum, Germany — [2]Walter Schottky Institut and Physik Department, Technische Universitaet Muenchen, Am Coulombwall 4, 85748 Garching, Germany — [3]Walter Schottky Institut and Department of Electrical and Computer Engineering, Technische Universitaet Muenchen, Am Coulombwall 4, 85748 Garching, Germany

The effect of nanoscale surface roughness on the nucleation of self-assembled InAs quantum dots (QD) is investigated with photoluminescence spectroscopy and atomic force microscopy. We show in-situ control of the roughness modulation by common epitaxial layer-by-layer growth, leaving alternating atomically smooth (rough) surfaces for integer (fractional) completion of a monolayer. We report significant differences in both PL intensity and QD surface density at the critical threshold of nucleation. By varying the underlying GaAs thickness gradients, we create and control 1- and 2-dimensional density modulation patterns on entire 3-inch wafers with modulation periods between a few mm and down to hundreds of μm and densities between 1 and 10 QDs/μm^2.

Bart, N., Dangel, C. et al. Wafer-scale epitaxial modulation of quantum dot density. *Nat Commun* **13**, 1633 (2022).

HL 42.6 Thu 16:45 POT 151

Statistical Analysis of the Spatial Distribution of MBE Grown InAs Quantum Dots on GaAs(100) — •Normen Auler, Akshay Kumar Verma, Ziyang Zhang, and Dirk Reuter — Universität Paderborn, Warburger Str. 100, 33098 Paderborn

Self-assembled InAs quantum dots (QDs) have been intensively studied as model systems for strong three-dimensional confinement over decades and gained considerable interest for applications in quantum technology. The growth by molecular beam epitaxy has been widely studied. In this contribution, we discuss the spatial distribution of InAs QDs grown by solid source molecular beam epitaxy on a GaAs(100) surface for different QD densities. Therefore, we determine the distribution of nearest-neighbor distances from atomic force microscope (AFM) images and compare them to simulated random distributions. We find good agreement under the assumption of a "denuded" zone of ca. 40 nm around each quantum dot center. This means that the QDs are basically randomly distributed as one would expect from the statistical nature of the nucleation process. The diameter of the denuded zone can either be interpreted as the average geometrical diameter of the QDs or the geometrical diameter plus a small distance due to a repelling interaction between QDs mediated by the strain field. We cannot decide this from our experimental data because AFM overestimates the geometrical diameter. For very low quantum dot densities as often required for single dot experiments, it is very difficult to obtain experimental data with statistical significance, whereas simulations can give insight into the spatial distribution.

HL 42.7 Thu 17:00 POT 151

Controlled MOF Growth on Functionalized Carbon Nanotubes — •Marvin J. Dzinnik[1], Necmettin E. Akmaz[1], Adrian Hannebauer[2], Peter Behrens[2], and Rolf J. Haug[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, Appelstraße 2, 30167 Hannover, Germany — [2]Leibniz Universität Hannover, Institut für Anorganische Chemie, Callinstraße 9, 30167 Hannover, Germany

The class of metal organic frameworks (MOFs) is continuously growing. These materials consist of inorganic building blocks, held together by organic linker molecules. Schulze *et al.* [1] showed that adding functionalized multi-walled carbon nanotubes (MWCNTs) to a UiO-66 synthesis drastically decreased the nucleation time. The MOFs preferably grow on the MWCNT until they fully encapsulate it. We demonstrate a mechanism to spatially control the UiO-66 MOF growth on individual carbon nanotubes and deplete the encapsulation. The MWCNTs are drop-casted on a silicon dioxide surface and then locally modified. The samples are then submerged in the synthesis solution. This process leads to a growth of MOF crystals on the MWCNT surface leaving the modified areas depleted. With this method we are able to define lines free of MOF on the length of a single MWCNT down to several hundred nanometres for example to electrically contact the tubes ends.

[1] Schulze, H. A., et al. Electrically Conducting Nanocomposites of Carbon Nanotubes and Metal-Organic Frameworks with Strong Interactions between the two Components. ChemNanoMat, 5(9), (2019), 1159-1169.

HL 43: Semiconductor lasers II

Time: Thursday 15:00–16:45 Location: POT 251

Invited Talk HL 43.1 Thu 15:00 POT 251

Superradiance as a witness to multipartite entanglement — •Frederik Lohof[1,2] and Christopher Gies[1,2] — [1]Institute for Theoretical Physics, University of Bremen, Bremen — [2]BCCMS, University of Bremen, Bremen

Generation and detection of entanglement is at the forefront of most quantum information technologies. There is a plethora of techniques that reveal entanglement on the basis of only partial information about the underlying quantum state including, in particular, entanglement witnesses. Superradiance refers to the phenomenon of highly synchronized photon emission from an ensemble of quantum emitters that is caused by correlations among the individual particles and has been connected to the presence of multipartite entangled states. We investigate this connection in a quantitative way and discuss the question, whether or not signatures of superradiance from semiconductor nanolasers, e.g. as revealed by photon-correlation measurements, can be interpreted as a witness to detect entanglement in the underlying state of the emitters.

HL 43.2 Thu 15:30 POT 251

Towards a quantum dot based semiconductor optical amplifier for sensing applications in the telecom O-band — •Philipp Noack, Michael Zimmer, Sergej Vollmer, Michael Jetter, and Peter Michler — Universität Stuttgart, IHFG

Optical methods for gas sensing are of great interest in recent technologies. To facilitate the optical detection of gases, a swept laser source can be realized through a semiconductor optical amplifier (SOA) and a tunable MEMS filter.

MOVPE grown quantum dots (QDs) are a prime candidate for providing gain in such a SOA system because of fast charge carrier recovery times and broad gain spectrum created by the statistical distribution of QD sizes.

To this end, we grow InGaAs QDs on a GaAs substrate. We control the growth parameters, such as material flow and growth time, to produce QDs at high densities. We incorporate a dots-in-well structure to shift the emission into the telecom O-band and to improve charge carrier confinement. To provide sufficient gain in a broad spectrum, we especially investigate the properties of vertically stacked QD layers.

After the optimization of the gain structure we perform optical simulations to find the electric field modes of edge-emitting laser structures. Then we incorporate the investigated QDs into electrically pumped edge-emitting structures and characterize the net modal absorption and net modal gain spectra of the devices as antecedent of the SOA.

HL 43.3 Thu 15:45 POT 251

Optical and quantum optical studies of feedback induced chaotic emission in bimodal VCSELs — •Aris Koulas-Simos, Timo Willburger, Niels Herrmeier, Ching-Wen Shih, Imad Limame, James Lott, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany

Vertical Cavity Surface Emitting Lasers (VCSELs) have proven to be a key building block for commercial applications in data communication, automotive systems and sensing as well as for novel complex neuromorphic photonic platforms. Here, we report on signatures of chaotic emission in bimodal GaAs-based quantum well VCSELs subject to delayed optical feedback. In excitation power-dependent microelectroluminescence studies, a clear lasing transition is evident for the strong mode reflected in the strong s-shape form of the I/O-curve accompanied by an abrupt linewidth narrowing, in contrast to the weak mode which exhibits intensity saturation and rollover at high injection currents. In power-dependent photon autocorrelation measurements, super thermal bunching is observed with $g^{(2)}(0)$ reaching values of 3. Revival peaks with a period equal to the round trip time of the external cavity emerge, indicating that the chaotic emission is induced from the optical feedback. This is further validated from signatures of chaotic emission, directly observed in single-shot intensity measurements with a streak camera.

HL 43.4 Thu 16:00 POT 251

Monolithic 850 nm VCSEL Array for QKD via the decoy state protocol — •Michael Zimmer, Moritz Birkhold, 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, the need for secure data communication has increased. Here, the usage of quantum key distribution (QKD) offers fundamental advantages over classical key distribution. However, despite its high level of security, QKD comes a long with numerous challenges regarding the application of single photons. In this view, the decoy state protocol offers the possibility to implement QKD using classical light sources such as semiconductor lasers. Here, we present an approach for the realization of a monolithic 850 nm eight VCSEL array capable for QKD via the BB84 and decoy state protocol. Growth of the VCSEL structure takes place by metal-organic vapor-phase epitaxy (MOVPE) on a GaAs substrate. In order to obtain defined light polarization states, each VCSEL features an integrated polarization grating in its light emission window. To allow for operation in the GHz-regime and hence a high key rate generation, the VCSEL are arranged in a coplanar contact design. Electro-optical device characteristics regarding light polarization and high frequency operation are presented.

HL 43.5 Thu 16:15 POT 251

In-situ EBL fabrication of highly homogeneous micropillar laser arrays based on InGaAs quantum dots for neuromorphic computing — •Imad Limame[1], Ching-Wen Shih[1], Sven Rodt[1], Daniel Brunner[2], and Stephan Reitzenstein[1] — [1]Technical Univ. of Berlin, Germany — [2]Univ. Bourgogne Franche-Comté, France

As classical computers are reaching their limit, especially in novel fields such as machine learning and artificial intelligence, cost-effective hardware platforms, and new computing architectures are needed. We combine reservoir computing with a nanophotonic platform in an all-optical computing architecture, taking inspiration from neuroscience. Our approach aims to utilize diffractive coupling between 900 micropillars to create a large-scale processing reservoir. Due to the high number of microlasers and the use of a spatial light modulator, laser arrays with low lasing threshold powers and high spectral homogeneity are required. We develop the necessary nanophotonic platform by optimized growth and in-situ electron beam lithography (EBL) fabrication of micropillar laser arrays. The MOCVD growth focuses on increasing the optical gain of the InGaAs quantum dots, used as the gain medium and on the design of the microresonator to decrease the lasing threshold. The realized devices feature thresholds as low as 20 μW. In the second phase, low temperature in-situ EBL is performed. In this process, first a CL map is recorded to determine the local resonance of the planar microcavity before micropillar with suitable diameter to match a target wavelength are patterned by electron beam lithography. Finally, the resulting micropillar array is investigated via photoluminescence.

HL 43.6 Thu 16:30 POT 251

Multimode lasing in a microdisk nanolaser — •M. L. Drechsler[1], F. Nippert[2], L. Sung-Min Choi[2], M. R. Wagner[2], P. Boucaud[3], S. Reitzenstein[2], and Frank Jahnke[1] — [1]Institute for Theoretical Physics, University of Bremen, Bremen, Germany — [2]nstitute of Solid State Physics, Technische Universität Berlin, Berlin, Germany — [3]CRHEA, Université Côte d*Azur, 06560 Valbonne, France

We investigate the quantum emission properties of a GaN-based microdisk nanolasers with a diameter of 2 μm and β-factor close to unity, pushing the device in the regime of strongly reduced laser threshold. A quantum optical semiconductor laser model based on the cluster expansion technique is used to describe the pump-power dependent emission with one consistent set of material parameters, thereby identifying laser action. Photon correlations quantified by $g^{(1)}(\tau)$ and $g^{(2)}(\tau)$ are an essential tool for this research. Information about the energy spectrum and the detection characteristics of photons is encoded in them. In this device we observe multimode lasing. We show that the mode coupling between well-separated resonator modes has a significant influence on the emission characteristics. Furthermore, we analyze what influence the mode couplings have on photon correlations.

HL 44: Nitrides: Devices

Time: Thursday 15:00–17:00 Location: POT 112

HL 44.1 Thu 15:00 POT 112

Highly doped GaN:Ge/GaN:Mg tunnel junctions for novel GaN-based optoelectronic devices — •Christoph Berger, Armin Dadgar, and André Strittmatter — Otto-von-Guericke-Universität Magdeburg

We report on low resistive GaN-based tunnel junctions (TJs) implemented into optoelectronic devices grown by metalorganic vapor phase epitaxy. Very high donor concentrations, which are mandatory for low-resistive TJs, are achieved by using germanium instead of commonly used silicon. Fabricated TJ-LEDs show an increased light output by more than 60 % in comparison to conventional LEDs employing indium tin oxide contacts while exhibiting a comparable differential resistance of 1.2x10^{-2} Ωcm^2 at a current density of 100 A/cm^2 and no voltage penalty by the TJ. Higher light output is attributed to a better light extraction efficiency due to V-pits formed within the GaN:Ge layer. We currently apply such tunnel-junctions in edge-emitting laser diodes as well as in vertical-cavity surface-emitting lasers. Furthermore, we will demonstrate cascaded LEDs featuring three tunnel junctions and three pn-junctions stacked on top of each other. Overgrowth of the lower LED sections affects their radiative efficiencies. We investigate different annealing concepts for acceptor activation but also the impact of annealing on the radiative recombination in the InGaN active regions.

HL 44.2 Thu 15:15 POT 112

Mitigating damage induced by strongly ionising radiation in nitride layered structures — •Miguel C. Sequeira[1], Mamour Sall[2], Flyura Djurabekova[3], Kai Nordlund[3], Isabelle Monnet[2], Clara Grygiel[2], Christian Wetzel[4], and Katharina Lorenz[5] — [1]HZDR, Dresden, Germany — [2]CIMAP, Caen, France — [3]University of Helsinki, Finland — [4]RPI, New York, USA — [5]INESC-MN, & IST-Universidade de Lisboa, Portugal

Group-III nitrides are well-known for their high radiation resistance, which brings them to extreme radiation environments. GaN is known for having a high resistance to strongly ionising radiation, such as Swift Heavy Ions (SHI) [1,2]. However, the behaviour of other nitrides under this radiation is not well understood especially when in layered structures (e.g. InGaN/GaN in LED). Here, we inspect how InGaN/GaN quantum wells (QW) resist SHI. We solve the Two-Temperature Model (TTM) using Finite Element Methods to show how the high electronic conductivity of InGaN in a QW acts as a heat sink, reducing the intensity of the ion-induced thermal spike in the entire InGaN/GaN structure. Combining TTM-Molecular Dynamics simulations and Transmission Electron Microscopy images show that the presence of QW significantly decreases the overall radiation damage in a device. The results presented here can lead to new radiation damage mitigation techniques, predict functional changes in devices under long radiation exposure, and ultimately improve device design.

[1] M. C. Sequeira et al., Communications Physics (2021); [2] M. C. Sequeira et al., Small (2022)

HL 44.3 Thu 15:30 POT 112

A guide on designing high performance porous GaN DBRs — •Matthias Hoormann[1,2], Frederik Lüssmann[1,2], Florian Meierhofer[1,2], Jana Hartmann[1,2], and Andreas Waag[1,2] — [1]Institute of Semiconductor Technology, Technische Universität Braunschweig, Hans-Sommer-Str. 66, 38106 Braunschweig, Germany — [2]Laboratory for Emerging Nanometrology (LENA), Technische Universität Braunschweig, Langer Kamp 6, 38106 Braunschweig, Germany

Recently, porous GaN etching has gained significant attention, due to its broad variety of convenient applications for optoelectronic devices. Specifically, the introduction of nanoporous layers enables the quasi-epitaxial growth of low refractive index GaN-based compounds for applications such as vertical DBR mirror structures.

Whilst classical DBRs are designed in order to satisfy the quarter-wavelength-condition, porous GaN DBRs are subject to a competition between porosity and optimal constructive interference from the layer thicknesses. It is vital to understand the influence of the porosity, as deviations from typical DBR designs might be advantageous for the device performance as inferred from simulations.

In this contribution, we investigate the influence of different designs and etching parameters on the optical performance of a defined layer structure. Particularly, the interdependency between the etched porosity and the design porosity with respect to the optical device performance is investigated. To determine the porosity, a combination of optical measurements, simulations and a gravimetric approach is used.

HL 44.4 Thu 15:45 POT 112

PL enhancement from Mie resonant silicon-rich-nitride nanodisks — •Krishna Koundinya Upadhyayula and Jörg Schilling — Martin Luther Universität Halle-Wittenberg, Halle

PECVD grown silicon-rich-nitride (SRN) exhibits refractive indices up to 3.5 and a broad luminescence in the visible up to near IR wavelengths making it a viable candidate for a photonic platform for biosensing at the therapeutic window. After a fundamental study on the origin of this photoluminescence (PL) in SRN using spectral and time resolved PL, we demonstrate the impact of Mie resonances on the luminescence by fabricating single Mie resonant SRN nano-disks with sizes on the order of a few 100nm. Comparing the measured PL-spectra with theoretically modelled transmission and emission spectra from finite element simulations, the observed PL-peaks could be attributed to the coupling of the emitters to electric dipole, magnetic dipole and higher order multipole Mie resonances. Furthermore, we created 2D periodic arrays of such SRN-Mie resonators with periods between 300-500nm and an absolute size of 100mm2 using interference lithography. The fabricated arrays exhibited an up to 27x enhancement of the room-temperature PL compared to that of an unstructured sample increasing further up 54x after hydrogen passivation. Tuning the structure parameters, we identify the remaining impact of the individual Mie-resonances in the spectra and the features caused by the grating/Bragg-resonances of the collective photonic crystal structure. Ongoing time resolved measurements will elucidate the impact of Purcell enhancement on the observed PL due to the Mie resonances.

15 min. break

HL 44.5 Thu 16:15 POT 112

UVC-LEDs grown on HTA-AlN templates with low dislocation densities and high Si doping for strain management — •Tim Mampe[1], Sarina Graupeter[1], Giulia Cardinali[1], Sylvia Hagedorn[2], Tim Wernicke[1], Markus Weyers[2], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics, Hardenbergstraße 36, 10623 Berlin, Germany — [2]Ferdinand-Braun-Institut (FBH),Gustav-Kirchhoff-Straße 4, 12489 Berlin, Germany

High temperature annealing (HTA) of AlN layers reduces the threading dislocation density of such layers on sapphire substrates below 10^9 cm^{-2} enabling UVC-LEDs with improved efficiencies. However, the HTA AlN-layers are under high compressive strain after cooling down, which can lead to strain relaxation and defect formation during further LED heterostructure growth. The in-plane lattice constant can be increased by growing a Si-doped AlN layer on HTA-AlN. In this work we investigate the influence of such an AlN:Si-layer on the growth of UVC-LEDs emitting at 265nm on AlN/sapphire substrates with silicon doped as well as undoped AlN layer and different sapphire offcut angles (0.1°, 0.2°, 0.5°). We will discuss the morphology as well as the strain state of AlN and AlGaN layers as well as the electro-optical properties of multi quantum-well (MQW) and LED structures.

HL 44.6 Thu 16:30 POT 112

Intensity fluctuations of infrared and green photodiodes at constant current and its correlation with voltage fluctuations — •Danylo Bohomolov and Ulrich T. Schwarz — Chemnitz University of Technology, Chemnitz, Germany

One important issue for display and sensing applications in LEDs is the fluctuation of light intensity over time. The physical reasons behind this are not fully understood yet, e.g. defect-related blinking is dicussed. In addition, it is known that the noise of these devices has a strong correlation with their lifetime. Consequently, the noise of the infrared and green micro-LEDs will be measured here, after which the similarity of their behaviour will be investigated. Standard derivation and corner frequency between flicker noise and thermal noise are chosen as the main comparison parameters. For this purpose, their spectral power density of intensity fluctuations of the emitted light at

constant current is investigated. We use a linear controlled precision current source. A large area Si photodiode with amplification capability is used as detector, and the signal is measured using a low-noise transimpedance amplifier and a 24-bit analog-to-digital converter. In parallel, the voltage of the LED is measured to correlate fluctuations in voltage and intensity. We observe oscillations in the frequency range from 1 Hz to 15 kHz. The first measurements of the infrared LEDs showed the presence of 1/f and Johnson-Nyquist noise in this frequency range as expected.

HL 44.7 Thu 16:45 POT 112

Theoretical improvement of 40% in efficiency of AlGaN UV LED using evolution strategies optimization algorithm — •Lucie Leguay and Andrei Schliwa — Institute of Solid-State Physics, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin

Nowadays, LED light sources can be found in many technologies ranging from smart lamps to high-quality screen displays. In particular, ultraviolet (UV) LED light can be used to sterilise surfaces and food, to purify air and water and to detect gas and diseases.

However, the nitride-based existing technology is still lacking efficiency. One way to enhance the performance of such devices is to improve their design with optimization algorithms such as evolutionary algorithms which are inspired by biological evolution.

We report an increase of 40% in the theoretical internal quantum efficiency (IQE) of an AlGaN UV-emitting multiple quantum well nanostructure using an evolution strategies algorithm paired with the simulation sofware nextnano++.

HL 45: Functional semiconductors for renewable energy solutions II

Time: Thursday 15:00–17:15 Location: POT 6

HL 45.1 Thu 15:00 POT 6

Engineering interfaces in multilayer photoanodes for stable and efficient solar energy conversion — •Katarina-Sophie Flashar, Matthias Kuhl, Gabriel Grötzner, Laura Wagner, Lukas Wolz, Alex Henning, Ian D. Sharp, and Johanna Eichhorn — Walter Schottky Institute and Physics Department, Technical University Munich, Am Coulombwall 4, 85748 Garching, Germany

Photoelectrochemical (PEC) energy conversion is a promising approach for the direct conversion of solar energy into storable chemical fuels. In this context, tantalum nitride (Ta_3N_5) has attracted considerable interest due to a theoretical photocurrent density limit of 12.9 mA*cm^{-2} and a theoretical solar-to-hydrogen conversion efficiency of 15% under AM 1.5G illumination. However, currently Ta_3N_5 photoelectrodes suffer from poor stability, such as oxidative decomposition, under the harsh PEC operation conditions. To overcome these limitations, we investigate the protection of Ta_3N_5 photoelectrodes with ultra-thin catalyst layers deposited via plasma-enhanced atomic layer deposition. In these multilayer architectures, the metal oxide catalyst decreases the activation energy, provides active sites for water oxidation, and promotes charge extraction of photogenerated holes. Here, we use a combination of spectroscopic and microscopic methods to elucidate the impact on interfacial energetics, defect properties, charge transport, recombination, and catalytic reactions. The gained understanding of interfacial properties is applied to design efficient interfaces between semiconductor photoelectrodes and functional catalyst coatings for the realization of highly stable and efficient PEC systems.

HL 45.2 Thu 15:15 POT 6

Discovery of multi-anion antiperovskite as promising thermoelectric materials by computational screening — •Dan Han[1], Bonan Zhu[2], Kieran B. Spooner[2], Stefan S Rudel[1], Wolfgang Schnick[1], Thomas Bein[1], David O. Scanlon[2], and Hubert Ebert[1] — [1]Department of Chemistry, University of Munich, Germany — [2]Department of Chemistry, University College London, United Kingdom

The thermoelectric performance of existing perovskites lags far behind the state-of-the-art thermoelectric materials such as SnSe, PbTe and Bi2Te3. Despite halide perovskites showing promising thermoelectric properties, namely, high Seebeck coefficients and ultralow thermal conductivities, their thermoelectric performance is significantly restricted by low electrical conductivities. Here, we explore new multi-anion antiperovskites by global structure searches, and demonstrate their phase stability by first-principles calculations. Ca6NFSn2 and Sr6NFSn2 exhibit decent Seebeck coefficients and ultralow lattice thermal conductivities (< 1 W m-1 K-1). The weak chemical bonding between the heavy-atom cage-rattler Sn and alkaline-earth metal (Ca and Sr) inducing low-frequency optical modes coupling with heat carrying acoustic phonons in combination with strong bond anharmonicity give rise to ultralow lattice thermal conductivities. Notably, Ca6NFSn2 and Sr6NFSn2 show remarkably larger electrical conductivities compared to halide perovskite CsSnI3. Our exploration of multi-anion antiperovskites X6NFSn2 (X = Ca, Sr) realizes the "phonon-glass, electron-crystal" concept within perovskite structures.

HL 45.3 Thu 15:30 POT 6

Template realized well-defined nanostructures for energy storage and conversion — •Mo Sha, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Template-based technique provides a perfect approach to realize well-defined arrayed nanostructures within large-scale. We have developed nanostructuring techniques mainly using anodic aluminum oxide templates for fabricating functional nanostructures. The obtained well-defined nanostructures possess large-scale arrayed configuration, high structural density, perfect regularity and cost-effectiveness, and are highly desirable for constructing different nano-devices especially for energy storage and conversion applications, including rechargeable sodium-ion and potassium-ion batteries, supercapacitors, and photo electrochemical devices. The device performances demonstrated that the obtained nanostructures benefit these applications through the precise control over the structural features enabled by the geometrical characteristics of the templates. Refs: Nat Commun, 2022, 13 (1), 2435; Adv Energy Mater, 2021, 11 (15), 2001537. Nat Commun 2020, 11 (1), 299; Nat Nanotechnology, 2017, 12 (3), 244.

HL 45.4 Thu 15:45 POT 6

Optical and Photocatalytic Properties of $BiVO_4$ Nanoplatelets — •Philipp Bootz[1], Bharati Debnath[1], Kilian Frank[2], Markus Döblinger[3], Bert Nickel[2], Jacek Stolarczyk[4], and Jochen Feldmann[1] — [1]Chair for Photonics and Optoelectronics, Nano-Institute Munich, Physics Department, Ludwig Maximilians Universität (LMU), 80539 Munich, Germany — [2]Chair for Soft Condensed Matter, 80539 Munich, Germany — [3]Chair for Functional Nanosystems (Prof. Bein), Department Physical Chemistry, 81377 Munich, Germany — [4]Smoluchowski Institute of Physics, Jagiellonian University, 30-348 Krakow, Poland

Bismuth vanadate ($BiVO_4$) with a bandgap of about 2.4 to 3.1 eV is known as one of the best water-oxidizing semiconductors in the field of photocatalysis. It is a material which can crystallize in three different phases - orthorhombic, tetragonal and monoclinic - and is often used as thin films or micron-sized crystals. In this study, we report a novel solvothermal synthesis method to obtain colloidal BiVO4 nanoplatelets with a lateral size of less than 30 nm. We have performed X-ray diffraction and transmission electron microscopy measurements for their structural characterization. We compare the linear optical properties of the nanoplatelets with their three-dimensional pendants and discuss the microscopic origins for the observed differences. Finally, we present the results of photocatalytic experiments, where a gas chromatograph is used to measure the produced oxygen from water during illumination with light.

30 min. break

HL 45.5 Thu 16:30 POT 6

beneficial impact of KF post-deposition treatment on optical diode factor and non-radiative recombination of CIGSe absorbers — •Sevan Gharabeiki, Mohit Sood, Valentina Serrano Escalante, Taowen Wang, and Susanne Siebentritt — Department of Physics and Materials Science, University of Luxembourg, 4422 Belvaux, Luxembourg

The efficiency of the solar cells depends on the open circuit voltage (VOC), short circuit current (JSC), and fill factor (FF) which in turn depends on the diode factor. The quasi-Fermi level splitting (QFLS) is the upper limit for VOC and the optical diode factor (ODF) is the lower limit of the diode factor. It has been long known that post-deposition treatment (PDT) with heavy alkalis has a beneficial impact on CIGSe solar cells. An increase in the hole concentration, decrease in non-radiative recombination, and surface passivation have been reported by many studies. We present the effect of the KF PDT on the CIGSe absorbers with different deposition temperature. Our study shows that the KF PDT increases the (QFLS) and decreases non-radiative recombination for the samples deposited on soda lime glass with high deposition temperature. For the samples with low deposition temperature, the improvement in QFLS is mainly due to an increase in doping level. A combination of QFLS, lifetime and capacitive-voltage measurements were conducted to separate the doping effect from the non-radiative recombination effect. We propose that high concentration of Na is required to get the full effect of KF PDT, i.e. increase in the doping and decrease in the non-radiative recombination.

HL 45.6 Thu 16:45 POT 6

Tuning optical properties of graphitic carbon nitrides for photocatalytic applications — •Julian Hirschmann[1], Bharati Debnath[1], Matthias Kestler[1], Kilian Frank[2], Bert Nickel[2], and Jochen Feldmann[1] — [1]Chair for Photonics and Optoelectronics, Nano-Institute Munich and Department of Physics, Ludwig Maximilians Universität (LMU) — [2]Chair for Experimental Physics Prof. Rädler, Department of Physics, Ludwig Maximilians Universität (LMU)

In the field of photocatalysis, graphitic carbon nitrides have proven to be a promising and cost-effective material. The organic graphene like material built from heptazine or triazole rings enable various photocatalytic applications such as hydrogen evolution and ammonia production.

Graphitic carbon nitrides have a two-dimensional sheet-like structure, which is advantageous for photocatalytic applications. Our refined synthesis process provides a simple way to obtain nanosheets of different thicknesses and varying π-conjugation areas. Their impact on the optical properties such as absorption and photoluminescence are presented. The results are compared with recently published electronic band structure calculations and with more molecularly based exciton models. Finally, photocatalytic measurements have been carried out and the obtained efficiencies are compared with our data from time-integrated and time-resolved optical experiments.

HL 45.7 Thu 17:00 POT 6

Functionalization of TiO2 thin films with gold nanoparticles aiming at plasmonic photocatalysis — •Narmina O. Balayeva[1,2], Lu He[1], Dietrich R.T. Zahn[1,2], and Teresa I. Madeira[1,2] — [1]Semiconductor Physics, Institute of Physics, Chemnitz University of Technology, Reichenhainer Str. 70, 09126 Chemnitz, Germany — [2]Research Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, Rosenbergstraße 6, 09126 Chemnitz, Germany

Developing novel photocatalytic systems with improved charge separation that can exploit visible light is of great interest. Here, we investigated the functionalization of anatase TiO2 thin films with gold nanoparticles (Au NPs) for enhanced photocatalytic activity. The LSPR effect of Au NPs is studied by depositing them either on top of or embedding them beneath TiO2 thin films or mixing them homogeneously into the precursor solution before the films are prepared using the spin-coating technique. An amount of Au NPs relative to TiO2 (0.01 wt% -1 wt%) was employed to study the effect of photocatalytic degradation of acetone using an FTIR-based gas photo-reactor chamber with a set of 6 cool white light-emitting diodes (LED). The structure and morphology of the Au/TiO2 films were characterized with different techniques, i.e., Raman spectroscopy and X-ray diffraction (XRD), X-ray reflectivity (XRR), scanning electron microscopy (SEM), as well as atomic force microscopy (AFM). Spectroscopic ellipsometry (SE) was used for a complementary analysis of thickness, roughness, and, in addition, dielectric properties of the thin films.

HL 46: Members' Assembly

Themen unter anderem:

- Bericht
- Wahl der Fachverbandsleitung
- Informationen zur Frühjahrstagung 2024
- Verschiedenes

Time: Thursday 18:00–19:00 Location: POT 6

All members of the Semiconductor Physics Division are invited to participate.

HL 47: Oxide Semiconductors II

Time: Friday 9:30–11:30 Location: POT 81

HL 47.1 Fri 9:30 POT 81

Origin of Resistive Switching in $SrTiO_3$ — •Wahib Aggoune[1], Christian Carbogno[1], Martin Albrecht[2], and Matthias Scheffler[1] — [1]The NOMAD Laboratory at the FHI of the Max-Planck-Gesellschaft and IRIS-Adlershof of the Humboldt-Universität zu Berlin. — [2]Leibniz-Institut für Kristallzüchtung, 12489 Berlin.

Memristors may play a key role for the next generation of non-volatile memory devices. They are typically realized using materials that allow to switch between a low- and a high-resistance state. This effect has been recently observed in $SrTiO_3$ thin films, whereby a pronounced dependence of the switching properties on the growth conditions was found [1,2]. To shed light on the underlying atomistic mechanisms, we performed density-functional theory calculations and carefully analyzed the critical effects of different exchange-correlation functionals. We explored the most stable defects (vacancies, interstitial, substitutional) under Ti-*rich* conditions. The study reveals that the formation of a Ti_{Sr} antisite defect is energetically favorable and also induces a spontaneous polarization. It can be further stabilized by an additional nearby Sr-vacancy (Ti_{Sr}+V_{Sr}). Furthermore, such a defect complex increases the observed polarization. We discuss these results with respect to the experimentally observed resistive switching by analyzing the electronic properties and the polarization as well as the energy barriers for switching it.

[1] A. Baki, *et al.*, *Sci. Rep.* **11**, 7497 (2021).
[2] K. Klyukin, *et al.*, *Phys. Rev. B* **95**, 035301 (2017).

HL 47.2 Fri 9:45 POT 81

Second harmonic generation of blue series excitons in Cu_2O — •Andreas Farenbruch[1], Dietmar Fröhlich[1], Heinrich Stolz[2], Dmitri R. Yakovlev[1,3], and Manfred Bayer[1,3] — [1]Experimentelle Physik 2, TU Dortmund, Dortmund, Germany — [2]Institut für Physik, Universität Rostock, Rostock, Germany — [3]St. Petersburg, Russia

Excitons are Coulomb-bound complexes of electrons and holes in semiconductors with a discrete hydrogen-like energy series. The yellow exciton series in Cu_2O involves excitations between the highest valence and lowest conduction band and it presents an ideal platform for investigations of exciton physics with Rydberg states up to a principal quantum number of n=28. Excitations, that involve the same valence band but the second lowest conduction band belong to the so-called blue series. Access in linear optical spectroscopy to these states is hard to achieve due to the high absorption in this spectral range. Optical second harmonic generation (SHG) is therefore a suitable investigation method. By analyzing the measured polarization dependence of the SHG signal and comparing it with group theoretical simulations, the magneto-Stark and Zeeman effects are identified as the SHG mechanisms involved. The 1S, 2S and 2P excitons and magneto-excitons up to n=8 in magnetic fields up to 10 T are detected. By analyzing their magnetic-field shift and polariton effect, key properties such as the energies of the exciton resonances, the Rydberg energy, the band gap, the reduced exciton mass, the anisotropy of the conduction band mass and the exciton radius are obtained for the blue exciton series.

HL 47.3 Fri 10:00 POT 81

Electrical and thermoelectrical properties of the two-dimensional electron gas in polar discontinuity doped BaSnO3/LaInO3 heterostructure — •Fazeel Zohair, Georg Hoffmann, and Oliver Bierwagen — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 7, Berlin, Germany

Transparent semiconducting oxides (TSOs) are key players for optoelectronic devices, among which high frequency applications benefit from electrical properties of two-dimensional electron gases (2DEGs) . In this contribution we demonstrate the electrical and thermoelectric properties of the 2DEG at the interface between a nonpolar perovskite oxide BaSnO3 and a polar perovskite oxide LaInO3, grown by plasma assisted molecular beam epitaxy. The electrical and thermoelectric properties are analyzed using Seebeck measurements and van der pauw-Hall measurements. Integrating the charge carrier concentrations from both measurements, we were able to deduce the thickness of the charge carrier system.

HL 47.4 Fri 10:15 POT 81

Analysis of thickness distributions for combinatorial pulsed laser deposition — •Clemens Petersen, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig Felix-Bloch-Institut, Leipzig, Deutschland

Recently combinatorial deposition methods have increasingly gained scientists* attention, due to the high experimental throughput and resource-wise efficiency they offer in materials discovery. This enables fast screening of material properties of multinary material systems using just a single sample. By employing pulsed laser deposition with our segmented target approach [1] we successfully realized the deposition of α-$(Al_xGa_{1-x})_2O_3$ with continuous composition spread over the whole composition range on a single 2-inch sapphire wafer [2]. Accompanied by the usage of high-throughput measurements such as spectroscopic ellipsometry and x-ray diffraction, the characterization of the material systems' physical properties with high chemical resolution and comparably low efforts becomes feasible. By employing the plasma plume expansion model suggested by Anisimov *et al.* [3] and the resulting spatial material-deposition distribution we calculate binary growth rates as function of position enabling us to predict film thickness and composition locally. Thereby the deposition of group III sesquioxides can be described exceptionally well. We further show that the binary distributions can be used to predict the combinatorial deposition of ternary alloys with high precision. [1] H. von Wenckstern *et al.*, pss(b), Vol. 257, 1900626 [2] A. Hassa *et al.*, pss(b), Vol. 258, 2000394 [3] S. I. Anisimov *et al.*, Phys. rev. B, Vol 48, 12076.

15 min. break

HL 47.5 Fri 10:45 POT 81

Cloud in cell scheme based stochastic modelling of $BiFeO_3$ memristor for circuit simulations — •sahitya yarragolla[1], nan du[2,3], torben hemke[1], xianyue zhao[2,3], ziang chen[2], and thomas mussenbrock[1] — [1]Chair of Applied Electrodynamics and Plasma Technology, Ruhr University Bochum, Germany — [2]Institute for Solid State Physics, Friedrich Schiller University Jena, Jena, Germany — [3]Department of Quantum Detection, Leibniz Institute of Photonic Technology , Jena, Germany

In recent years, analog memristive devices have been extensively investigated for neuromorphic computing and hardware security applications. It is found that these devices show excellent properties such as long retention time, intrinsic stochasticity, and fast switching. However, the switching mechanism in these devices from the physics point of view is still under discussion. Therefore, in this work, we focus mainly on understanding the resistive switching based on the transport of oxygen vacancies in the interface-type Au/$BiFeO_3$ (BFO)/Pt/Ti memristive devices using a 1D cloud-in-a-cell model. The proposed model combines the advantages of both 1D concentrated and 3D distributed models in a single model. The model is stochastic and computationally less expensive, making it suitable for circuit simulations. The calculated I-V characteristics of BFO memristor using the proposed are in excellent agreement with the experimental results. Furthermore, the response of the BFO memristor to changes in electrical properties, temperature and retention characteristics are analyzed, and the results show reasonable agreement with experimental findings.

HL 47.6 Fri 11:00 POT 81

Comparing processing strategies for Indium oxide field-effect transistors — •Fabian Schöppach, Clemens Petersen, Holger von Wenckstern, and Marius Grundmann — Felix Bloch Institute for Solid State Physics, Universität Leipzig, Germany

Indium oxide (In_2O_3) combines promising physical properties such as high carrier mobility and transparency in the visible. However, due to its tendency to form an electron accumulation layer on its surface (SEAL), the use of In_2O_3 in active devices is generally difficult. We use the published strategies, compensating Mg doping [1] and oxygen plasma treatment [2], to suppress SEAL formation and allow the films to be used in FET devices. In addition, In_2O_3 as sesquioxide is a very robust material that resists classical patterning processes such as wet chemical etching.

We identified two different fabrication strategies to structure our films laterally: Plasma-assisted etching and using a wet-chemical soluble sacrificial layer. In this work, both strategies are compared re-

garding additionally necessary processing steps and the final devices' performance. We used In_2O_3 films grown by pulsed laser deposition. For the source and drain contacts, gold was deposited via inert ambient sputtering. Schottky gate diodes were fabricated in a reactive sputtering process, which is a prerequisite for obtaining electrically rectifying contacts to In_2O_3 [3].

[1] Schmidt, et al. physica status solidi (b) 252.10, 2304–2308 (2015)
[2] Michel, et al. ACS Appl. Mater. Interf. 11, 27073–27087 (2019)
[3] von Wenckstern, et al. APL Materials 2.4, 046104 (2014)

HL 47.7 Fri 11:15 POT 81

Charge carrier diffusion and localization in metal oxide photoabsorbers — •Hannes Hempel, Markus Schleuning, Klaus Schwarzburg, Rainer Eichberger, Roel van de Krol, Moritz Kölbach, Fatwa F. Abdi, and Dennis Friedrich — Helmholtz-Zentrum Berlin, Germany

Long diffusion lengths of photo-excited charge carriers are crucial for high power conversion efficiencies of photoelectrochemical and photovoltaic devices. However, in metal oxids are effects such as (multiple-)trapping, carrier localization and polaron formation can lead to time-varying mobilities and lifetimes that are not accounted for in the conventional analysis. Therefore, here, a generalized analysis is presented that determines the diffusion length directly from the integral of a photoconductivity transient, regardless of the nature of carrier relaxation. This approach is presented on amorphous silicon, a prototype of disordered materials, and BiVO4, one of the most studied photoanode materials for solar water splitting. Our generalized analysis allows monitoring the temporal evolution of the charge carrier displacement, which converges for both materials after ˜100 ns to a diffusion length of a few tens of nanometers. For BiVO4, the obtained diffusion length is significantly shorter than the typical thin film thickness, which rationalizes the photocurrent loss in the corresponding photoelectrochemical device. Finally, we probe several metal other prominent metal oxide photoabsorbers, namely Fe2O3, FeVO4, CuFeO2, α-SnWO4, BaSnO3, and CuBi2O4, and find sings of carrier localization on the nanometer scale, which limits the charge carrier diffusion.

HL 48: Ultra-fast Phenomena

Time: Friday 9:30–12:00 Location: POT 361

HL 48.1 Fri 9:30 POT 361

Characterizing the nonadiabatic tunneling dynamics in solid-state high harmonic generation — •Ruixin Zuo[1], Xiaohong Song[2], Shuai Ben[2], Weifeng Yang[2], and Torsten Meier[1] — [1]Department of Physics, Paderborn University, Warburger Str. 100, D-33098 Paderborn, Germany — [2]School of Science, Hainan University, Hainan 570288, China

Tunneling is a fundamental quantum process which may result from light-matter interaction. High-harmonic radiation, as an ultrafast phenomenon initiated by the tunneling excitation, carries information about the electronic dynamics in the classically forbidden region. We introduce a quantum trajectory analysis to identify the underlying quantum dynamics governing solid-state high harmonics which improves the understanding of neighboring-atoms collisions [1]. It is revealed that properties of the electron-hole pairs when emerging in the classically allowed region like the group velocity and the relative displacement are dictated by the nonadibaticity of tunnel ionization and are crucial in determining the subsequent propagation and radiation. Furthermore, we show that the two-color high harmonic spectroscopy validates the quantum trajectory analysis and enables us to probe the tunneling dynamics in strongly driven solid-state systems.
[1] R. Zuo, A. Trautmann, G. Wang, W.-R. Hannnes, S. Yang, X. Song, T. Meier, M. Ciappina, H. T. Duc, and W. Yang, Neighboring atom collisions in solid-state high harmonic generation, Ultrafast Science **2021**, 9861923 (2021).

HL 48.2 Fri 9:45 POT 361

Compact, CEP-stable, few-cycle OPCPA for single attosecond pulse generation — •Bastian Manschwetus, Filippo Campi, Thomas Braatz, Sebastian Starosielec, Jan-Heye Buss, Michael Schulz, and Robert Riedel — Class 5 Photonics, Hamburg, Germany

Attosecond technology pathed the way for studying ultrafast electronic processes in atoms, molecules, solids, and complex many body systems. Carrier envelope phase (CEP) stabilization in the few-cycle regime is a key enabler of this technology. A crucial step forward is the demonstration of high-repetition rate optical parametric chirped-pulse amplifier (OPCPA) systems for the generation of phase-stable few-cycle, μJ-level driver pulses for high-harmonic-generation (HHG). In this work, we present an OPCPA providing white light seeded, actively controlled CEP stable, 9 fs pulses around 900 nm center wavelength with 30 μJ pulse energy as a high-harmonic driver for attosecond experiments at 200 kHz repetition rate.

HL 48.3 Fri 10:00 POT 361

Transient Optical Property Changes in Semimetals with Strong Electron-Phonon Coupling — •Fabian Thiemann[1], Germán Sciaini[2], Alexander Kassen[1], Tyler Lott[2], and Michael Horn-von Hoegen[1] — [1]University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany — [2]University of Waterloo, 200 University Avenue West, Waterloo, ON N2L 3G1, Canada

Group V semimetals, such as bismuth used in this study, are well known for their strong electron-phonon coupling due to the inherent Peierls distortion of their lattice. In particular, the displacively excited coherent A_{1g} phonon mode plays an important role in ultrafast studies on Bi. With knowledge of the excitation density we used a series of thin Bi films on Si(111) to reconstruct the transient dielectric function in an all optical pump-probe experiment. Though we only access the first half ps of dynamics, we separate the contributions from the excited carrier system and the coherent atomic motion. Our results suggest that we can describe the changes in optical properties caused by the non-equilibrium distribution of carriers still similar to a thermal dependency in equilibrium. In the regime of high excitation densities, we no longer can use the two-band Raman susceptibility approach to describe changes caused by the coherent phonons. We suggest that the light scattering is greatly enhanced by the excited carriers and that recently proposed band shifts in the time domain mainly define this part of changes of the dielectric function.

HL 48.4 Fri 10:15 POT 361

Ultrafast optical control of polariton energy in an organic semiconductor microcavity — •K.E. McGhee[1,2], M. Guizzardi[3], R. Jayaprakash[1], K. Georgiou[1,4], G. Cerullo[3,5], T. Jessewitsch[6], A. Zasedatelev[7], U. Scherf[6], T. Virgili[5], P.G. Lagoudakis[7], and D.G. Lidzey[1] — [1]University of Sheffield, UK — [2]Universität Leipzig, Germany — [3]Politecnico di Milano, Italy — [4]University of Cyprus, Cyprus — [5]Istituto di Fotonica e Nanotecnologia-CNR, Italy — [6]Universität Wuppertal, Germany — [7]University of Southampton, UK

Exciton-polariton condensates are of great interest due to their potential applications in polariton logic devices, nonlinear photonic integrated circuits and quantum simulators. In this work, we have fabricated polariton microcavities designed to allow the dynamic trapping and manipulation of such condensates using ultrashort laser pulses. Using transient pump-probe spectroscopy, we have saturated the electronic transition of a weakly-coupled dye in a cavity containing a second strongly-coupled dye. In doing so, we alter the cavity effective refractive index and therefore the position of the lower polariton branch. We demonstrate a maximum blueshift of this mode of 12 meV, dependent on the pump fluence, and show that this effect is ultrafast, with switch 'on' and 'off' times of less than 1 ps. Utilising this controllable energy shift, it should be possible to dynamically 'write' energy barriers into organic polariton microcavities without affecting the coupling strength. This would allow important studies on interacting polariton condensates for the development of next generation quantum devices.

HL 48.5 Fri 10:30 POT 361

Imaging nanoscale electron dynamics with extreme ultraviolet radiation — •Hung-Tzu Chang[1], Sergey Zayko[1], Jakob Hagen[1], Murat Sivis[1,2], and Claus Ropers[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, 37077 Goettingen, Germany — [2]4th Physical Institute, University of Goettingen, 37077 Goettingen, Germany

Non-equilibrium electronic processes such as electron thermalization, ballistic transport, and spin diffusion, occur at femtosecond time- and nanometer length-scales. While ultrafast spectroscopic methods can trace the temporal evolution of electronic states [1], capturing those dynamics in real space remains challenging. Here we demonstrate time-resolved coherent diffractive imaging using a table-top extreme ultraviolet (EUV) source based on high harmonic generation [2,3], where the sample is first excited by a near-infrared pump pulse and probed with core-level absorption induced by a time-delayed EUV pulse. The valence electron dynamics can be retrieved from the spatially resolved changes of the EUV field amplitude and phase exiting the sample after localized photoexcitation. This technique provides nanometer spatial resolution in addition to the time resolution and element specificity of femtosecond table-top core-level spectroscopy, and paves the way for further understanding of the mechanisms of photophysical processes in condensed matter.

[1] Chang et al., Phys. Rev. B 103(6), 064305 (2021). [2] Kfir et al., Sci. Adv. 3(12), eaao4641 (2017). [3] Zayko et al., Nat. Commun. 12(1), 6337 (2021)

15 min. break

HL 48.6 Fri 11:00 POT 361

Coherent-to-incoherent crossover of photoexcited electron-phonon dynamics in 2D materials — •Enrico Perfetto[1,2] and Gianluca Stefanucci[1,2] — [1]Dipartimento di Fisica, Universita' di Roma Tor Vergata, Via della Ricerca Scientifica 1, 00133 Rome, Italy — [2]INFN, Sezione di Roma Tor Vergata, Via della Ricerca Scientifica 1, 00133 Rome, Italy

We present a first principles nonequilibrium Green's function approach to describe the carrier and nuclear dynamics of 2D materials. Our scheme is based on the simultaneous propagation of the electronic and phononic degrees of freedom and includes the GW, Ehrenfest, and Fan-Migdal self-energies. The method scales linearly with the propagation time, and allows to describe in a conserving fashion the retarded Coulomb screening and the cooling dynamics of hot carriers via phonon emission. Numerical results are provided for a monolayer MoS2 photoexcited above the gap. The intra-valley scattering is responsible for an ultrafast carriers migration toward the band edges already during pumping. Intervalley scattering occurs on a longer timescale, of the order of a few hundreds of femtoseconds. At high carrier density the energy exchange between electrons and phonons is very efficient, leading to a sizable increase of the lattice temperature within one picosecond. During this processes the electronic coherence is lost. The lattice coherence, instead, survives for much longer. Several hundreds of femtoseconds after the dephasing of the electronic polarization the nuclear displacements still exhibit undamped oscillations.

HL 48.7 Fri 11:15 POT 361

Coherent versus incoherent excitons: Stability, time-dependent ARPES spectrum and Floquet topological phases — •Gianluca Stefanucci[1,2] and Enrico Perfetto[1,2] — [1]Dipartimento di Fisica, Universita' di Roma Tor Vergata, Via della Ricerca Scientifica 1, 00133 Rome, Italy — [2]INFN, Sezione di Roma Tor Vergata, Via della Ricerca Scientifica 1, 00133 Rome, Italy

We consider a band insulator turning into a nonequilibrium (NEQ) exciton superfluid (XS) after resonant pumping. The NEQ-XS is characterized by self-sustained coherent oscillations of the superfluid condensate. We show that the ARPES spectrum from long probe pulses features a subgap excitonic sideband; it originates from the condensate-dressing of the conduction states and it has an intensity proportional to the excitonic wavefunction squared [PRB94, 245303 (2016); PRM3, 124601 (2019)]. Reducing the probe duration below the condensate period the ARPES signal becomes periodic in the impinging time of the probe [PRB101, 041201(R)(2020)]. The stability of the NEQ-XS as the conduction density grows is jeopardized by the increased screening efficiency of the looser excitons. Nonetheless, a proper nonequilibrium self-consistent treatment of screening indicates that NEQ-XS is stable up to relatively high densities [PRB102, 085203 (2020)]. We also show that a p-wave NEQ-XS at high enough density undergoes a Floquet topological transition [PRL125, 106401 (2020)]. Phonon-induced decoherence eventually transforms the XS phase into an incoherent exciton-polaron fluid. During this process the excitonic sideband broadens and red-shifts (Stokes shift) [PRB103, 245103 (2021)]

HL 48.8 Fri 11:30 POT 361

Intermolecular conical intersections in acceptor-donor-acceptor aggregated molecules — •Somayeh Souri[1], Katrin Winte[1], Antonietta De Sio[1], Christoph Lienau[1], Elena Mena-Osteritz[3], Peter Bäuerle[2], Teresa Kraus[3], Fulu Zheng[2], Mohamed Madjet[2], and Sergei Tretiak[4] — [1]University of Oldenburg, Germany — [2]University of Bremen, Germany — [3]Ulm University, Germany — [4]Los Alamos National Laboratory, USA

In molecules, strong coupling between electronic excitations and vibrational modes may result in conical intersections (CoIns) of multidimensional potential energy surfaces. At CoIns different electronic states cross and couple strongly via vibrational modes. This results in large nonadiabatic couplings violating the Born-Oppenheimer approximation. While CoIns are ubiquitous in molecules, not much is known about their occurrence and relevance for intermolecular ultrafast energy and charge transfer dynamics in the solid state. Here, we reveal the existence of intermolecular CoIns in thin films of aggregated acceptor-donor-acceptor-type oligomers by ultrafast two-dimensional electronic spectroscopy (2DES). The 2DES maps show a grid-like peak pattern at early times, followed by a rapid reduction of the peak spacings which transforms into a featureless map after only ~40 fs. We take this abrupt change in the 2DES maps as clear evidence for the passage of the optically launched vibrational wave packet through the intermolecular CoIn in the thin films. Our results, which are confirmed by simulations, suggest new opportunities for guiding the coherent flow of energy and charge in solid-state nanostructures.

HL 48.9 Fri 11:45 POT 361

Potential signatures of hydrodynamic transport captured by THz high harmonic generation — •Tim Priessnitz[1], Thales de Oliveira[2], Liwen Feng[1,3], Min-Jae Kim[1,3], Sergey Kovalev[2], Bernhard Keimer[1], and Stefan Kaiser[1,3] — [1]Max-Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [3]Institute of Solid State and Materials Physics, Technical University Dresden, 01069 Dresden, Germany

Terahertz high harmonic generation (THz HHG) is a common property of nonlinear systems. Recently it has been used to investigate fundamental principles that govern transport and nonlinear dynamics in novel quantum materials like graphene or Dirac semimetals. However, these studies have not yet been successfully extended to low temperatures where hydrodynamic effects come into play. Optical phenomena such as THz HHG are proposed to provide a more efficient way to probe hydrodynamic effects than previously studied DC transport measurements, which identified the delafossite $PdCoO_2$ as a candidate to observe such properties. Here, we report on THz HHG in thin films of $PdCoO_2$ at low temperatures and we will discuss potential signatures of hydrodynamics, contributing to the ongoing puzzle of low-temperature origins of THz HHG.

HL 49: Quantum dots: Devices

Time: Friday 9:30–11:45 Location: POT 151

HL 49.1 Fri 9:30 POT 151

Gate-based protocol simulations for quantum repeaters using quantum-dot molecules in switchable electric fields — •Steffen Wilksen, Frederik Lohof, and Christopher Gies — Institute for Theoretical Physics, University of Bremen, Bremen, Germany

Semiconductor quantum dots provide a promising platform for applications in quantum information technologies, such as quantum repeaters, which enable secure quantum communication over long distances. Two quantum dots, separated by a small tunnelling layer, form a so-called quantum dot molecule (QDM), which exhibits properties similar to classical molecules. Their energy levels can be tuned by applying an external electric field, thereby allowing to perform gate operations. We consider QDMs in switchable electric fields towards quantum-repeater realizations. The time dependence that arises from performing gate operations requires a careful treatment of the system-bath interaction. We treat the QDM as an open quantum system using an explicitly time-dependent Redfield master equation approach, accounting for the time dependence of the interaction rates beyond more simple Lindblad approaches. Based on our approach, we investigate the adiabatic and non-adiabatic behaviour of the system for different switching speeds and determine achievable execution times for gate operations with currently existing QDMs.

HL 49.2 Fri 9:45 POT 151

Heterogeneous integration of telecom c-band emitting quantum dots on silicon photonics platform by adhesive bonding — •Ponraj Vijayan, Fiona Braun, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart, Germany

Silicon photonics for telecommunications applications has garnered much attention recently. The optical transparency and the large refractive index contrast of silicon in the telecommunication wavelengths allow the implementation of high-density photonic integrated circuits. The drawback of silicon photonics is that there is no native light source due to the indirect band-gap nature of silicon. Integration of III-V material, which offers outstanding optical emission properties, on silicon provides a potential solution. The direct growth of III-V materials on silicon is the most desired approach because it is economically favourable. However, it is challenging because of large lattice mismatch between the III-V materials and silicon. An alternate approach for large-scale integration is through heterogeneous integration of thin III-V membrane using adhesive bonding technique. For such integration, it is crucial to have a robust bonding procedure which provides a uniform bonding layer with a desired thickness for efficient light coupling between III-V active layer and the silicon photonic platform. Our group has previously developed InAs QD/InGaAs MMB/GaAs substrate structures for long-distance optical fiber applications [3]. Here, we report on the route to integrate the telecom C-band emitting InAs QD on silicon photonic platform using adhesive bonding.

HL 49.3 Fri 10:00 POT 151

Investigation of optical properties of open-fiber cavities embedding semiconductor quantum dots emitting in the telcom O-band — •Nam Tran[1], Julian Maisch[1], Jonas Grammel[2], Julia Wecker[1], Thomas Herzog[1], Robert Sittig[1], Ponraj Vijayan[1], Michael Jetter[1], Simone L. Portalupi[1], David Hunger[2], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen , Center for Integrated Quantum Science and Technology (IQST) and SCoPE , University of Stuttgart, Stuttgart, Germany — [2]Physikalisches Institut , Karlsruher Institut für Technologie (KIT), Karlsruhe, Germany

Single photon sources operating at telecom wavelength play a central role in quantum information, in particular when long-distance implementations are targeted. Highly promising candidates are semiconductor quantum dots (QD). Cavity quantum electrodynamics is often used to tailor the emission properties and, in case of photon sources, enhance their performances. However, limiting factors like spatial and spectral mismatch can be detrimental to the cavity-emitter interaction. Using tunable fiber cavities can overcome these limitations. Additionally, since the fiber coupling is intrinsically given in these cavities the integration into the already existing fiber network is facilitated. Here, we made a thorough investigation of the optical properties of open fiber cavities embedding semiconductor QDs emitting in the telecom O-band. Moreover, deterministic positioning of individual QDs enables the comparison of the optical properties within and outside the cavity.

HL 49.4 Fri 10:15 POT 151

Higher order effective coefficients in Ge/Si core/shell nanowire devices — •Sebastian Miles[1,2], Piotr Rozek[1,2], Mert Bozkurt[1,2], Dániel Varjas[3], and Michael Wimmer[1,2] — [1]QuTech, Delft University of Technology, Delft 2600 GA, The Netherlands — [2]Kavli Institute of Nanoscience, Delft University of Technology, Delft 2600 GA, The Netherlands — [3]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany

Germanium based nanowires are prominent platforms in mesoscopic physics because of their tunable spin-orbit interaction. This property makes them an interesting candidate for hole-qubit devices or as a platform for Majoranas. Hence, a good understanding of effective models for the relevant degrees of freedom in these devices is of great importance. We revisit the subject of effective Hamiltonians and effective coefficients for efficient nano-device control in Ge/Si core/shell semiconductor nanowires from a perturbation theory perspective. We elaborate on relevant terms and present numerical and semi-analytical results of Lowdin perturbation theory to second order. We discuss the consequences of higher order terms on the effective models of interest for device applications.

30 min. break

HL 49.5 Fri 11:00 POT 151

Interfacing Semiconductor Quantum Dots with Photonic Wire Bonds — •Marco De Gregorio[1], Shangxuan Yu[2,3], Donald Witt[2,3], Becky Lin[2,3], Matthew Mitchell[2], Tobias Huber-Loyola[1], Lukas Chrostowski[2,3], Jeff F. Young[2,4], Andreas Pfenning[1,2], and Sven Höfling[1] — [1]Lehrstuhl für Technische Physik, Julius-Maximilians-Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Stewart Blusson Quantum Matter Institute, University of British Columbia, Vancouver, British Columbia V6T 1Z4, Canada — [3]Department of Electrical and Computer Engineering, University of British Columbia, Vancouver, British Columbia V6T 1Z4, Canada — [4]Department of Physics and Astronomy, University of British Columbia, Vancouver, British Columbia V6T 1Z1, Canada

We present first experimental results of an alternative extraction technique of single photons emitted by semiconductor quantum dots. For this purpose, a photonic wire bond is directly attached to the end facet of a waveguide containing In(Ga)As semiconductor quantum dots grown by molecular beam epitaxy and connected to a single-mode optical fiber. We perform above-band and optical resonant excitation of the quantum dot and find that in this configuration, cross-polarization filtering of the single photons can be avoided, while measuring a steady stream of single-photons in fiber. The coupling efficiency can be further improved by optimized mode matching between photonic wire bond and waveguide.

HL 49.6 Fri 11:15 POT 151

Deterministically fabricated InAs quantum dot based single-photon sources at telecom wavelengths — •Monica Pengerla[1], Alkaales Mohanad[2], Ranbir Kaur[2], Jan Donges[1], Lucas Bremer[1], Johannes Schall[1], Sven Rodt[1], Mohamed Benyoucef[2], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany — [2]Institute of Nanostructure Technologies and Analytics (INA), Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

Quantum dot (QD) based single-photon sources are key elements of photonic quantum networks. Most interesting are sources emitting at telecom wavelengths to enable long distance fiber-based quantum communication. Here, we report on deterministically fabricated single-photon sources based on InAs QDs grown on InP substrate. Numerical simulations of such QD heterostructures with backside distributed

Bragg reflector reveal photon extraction efficiency exceeding 50% when QDs are integrated into mesa or circular Bragg grating structures. A state-of-the-art electron beam lithography (EBL) system with integrated low temperature cathode luminescence (CL) system allows us to perform in-situ EBL at telecom wavelengths. For noisy CL maps, an advanced approach for machine learning enhanced in-situ EBL to enhance the maps at telecom wavelengths for better integration of QDs into photonic structures is used. Micro-photoluminescence studies reveal the optical properties of the fabricated quantum devices.

HL 49.7 Fri 11:30 POT 151

GaSb Quantum Dots as Emitters of Telecom S-Band Single Photons — •Johannes Michl[1], Giora Peniakov[2], Andreas Pfenning[1], Joonas Hilska[2], Abhiroop Chellu[2], Teemu Hakkarainen[2], Tobias Huber-Loyola[1], Mircea Guina[2], and Sven Höfling[1] — [1]Technische Physik, Julius-Maximilians-Universität Würzburg, Germany — [2]Physics Unit / Photonics Faculty of Engineering and Natural Sciences, Tampere University, Finland

Over the last few years, several semiconductor quantum dot (QD) material platforms like In(Ga)As)/ GaAs and InAs/InP have emerged as resources for non-classical light and spin-photon interfaces in the telecom wavelength range. However, there is not much data on the optical and spin properties of GaSb QDs, despite it being a physically rich system. For example, it is possible to switch between direct and indirect bandgap by controlling the size of the quantum dots. Moreover, due to reduced strain, it is expected to have less quadrupole nuclear interaction resulting in enhanced spin dephasing times, similar to what was recently observed in GaAs QDs in AlGaAs. Here, we investigate the (quantum-) optical properties of GaSb quantum dots which are fabricated by filling droplet-etched nanoholes in an AlGaSb matrix and exhibit photoluminescence (PL) with a narrow linewidth in the telecom S-band. We perform polarization resolved magneto-PL studies to investigate charge complexes in our sample and perform correlation measurements to evaluate the use of GaSb quantum dots as a source of indistinguishable single photons.

HL 50: Materials and devices for quantum technology III

Time: Friday 9:30–13:00 Location: POT 251

HL 50.1 Fri 9:30 POT 251

3D magnetic resonance tomography of nitrogen vacancy centers with sub-10nm resolution — •Mohammad T Amawi[1,2], Andrii Trelin[1], You Huang[1], Georg Braunbeck[2], Francesco Poggiali[1], and Friedemann Reinhard[1] — [1]Institute for Physics, Quantum Technology, University of Rostock, Germany — [2]Physics Department, Technical University of Munich, Germany

We present a device for three-dimensional magnetic resonance tomography with nanoscale resolution, and apply it to image the spatial position of a nitrogen-vacancy center (NV) cluster in bulk diamond. Three orthogonal magnetic field gradients, generated from currents in microfabricated gold conductors, are used to create a position-specific Larmor frequency of the NV ground state spins. Measuring this frequency by pulsed optical-microwave spectroscopy, we determine the position of each NV center in 3D.

I will report on fabrication of the device, based on a liftoff process and maskless lithography, as well as the geometry required to create three orthogonal magnetic fields. The measurement protocol for 3D imaging will be discussed, as well as hardware and software means to reduce the shot-to-shot field variation, caused by electrical noise, down to 0.1%. This level of stability enabled us to demonstrate 3D imaging with around 5 nm spatial resolution. I will conclude with an outlook addressing how the resolution can be further improved by reducing the dimensions of the micro wires, and how it could be extended to image spins deposited on the diamond surface.

[1] Arai, K. et al. Nat. Nanotechnol. 10 (2015)

HL 50.2 Fri 9:45 POT 251

3D printing as an enabling tool for quantum technologies — •Pavel Ruchka[1], Ksenia Weber[1], Sina Hammer[2], Carlos Jimenez[3], Simon Thiele[3], Johannes Drozella[3], Tim Langen[2], Alois Herkommer[3], and Harald Giessen[1] — [1]4th Physics Institute, Research Center SCoPE and Center for Integrated Quantum Science and Technology, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]5th Physics Institute and Center for Integrated Quantum Science and Technology, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [3]Institute of Applied Optics (ITO) and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 9, 70569 Stuttgart, Germany

Nowadays, a lot of effort is given to making quantum technologies more usable for day-to-day life. This involves many aspects, such as developing quantum computers with a large number of qubits, creating quantum gates with high fidelity, and establishing a large-scale communication links with quantum repeaters. Miniaturizing such quantum devices remains nevertheless a highly relevant issue. For this, the 2-photon polymerization (2PP) based 3D printing comes in handy. In this talk, we present several miniature 3D printed optical and mechanical components, which enable the optical trapping of atoms and coupling quantum emitters and detectors to fibers or chips. These devices have an exceptionally compact footprint and a comparably high efficiency. With the ease of production of such components, 2PP can be scaled for the future requirements of highly compact and efficient quantum devices.

HL 50.3 Fri 10:00 POT 251

Spatially controlled fabrication of telecom single-photon emitters in Si by focused ion beam implantation — •Nico Klingner[1], Michael Hollenbach[1,2], Nagesh Jagtap[1], Lothar Bischoff[1], Ciaran Fowley[1], Ulrich Kentsch[1], Gregor Hlawacek[1], Artur Erbe[1], Nikolay Abrosimov[3], Manfred Helm[1], Yonder Berencen[1], and Georgy Astakhov[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany — [2]Technische Universität Dresden, 01062 Dresden, Germany — [3]Leibniz-Institut für Kristallzüchtung (IKZ), 12489 Berlin, Germany

Single photon emitters (SPE) are the starting point and foundation for future photonic quantum technologies. We present the laterally controlled fabrication of single G and W centers in silicon that emit in the telecom O-band. We utilized home built gold-silicon liquid metal alloy ion sources (LMAIS) in a focused ion beam (FIB) system to perform mask-free implantation of 40 keV Si ions from 6 to 500 ions per spot. Analysis and confirmation of SPEs has been done in a home-build cryo-photoluminescence setup. We will demonstrate a success rate of more than 50% and upscaling to wafer-scale. We will also provide an insight and overview on the LMAIS technology and an outlook on other potential applications of FIB implantation. arXiv:2204.13173

HL 50.4 Fri 10:15 POT 251

Plasma studies by optical emission spectroscopy for phosphorus doped diamond — •Felix Hoffmann[1], Nicola Lang[1], Philipp Reinke[2], Peter Knittel[1], and Volker Cimalla[1] — [1]Fraunhofer Institute for Applied Solid State Physics, Tullastraße 72, D-79108 Freiburg, Germany — [2]Quantum Brilliance GmbH, Industriestraße 4, D-70565 Stuttgart, Germany

While p-doping of diamond by Boron is a well-controlled process, n-doping by Phosphorus (P) remains challenging due to its low solubility and big covalent radius in comparison to carbon. The control of plasma conditions and the understanding of its influence on growth parameter is crucial for single crystal diamond growth by microwave plasma assisted chemical vapor deposition (MPCVD) [1]. Hydrogen-methane plasmas with dopant-carrier gases have been analyzed with respect to kinetic gas temperature (of the C2 band) and radical concentration by optical emission spectroscopy (OES) under various experimental conditions such as excitation power, operating pressure and gas concentrations [2]. Here we present results of P-doped diamond growth using the carrier gas trimethylphosphine (TMP) and point out the influence of TMP on plasma properties and its relation to growth parameter of P-doped {111} diamond grown by MPCVD.

[1] V. Mortet et al. Diamond and Related Materials, 2022, 124, 108928

[2] Mikhail Aleksandrovich Lobaev et al. Phys. Satus Solidi A, 2019, 216, 1900234

HL 50.5 Fri 10:30 POT 251

Modifying dipole selection rules in cuprous oxide Rydberg excitons — •Annika Neubauer and Harald Giessen — 4th Physics Institute, University of Stuttgart

Excitons in cuprous oxide have large binding energies, which implies that different principal quantum number state excitons can be created as they are energetically not spaced too closely to each other nor to the ionization continuum. High principal quantum number Rydberg excitons in cuprous oxide are macroscopic quantum systems with spatial extensions in the several hundreds of nm up to several μm range. This implies, that excitation with a focused light beam leads to a large overlap of light and matter wavefunctions and should lead to an enhanced optical transition.

We are going to show that the dipole selection rules in cuprous oxide Rydberg excitons can be manipulated via excitation with orbital angular momentum light or via the quadrupole field of plasmonic antennas. Both such light fields posses a strong field gradient or an additional angular momentum. This way, different angular momentum quantum number state excitons can be switched on and off, which is attractive for quantum state engineering. The mesoscopic size of cuprous oxide Rydberg excitons also implies that already μm-sized structures lead to mesoscopic quantum size effects. This can be advantageous for the realization of quantum technologies, such as optical switching applications, based on cuprous oxide Rydberg excitons.

HL 50.6 Fri 10:45 POT 251

Strong coupling of a single quantum dot to a tunable plasmonic nanogap antenna at room temperature using a novel scanning probe technique — •Michael A. Becker[1], Hsuan-Wei Liu[1,2], Burak Gurlek[1,2], Korenobu Matsuzaki[1], Randhir Kumar[1], Stephan Götzinger[2,1], and Vahid Sandoghdar[1,2] — [1]Max Planck Institute for the Science of Light, Staudtstr. 2, 91058 Erlangen, Germany — [2]Friedrich Alexander University of Erlangen-Nürnberg, Schloßplatz 4, 91054 Erlangen, Germany

In the strong coupling regime of cavity quantum electrodynamics, the spectrum of an isolated quantum system hybridizes with a mode of a resonator. At room temperature, coupling to the environment leads to a fast dephasing of the transition dipole, and strong near-field enhancements in plasmonic nanoantenna geometries need to be exploited to reach the strong light-matter coupling regime. For an efficient coupling, the antennas need to be placed within a few nanometer with respect to the individual emitters. Here, we exploit our novel and simple press-roll scanning probe technique (PROscan) capable of performing high-precision optical near-field measurements with remarkable stability. We demonstrate an open nanogap antenna that can be tuned in resonance with the exciton transition of a single quantum dot. With this approach, we drive the system from the weak to the strong light-matter coupling regime, evidenced by a vacuum Rabi splitting. Our results elucidate the complex interplay between the nanoantenna's mode volume and the physics of its eigenmode.

30 min. break

HL 50.7 Fri 11:30 POT 251

Optimal quantum control of Si/SiGe spin qubits in a Quantum bus architecture — •Akshay Menon Pazhedath[1], Alessandro David[1], Lars R. Schreiber[2], Hendrik Bluhm[2], Tommaso Calarco[1], and Felix Motzoi[1] — [1]Peter Grünberg Institute-Quantum Control (PGI-8), Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany — [2]JARA-FIT Institute for Quantum Information, Forschungszentrum Jülich GmbH and RWTH Aachen University, Aachen, Germany

Quantum bus architecture based on electron spin-shuttling is a promising candidate for scalable quantum computing, as the number of control lines required to control the spin remains constant irrespective of the length of the device. A gated Si/SiGe quantum well with a carefully placed micro-magnet acts as an addressable qubit system in such an architecture. We investigate the feasibility of performing single qubit operations using optimal quantum control techniques. Spin decoherence due to interaction with the valley degree of freedom in the Si/SiGe heterostructure is identified as a potential decay mechanism and optimal pulses are engineered to maximize single qubit state transfer and unitary operation fidelities, so that the operations are compliant with the fault tolerant error threshold.

HL 50.8 Fri 11:45 POT 251

Generating spatially distributed entanglement as a resource for novel quantum computing paradigms on a platform of coupled microcavities — •Marc Bostelmann, Steffen Wilksen, Frederik Lohof, and Christopher Gies — Institute for Theoretical Physics and Bremen Center for Computational Material Science, University of Bremen, Bremen, Germany

Spatially distributed entanglement is important for the realization of novel quantum-photonic applications in quantum computing and quantum machine learning. We consider photonic arrays made from quantum emitters in optically coupled microcavities as hardware platform for entanglement generation. These offer a large degree of tunability with the possibility of site-selective optical excitation. We present a scalable numerical scheme for the determination of excitation parameters to generate different classes of multipartite entangled states, and a quantum bath engineering approach to create entanglement in the steady-state [arXiv:2211.13639].

HL 50.9 Fri 12:00 POT 251

Towards the Development of Cryogenic Integrated Power Management Units — •Alfonso Rafael Cabrera Galicia — Forschungszentrum Jülich GmbH Wilhelm-Johnen-Straße 52428 Jülich

Integrated Circuits (ICs) in cryogenic environments are expected to allow the development of scalable quantum computers consisting of thousands of physical quantum bits (qubits). However, since these ICs require undistorted power supply for optimal performance, the development of Power Management Units (PMUs) capable of cryogenic operation is also needed for the quantum computing systems scalability. To develop such PMUs, it is necessary to understand the cryogenic electrical behavior of its components. Therefore, this talk will present the measurement results obtained from an exploratory cryogenic DC characterization of some of the passive and active components belonging to a commercial 22nm FDSOI IC technology.

HL 50.10 Fri 12:15 POT 251

Physical Integration of Cryogenic Control Electronic Together with a Spin Qubit Sample at mK Temperatures — •Lea-Marie Schreckenberg[1], Patrick Vliex[1], René Otten[2], and Stefan van Waasen[1,3] — [1]Central Institute of Engineering, Electronics and Analytics, Electronic Systems, Forschungszentrum Jülich GmbH, Jülich, Germany — [2]JARA Institute for Quantum Information, Forschungszentrum Jülich GmbH and RWTH Aachen University, Aachen, Germany — [3]Faculty of Engineering, Communication Systems, University of Duisburg-Essen, Germany

A universal quantum computer requires the control and read out of millions of physical quantum bits (qubits). Due to wiring limitation in current state-of-the-art dilution refrigerators scaling up to millions of qubits with room-temperature electronics is challenging. Integrated Circuits (ICs) operating next to the qubits will help solving this scalability problem but require novel approaches for cryogenic circuits. This talk will focus on the physical design layer of the integration of a custom-designed 65nm CMOS low-power digital to analog converter (DAC) for qubit bias together with a spin qubit sample. In total, eight DAC channels are integrated at the mixing chamber stage of a dilution refrigerator and are operated at milli-kelvin temperatures. Additionally, engineering aspects regarding the sample space setup, cryostat wiring and the tight density are pointed out.

HL 50.11 Fri 12:30 POT 251

Design of power efficient digital low-dropout circuit for quantum computers — •Swasthik Baje Shankarakrishna Bhat[1], Alfonso Rafael Cabrera Galicia[1], Arun Ashok[1], Patrick Vliex[1], Andre Zambanini[1], Christian Grewing[1], and Stefan van Waasen[1,2] — [1]Forschungszentrum Jülich GmbH, Germany — [2]Universität Duisburg-Essen

Quantum computing is an approach to enable new computing paradigms with qubits as the computing elements that require individual tuning. A limitation in current setups is the number of controllable qubits. To scale the number of qubits, a close integration of control circuits close to the qubits in the cryogenic environment is required. However, to deal with these cryostats* minimal thermal power budget, ultra-low power dissipation is required, also for biasing circuits.

This contribution presents the design and simulation results of a power-efficient digital low-dropout regulator developed with a commercial 22nm FDSOI technology. It is expected that the circuit will enable on-chip biasing for future quantum computers based on Cryogenic Electronics operating at 4 K. Unlike its Analog counterpart integrated Digital LDO is not prone to process and mismatches delivering

high efficiency at the same time The circuit concept and the system model investigation performed via Matlab-Simulink will be showed, as well as the expected circuit performance.

HL 50.12 Fri 12:45 POT 251

Design of Ultra-Low Power High Speed Communication Interface From Cryogenic to Room Temperature Electronics — •Ege Onat, Jonas Bühler, Christian Grewing, and Stefan van Waasen — Central Institute of Engineering, Electronics and Analytics, ZEA-2: Electronic Systems, Forschungszentrum Jülich GmbH

The objective of this research is to transfer high-speed data from deep cryogenic temperatures to room temperature while aiming for the lowest achievable power consumption in the cryostat. Quantum computers are operated inside dilution refrigerators under deep cryogenic temperatures and they need additional circuitry to ensure fault-free operations. Heating of the qubits caused by additional electronics degrades the system performance. Due to the limited power budget of the dilution refrigerators, each circuit should be designed considering power consumption. In contrast, the higher temperature stage can manage a higher power budget than the stage with the qubits. In this research, low-power data transmission methods for quantum computer applications are investigated and an asymmetric communication interface is designed and implemented. To achieve the asymmetric interface, only a varactor is placed into the cryogenic stage. To measure the capacitance on the room temperature stage, a capacitance readout circuitry is designed. It converts the capacitance into a measurable output such as voltage, frequency, or digital data. By implementing this interface, the data is carried on capacitance rather than voltages, which minimizes the power consumption at the transmitter compared to widely implemented communication interfaces.

HL 51: Nitrides: Preparation and Characterization

Time: Friday 9:30–12:15 Location: POT 112

HL 51.1 Fri 9:30 POT 112

High resistive buffer layers by Fermi-level engineering — •Armin Dadgar, Ralf Borgmann, and André Strittmatter — Otto-von-Guericke-Universität Magdeburg, FNW-IfP, Universitätsplatz 2, 39106 Magdeburg

We present a novel method to increase the resistivity of semiconductor buffer layers by aligning the Fermi level using a donor and an acceptor dopant of which one preferentially is a deep level placed in the lower (acceptor) or upper (donor) half of the energy band-gap. Potential doping sequences in GaN were simulated by nextnano software showing that the average Fermi-level position of alternately donor and acceptor doped layers can be shifted to the midgap position. This shift decreases the free carrier concentration and increases the resistivity as demonstrated for GaN:C / GaN:Si layer stacks. In structures grown by metalorganic vapor phase epitaxy, less charging and hysteresis effects are observed upon polarity changing between electrical contacts placed at surface and substrate. Also, the reduced total deep level concentration improves resistivity under electron and hole injection and the overall breakdown voltage by more than 20 %.

HL 51.2 Fri 9:45 POT 112

yolo-assisted object detection of dislocation-related pits on GaN surfaces using generative adversarial networks — •Mahdi Khalili Hezarjaribi[1,2], Uwe Rossow[1,2], Heiko Bremers[1,2], and Andreas Hangleiter[1,2] — [1]Institute of Applied Physics, Technische Universität Braunschweig, Germany — [2]Laboratory for Emerging Nanometrology, Technische Universität Braunschweig, Germany

In this paper, we present a model for detecting dislocation-related pits on GaN surfaces using SEM images, which strongly relies on the use of synthetic image generation. Pits mark dislocations in the layers and are widely used to assess crystalline quality; therefore, a considerable amount of images containing pits have to be evaluated. For this purpose, a Deep Learning (DL) algorithm is employed to achieve objective results, which are detecting the pits, and hence the dislocations, in SEM images. In order to train the algorithm to efficiently detect the objects, we need a host of SEM images containing pits in multiple sizes, numbers, formations, and noises. Due to the complexity of the microscopic structures and the lack of enough images, we incorporated a group of powerful algorithms called Generative Adversarial Networks to create artificial fake images just like real images and feed them, together with our real images, to our dataset to enrich the volume of the dataset. In the next stage, the YOLO algorithm (version 5) has been employed as the core deep learning algorithm for the object detection process using the above-mentioned dataset to train the network. A minimum average confidence of 86% for detecting real objects has been realized, corresponding to a high probability of detection.

HL 51.3 Fri 10:00 POT 112

Molecular beam epitaxy growth study and characterization of HoN thin films — •Anna Melendez-Sans[1], Vanda M. Pereira[1], Chun-Fu Chang[1], Chang-Yang Kuo[1,2,3], Chien-Te Chen[2], Liu Hao Tjeng[1], and Simone G. Altendorf[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [3]Department of Electrophysics, National Yang Ming Chiao Tung University, Hsinchu, Taiwan

Rare earth nitrides show potential for a wide range of applications due to their strong magnetic moment and semiconducting behavior. However, their synthesis and characterization has proven challenging since they rapidly oxidize when exposed to ambient conditions. Thanks to continuous developments in UHV-based thin film growth methods it is possible to grow high quality rare earth nitride films and, through the characterization of these, gain better insight into these compounds.

Whilst there have been many reports on GdN and SmN, not much is yet known about HoN. Now we present a systematic growth study on HoN thin films synthesized by molecular beam epitaxy (MBE), and using different substrates (MgO, $LaAlO_3$) and growth conditions (substrate temperatures and Nitrogen-gas pressure). These films were subsequently characterized using *in situ* techniques (Reflection high-energy electron diffraction, X-ray absorption and photoelectron spectroscopy) and *ex situ* techniques (X-ray diffraction, Superconducting quantum interference device) in order to evaluate their crystalline, electronic and magnetic structure.

HL 51.4 Fri 10:15 POT 112

Theoretical study on the (Al,Sc)N random alloy — •Jan M. Waack[1,2], Markus Kremer[1,2], Michael Czerner[1,2], and Christian Heiliger[1,2] — [1]Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Germany — [2]Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen, Germany

Aluminium scandium nitride ($Al_xSc_{1-x}N$, (Al,Sc)N or AlScN) is an random alloy. As such, the calculation of physical properties requires specific methods such as the coherent potential approximation (CPA)[1] and special quasi-random structures (SQS)[2]. We compare the CPA in the framework of the atomic sphere approximation (ASA) Korringa-Kohn-Rostoker (KKR) density functional theory (DFT) with the SQS using the plane-wave pseudopotential DFT to calculate the lattice parameters and electronic band structures of the face-centered cubic phase of $Al_xSc_{1-x}N$ (with $0 \leq x \leq 1$).

Using the low computational cost LDA-1/2 quasiparticle method [3] to calculate the electronic band structures within SQS and CPA, we present the first implementation of LDA-1/2 within the KKR DFT. We find that both the lattice parameter and the indirect band gap deviate from Vegard's law.

[1] C. Franz, M. Czerner, and C. Heiliger, Phys. Rev. B 88, 94421 (2013). https://doi.org/10.1103/PhysRevB.88.094421

[2] A. Zunger, S.-H. Wei, L. G. Ferreira, and J. E. Bernard, Phys. Rev. Lett. 65, 353 (1990). https://doi.org/10.1103/PhysRevLett.65.353

[3] L. G. Ferreira, M. Marques, and L. K. Teles, Phys. Rev. B 78, 125116 (2008). https://doi.org/10.1103/PhysRevB.78.125116

HL 51.5 Fri 10:30 POT 112

Thermal Transport in c-plane GaN Membranes Studied by Raman Thermometry — •Wilken Seemann[1], Joachim Ciers[2], Isabell Hüllen[1], Mahmoud Elhajhasan[1], Jean-François Carlin[3], Nicolas Grandjean[3], Åsa Haglund[2], and Gordon Callsen[1] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]Department of Microtechnology and

Nanoscience, Chalmers University of Technology, Gothenburg, Sweden — [3]Institute of Physics, École Polytechnique Fédérale de Lausanne (EPFL), Switzerland

Heating during operation often limits the lifetime or stability of semiconductor devices, like laser structures, e.g., via defect formation or by affecting the refractive index. Understanding how thermal energy is dissipated from the active region of such structures is therefore an important step towards device optimization.

We analyze the in-plane thermal transport in GaN-based membranes. The temperature is probed by the shift and width of Raman modes under heating with a UV laser. This allows for a non-contact characterization without the need for additional processing steps.

By varying the membrane underetching process, we can tune the membrane bottom facet roughness and porosity to study their impact on thermal conductivity κ, due to phonon boundary scattering. A reduction of κ is a sign of phonon frequency filtering, which is a first step towards engineering the phonon dispersion relation in GaN membranes. Controlling this effect, e.g., via the position and sizes of pores, might enable thermal concepts to locally reduce temperature rises.

15 min. break

HL 51.6 Fri 11:00 POT 112

SmN thin films: MBE-growth and spectroscopy studies — •Vanda M. Pereira[1], Anna Melendez-Sans[1], Chun-Fu Chang[1], Chang-Yang Kuo[1,2,3], Chien-Te Chen[2], Liu Hao Tjeng[1], and Simone G. Altendorf[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [3]Department of Electrophysics, National Yang Ming Chiao Tung University, Hsinchu, Taiwan

Although the rare earth nitrides have been in the scientific scene for many decades, their poor stoichiometry and reactivity in ambient conditions have severely conditioned their progress. It has been only rather recently that studies on thin films have started to unveil some of their unique characteristics and solve decades-old controversies, but there are still significant gaps left to explore.

Recent studies on the ferromagnetic semiconductor SmN suggest that the $4f$ bands are involved in electron transport and are crucial to the observed superconductivity in nitrogen-vacancy doped samples. Nevertheless, more concrete experimental evidence is needed.

Here we present a systematic study of SmN thin films grown by molecular beam epitaxy, exploring their crystalline quality and composition as the growth parameters (substrate temperature and nitrogen pressure) are varied. The films were characterized *in situ* making use of photoemission and x-ray absorption spectroscopies, thereby allowing to reliably gain more insight into the electronic structure of this material.

HL 51.7 Fri 11:15 POT 112

Growth of ScN and AlScN by reactive sputter epitaxy — •Florian Hörich, Christopher Lüttich, Ralf Borgmann, Jürgen Bläsing, André Strittmatter, and Armin Dadgar — Otto-von-Guericke University

Spontaneous polarization fields induced by a strained AlGaN/GaN layer structure lead to high-density two-dimensional electron gases which are key to current high-power and high-frequency transistor devices. Recent theoretical and experimental data demonstrated an even higher two-dimensional electron density when AlScN is used [1]. Up to now, growth of Sc-containing materials by conventional MOVPE is hampered by the lack of a suitable Sc precursor. Reactive sputter epitaxy using metallic Al and Sc targets together with ammonia or molecular nitrogen has the potential to fabricate high quality layers at low cost. We will discuss principle growth parameters such as temperature and nucleation conditions for ScN and AlScN on bare Si(111) substrates and on MOVPE grown GaN templates. A large impact of growth temperature is observed on crystal structure and surface morphology. Single-phase crystalline material is obtained at temperatures $>$ 800 °C. We find different optimum nucleation conditions for both kind of substrate surfaces. Growth on bare Si(111) surfaces with an initial metallic Sc thickness equivalent to $<$1 nm drastically improves crystallinity. For the GaN(0001) template surface, such sequence has no impact. Additionally, sputtering of AlScN and ScN with ammonia results in better structural quality than with nitrogen.

[1] I. Streicher, et. al. Phys. Status Solidi RRL 2200387

HL 51.8 Fri 11:30 POT 112

On the variation of PL intensity in GaInN/GaN quantum wells with different cladding thicknesses — •Nico Wagner[1], Shawutijiang Sidikejiang[1,2], Philipp Henning[1,2], Rodrigo de Vasconcellos Lourenço[1,2], Heiko Bremers[1], Uwe Rossow[1,2], and Andreas Hangleiter[1,2] — [1]Institute of Applied Physics, Technische Universität Braunschweig, Germany — [2]Laboratory for Emerging Nanometrology, Braunschweig, Germany

The absolute internal quantum efficiency (IQE) of GaInN/GaN quantum wells (QW) at low temperature can be determined using time-resolved photoluminescence (PL) measurements. If the IQE is 100 %, the PL intensity under steady state conditions is expected to be the same for all samples. We can verify that for some samples, but others show different intensities. It turns out that the difference varies for different cladding thicknesses, i.e. the layer between the QW and air. In this work, we present a model calculating the allowed modes inside the sample assuming that all the light is emitted into them if we have 100 % IQE. Due the small critical angle, it is important to determine the small ratio of intensity, which is coupled out and detected. The result yields an oscillating behavior as a function of the cladding thickness and shows a good agreement with the measured samples. It is important to note that this is a consequence of the Purcell effect, i.e. that spontaneous emission depends on the optical environment.

HL 51.9 Fri 11:45 POT 112

Optical properties of ScN films grown by HVPE and sputter epitaxy — •Jona Grümbel[1], Yuichi Oshima[2], Christopher Lüttich[1], Armin Dadgar[1], Martin Feneberg[1], and Rüdiger Goldhahn[1] — [1]Institut für Physik, Otto-von-Guericke-Universität, Universitätsplatz 2, 39106 Magdeburg — [2]Environment and Energy Materials Research Division, National Institute for Materials Science, 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan

We investigate the optical properties of rocksalt structured ScN films using spectrocopic ellipsometry and Raman spectroscopy. Two different sets of samples were used for our measurements: (I) ca. 300nm thick ScN grown by sputter epitaxy and (II) 0.4μm up to 40μm thick ScN grown by HVPE. The HVPE grown ScN exhibits a very good crystalline structure, so the carrier concentration varies around 10^{18}cm^{-3} - 10^{19}cm^{-3}, while for ScN grown by sputter epitaxy the carrier concentrations can reach 10^{22}cm^{-3} or more. Therefrom we obtain detailed information about their impact on optical properties, such as optical transitions, optical phonon modes or luminescence. Using spectroscopic ellipsometry we arrive at the dielectric function of ScN from 0.04eV to 6.5eV. Detailed analysis yields the main transitions regarding to direct bandgaps at X- and Γ-point as it was already shown in earlier theoretical works. Surprisingly, we observe characteristic peaks in a Raman scattering measurement, although first order Raman scattering is forbidden in rocksalt structured crystals. Detailed discussion and a possible interpretation will be presented as well as ScN materials parameters calculated from our measurements.

HL 51.10 Fri 12:00 POT 112

Temperature dependent spectroscopic ellipsometry on cubic GaN — •Jonas Rose[1], 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

Cubic Galliumnitride (c-GaN) is a promising material for designing and fabricating efficient optoelectronic devices, such as green LEDs, and can potentially replace hexagonal GaN for certain applications due to its lack of internal polarization fields. Therefore, the knowlegde and control of the optical properties is essential. Recently, several breakthroughs regarding crystal quality of c-GaN have been achieved by utilizing 3C-SiC as a substrate material. We present our investigation of thin film c-GaN deposited by plasma-assisted molecular beam epitaxy on 3C-SiC/Si substrates in (001) orientation. Temperature dependent spectroscopic ellipsometry between 80 and 300 K yields the optical properties (dielectric function, DF) in this temperature range. Hereby, the influence of the excitonic contribution to the DF is of special interest. Using Elliott's model, we describe the lineshape of the DF around the absorption onset. The obtained transition energies follow Pässler's temperature dependent model. Degenerately doped samples up to 10^{20} cm^{-3} are investatigated as well. A free-carrier dependent behaviour of the absorption onset is observed and explained for different temperatures.

HL 52: Focus: Self-Assembly of Plasmonic Nanostructures (joint session CPP/HL)

Organized by Tobias A. F. König and Markus Lippitz

Time: Friday 9:30–12:30 Location: GÖR 226

Invited Talk HL 52.1 Fri 9:30 GÖR 226

Self-assembled optical metamaterials — •Ullrich Steiner — Adolphe Merkle Institute, Chemin des Verdiers 4, 1700 Fribourg

The self-assembly of block-copolymers gives rise to numerous 2D and 3D morphologies with characteristic pattern sizes on the 10 nm length scale. These polymer structures can be transformed into plasmonic metals to fabricate 2D metasurfaces and 3D metamaterials. These plasmonic replicas have the appropriate structure sizes for the coupling of plasmon resonances to the visible light spectrum, yielding interesting optical materials.

This presentation will review recent progress in manufacturing and studying these materials and highlight interesting current developments.

HL 52.2 Fri 10:00 GÖR 226

In Situ Monitoring of Self-Assembly and Plasmonic Shifts during the Growth of AgCu Alloy Nanostructures — •Matthias Schwartzkopf[1], André Rothkirch[1], Niko Carstens[2], Thomas Strunskus[2], Franziska C. Löhrer[3], Senlin Xia[3], Volker Körstgens[3], Peter Müller-Buschbaum[3,4], Franz Faupel[2], and Stephan V. Roth[1,5] — [1]DESY, Notkestr. 85, D-22607 Hamburg — [2]CAU zu Kiel, Kaiserstr.2, 24143 Kiel — [3]TUM, James-Franck-Str. 1, D-85748 Garching — [4]MLZ, Lichtenbergstr. 1, D-85748 Garching — [5]KTH, Teknikringen 56-58,SE-100 44 Stockholm

While magnetron sputtering is a versatile routine method in industry for the deposition of large area metal and alloy coatings, it can be also used for the preparation of functional nanocomposites with e.g. adjustable optical properties [1]. We investigated in real-time the formation of supported silver, copper, and silver-copper-alloy nanoclusters during sputter deposition on poly(methyl methacrylate) by combining in situ surface-sensitive X-ray scattering with optical spectroscopy [2]. While following the transient growth morphologies, we quantify the early stages of phase separation at the nanoscale, track the shifts of surface plasmon resonances, and quantify the growth kinetics of the nanogranular layers at different thresholds. We are able to extract the influence of scaling effects on the nucleation and phase selection and demonstrate a route to tailor accurately the plasmon resonances of nanosized, polymer-supported clusters. [1] Faupel et al., Adv. Eng. Mater. 2010, 12, 12, 1177-1190. [2] Schwartzkopf et al., ACS Appl. Nano Mater. 2022, 5, 3, 3832-3842.

HL 52.3 Fri 10:15 GÖR 226

What happens to bovine serum albumin in-between two gold nanoparticles and how this biomolecule defines the plasmonic effect? — Nina Tverdokhleb, •Olga Guskova, Ziwei Zhou, Holger Merlitz, and Vladyslav Savchenko — Leibniz-Institut für Polymerforschung Dresden e. V.

In experiments, spherical gold nanoparticles (NPs) covered by bovine serum albumin (BSA) create 1D Au-BSA nanoarrays on a polymer film. The external mechanical strain applied to the film leads to plasmon-coupled circular dichroism (PCCD) enhancement. To explain this phenomenon, we perform all-atom MD simulations of plasmonic nanostructures, representing BSA in-between two gold NPs. The following steps were undertaken: (1) BSA was adsorbed on the gold wall (a model of NP) in implicit water with optimization of its geometry; (2) the second mobile gold wall was approaching adsorbed protein until the distance between NPs reaches the experimentally measured value; (3) mimicking mechanical stretching mentioned above, an external tensile force applied on the second wall has induced the backbone stretching of the initially compressed BSA. This process is accompanied by the crucial growth of BSA dipole moment along the directional deformation, restructuring of the protein secondary structure from helices to coils upon compression (2), the reorientation of the charged amino-acid residues, and subsequent partial back-folding of the secondary structure elements upon stretching (3). We correlate an observed plasmonic effect in the 1D Au-BSA arrays to the changes in dipole moment and chirality of BSA.

HL 52.4 Fri 10:30 GÖR 226

Uniform and sensitive Raman signal by self-assembled plasmonic nanoparticle gratings — •Sezer Seçkin[1] and Tobias A. F. König[1,2] — [1]Leibniz-Institut für Polymerforschung e.V., Hohe Straße 6, 01069 Dresden — [2]Center for Advancing Electronics Dresden (cfaed), Technische Universität Dresden, 01062 Dresden

Despite recent advancements in this field, it is still challenging to manufacture SERS substrates that provide high sensitivity and uniformity over large areas. One can overcome this challenge by employing a colloidal approach such as directed self-assembly of plasmonic nanoparticles into ordered structures [König et al. Advanced Functional Materials 31.36 (2021): 2105054]. Here, we have produced highly ordered 1D plasmonic lattice structures by assembling nanoparticles of various sizes. With the help of the low optical loss of colloidal gratings, we studied the enhancement capabilities of the SERS substrates by the excitation of a fluorescent reporter Rhodamine 6G, at different wavelengths. We conducted the polarization-dependent SERS enhancement by exciting colloidal gratings parallel and perpendicular to the polarization of the excitation lasers. Moreover, we studied the effect of the surface plasmon modes on the SERS enhancement at different orientations using the FDTD simulation. The mapping technique visually interpreted the SERS performances of other substrates, which supports the reproducibility and uniformity of the Raman signals over larger areas. Controlling the particle size while keeping the periodicity constant allows us to tune the SERS enhancement factor, which can be helpful for various sensing applications.

HL 52.5 Fri 10:45 GÖR 226

Investigating Charge Transfers in Colloidal Photonic Crystal Slabs — •Swagato Sarkar[1] and Tobias A. F. König[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Institute of Physical Chemistry, Hohe Str. 6, 01069 Dresden, Germany — [2]Center for Advancing Electronics Dresden (cfaed), Technische Universität Dresden, Helmholtzstraße 18, 01069 Dresden

The challenges of large-scale and low-loss plasmonic charge transfers are systematically investigated by optical designs with colloidal 1D plasmonic lattice structures. These plasmonic lattices are used as couplers to confine the incident energy into the underlying titanium dioxide layers, thus acting as colloidal photonic crystal (cPhC) slabs. Conventionally, photodetection is possible at energy levels close to the semiconductor bandgap; however, with the observed plasmonic-photonic hybrid modes, the extended solar spectrum can be used for energy harvesting. The photo-amplified current is measured locally with simple two-point contact on the centimeter-sized nanostructure by applying a bias voltage. The optical concepts for metallic grating composed of nanobars are extended for the first time to colloidal self-assembled gold nanoparticle (AuNP) chains to make large-scale charge injection accessible at a reasonable cost. Further, the possibility of photodetection by electric field vectors lying both along and perpendicular to the grating lines can be achieved by tuning the plasmonic grating periodicities.

HL 52.6 Fri 11:00 GÖR 226

Self-assembled plasmonic metasurfaces for sensing and photocatalysis — •Olha Aftenieva[1] and Tobias A.F. König[1,2] — [1]Leibniz-Institute for Polymer Research Dresden, Hohe Straße 6, 01169 Dresden, Germany — [2]Center for Advancing Electronics Dresden (cfaed), Technische Universität Dresden, 01062 Dresden, Germany

Self-assembly of colloids allows for robust and tunable manufacturing over centimeter-scaled areas. Here we present the soft lithographic approach for creating plasmonic lattices and demonstrate their usage for sensing applications and photocatalysis. First, a particular case of collective out-of-plane resonant coupling is considered. Such resonances are excited solely under oblique illumination with transverse magnetic polarization and provide field enhancement in the area above the metasurface that is easily accessible to an analyte and is particularly sensitive to the changes in the refractive index. On the other hand, we realize imprinting of such periodic plasmonic lattices on functional substrates, including glass, silicon wafers, carbon, gold, semiconductor, or polymer thin films, illustrating the versatility of the colloidal approach. In particular, the combination of titanium dioxide thin waveguiding layers and plasmonic metasurface gives rise

to narrow-bandwidth guided plasmon-polariton modes. Moreover, it induces the generation of hot charge carriers and enhances photocatalytic processes. Thus, colloidal self-assembly of plasmonic metasurfaces presents an application-oriented approach that is of potential use for optical sensors, photonic circuit applications, or hybrid device manufacturing.

15 min. break

Invited Talk HL 52.7 Fri 11:30 GÖR 226

Simulating quantum systems with plasmonic waveguide arrays — •Stefan Linden — Physikalisches Institut, Universität Bonn, 53115 Bonn

Coupled waveguides provide a powerful platform to simulate the evolution of quantum mechanical tight-binding systems in a classical wave environment. The basis for this is the mathematical equivalence between the time-dependent Schrödinger equation and the paraxial Helmholtz equation. In this presentation, we report on the observation of the Wannier-Stark ladder and Bloch oscillations in arrays of plasmonic waveguides with a propagation constant gradient acting as an effective external potential. Moreover, we show that Floquet engineering is a powerful method to tailor the topological properties of plasmonic waveguide arrays. In this context, we demonstrate that time-periodic modulation of dissipation can restore transport quantization in fast Thouless pumps and report on the observation of the anomalous Floquet topological π-mode at optical frequencies.

Invited Talk HL 52.8 Fri 12:00 GÖR 226

single molecule detection on a smartphone microscope enabled by DNA origami biosensors — •Philip Tinnefeld — Department of Chemistry and Center for NanoScience, Ludwig-Maximilians-Universität München, Butenandtstr. 5-13, 81377 München, Germany

DNA nanotechnology and especially the DNA origami technique allow well-defined assembly of optically active components and sensing units for novel biosensing approaches. We here demonstrate single-molecule detection on a battery driven smartphone microscope enabled by fluorescence enhancement with DNA origami nanoantennas. As further examples, we show DNA origami membrane sensors for curvature and membrane potentials. Finally, DNA origamis are used for a novel superresolution approach combining graphene energy transfer, pMINFLUX and DNA PAINT that enables nanometric 3D superresolution close to the coverslip.