HL 19: Poster Session IV

Topics:
- Semiconductor lasers
- Semiconductors for quantum technologies
- Ultra-fast phenomena
- Oxide semiconductors
- Tailored Nonlinear Photonics

Time: Thursday 13:30–16:30 Location: P

HL 19.1 Thu 13:30 P

Bandgap and Secondary Phase Analysis of (A)CIGS Solar Cell Absorber and Buffer Layers Using Electroreflectance Spectroscopy — •Michael Dao[1], Jonas Grutke[1], Wolfram Witte[2], Dimitrios Hariskos[2], Heinz Kalt[1], and Michael Hetterich[1,3] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70563 Stuttgart, Germany — [3]Light Technology Institute, KIT, 76131 Karlsruhe, Germany

Thin-film solar cells based on Cu(In,Ga)Se_2 (CIGS) absorbers have established themselves as highly efficient photovoltaic devices. To further optimize their properties, the incorporation of silver (Ag) into the absorber layer (ACIGS) is currently investigated by many groups. In this contribution, the effect of Ag on the absorber bandgap energy as well as the corresponding inhomogeneous broadening is investigated by electroreflectance spectroscopy (ER) which allows a destruction-free analysis of full device structures. Additionally, angle-resolved ER (ARER) is applied to study the impact of Ag on the formation of secondary phases as well as possible interdiffusion effects at the absorber-buffer interface. Using this technique, the bandgap energies of both the buffer layer as well as secondary phases can be determined despite interference effects in the multi-layered device structure and the small thickness < 60 nm of the buffer layer.

HL 19.2 Thu 13:30 P

Electroreflectance as a Powerful Tool to Investigate Internal Device Parameters in CIGS Solar Cells — •Lennart Meyer[1], Jonas Grutke[1], Wolfram Witte[2], Dimitrios Hariskos[2], Heinz Kalt[1], and Michael Hetterich[1,3] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70563 Stuttgart, Germany — [3]Light Technology Institute, KIT, 76131 Karlsruhe, Germany

Recently, our group has developed and successfully utilized various advanced electroreflectance (ER) spectroscopy techniques for the destruction-free analysis of Cu(In,Ga)Se_2 (CIGS) solar cell absorber and buffer layers in full devices, including investigations into interdiffusion phenomena and secondary phase formation. In this contribution, we present first steps towards a novel ER approach that shall enable the determination of internal device parameters such as the built-in potential drop at the absorber-buffer interface, the carrier concentration in the absorber, or the width of the space charge region. To this end, the variation of the CIGS bandgap resonance amplitude in the ER spectra is analysed as a function of the simultaneously applied AC and DC reverse biases, respectively. The cell parameters can then be obtained via theoretical modelling of the experimental data. First examples and applications of this method will be discussed.

HL 19.3 Thu 13:30 P

Atomic and electronic structure of the GaP/Si(001) heterointerface studied by HAXPES — •Agnieszka Paszuk[1], Oleksandr Romanyuk[2], Igor Bartoš[2], Regan G. Wilks[3], Manali Nandy[1], Jakob Bombsch[3], Claudia Hartmann[3], Raül Garcia-Diez[3], Shigenori Ueda[4], Ivan Gordeev[2], Jana Houdkova[2], Peter Kleinschmidt[1], Marcus Bär[3], Peter Jiříček[2], and Thomas Hannappel[1] — [1]Institute of Physics, University of Technology, Ilmenau, German — [2]Institute of Physics, Prague, Czech Republic — [3]Department Interface Design, Helmholtz-Zentrum Berlin, Germany — [4]SPring-8, National Institute for Materials Science, Japan

For highly efficient III-V-on-Si optoelectronic devices it is crucial to prepare defect-free heterointerfaces with defined electronic properties. Commonly a thin, pseudomorphic GaP epilayer is deposited on Si prior to further III-V buffer growth, due to its close lattice matching to Si. Here, the atomic and electronic structures of buried GaP/Si(001) heterointerfaces prepared by MOCVD were investigated by hard X-ray photoelectron spectroscopy combined with theoretical modelling. 4 - 50 nm thick GaP films with a different density of antiphase domain boundaries were grown on Si(001) H-terminated surfaces, as controlled by optical *in situ* spectroscopy. We found that the core-level positions and width change with GaP film thickness and Si substrate type. These observations were related to charge replacement and band bending effects at the interface. In consequence, an inter-diffused layer interface structure model based on the formation of Si-P bonds at the heterointerface and P-doping of the Si substrate is suggested.

HL 19.4 Thu 13:30 P

Electric-field-driven evolution of anti-Frenkel defects in ErMnO3 — •Jiali He[1], Ursula Ludacka[1], Donald Evans[1], Theodor Holstad[1], Erik Roede[1], Kasper Hunnestad[1], Konstantin Shapovalov[2], Zewu Yan[3,4], Edith Bourret[4], Antonius Van Helvoort[1], and Dennis Meier[1] — [1]Norwegian University of Science and Technology(NTNU), Trondheim, Norway. — [2]Institute of Materials Science of Barcelona, Bellaterra, Spain — [3]ETH Zurich, Zürich, Switzerland. — [4]Lawrence Berkeley National Laboratory, Berkeley, USA.

The electronic properties of complex oxides can readily be tuned via oxygen defects, offering intriguing opportunities for precisely controlling the conductivity of materials. Recently, anti-Frenkel defects moved into focus for minimally invasive property engineering. Anti-Frenkel defects are charge-neutral interstitial-vacancy pairs, and their injection makes it possible to adjust the transport behavior in oxides without causing long-range ionic migration or changes in stoichiometry. Here, we present a detailed analysis of the electric-field-driven formation and response of anti-Frenkel defects in hexagonal ErMnO3. The defects are generated via an electrically biased nano-sized probe tip and imaged by cAFM and SEM. We investigate the spatio-temporal evolution of the written defects for different drive voltages, complemented by numerical simulations, which reveal a non-trivial evolution, allowing to separate the initially paired vacancies and interstitials. The results provide new insight into the local electronic properties of ErMnO3 and the nanoscale defect physics of functional oxides in in general.

HL 19.5 Thu 13:30 P

Modification of epitaxial La0.6Sr0.3CoO3-δ thin films by ion irradiation — •Yunxia Zhou[1,2], Lei Cao[1], Andreas Herklotz[3], Diana Rata[3], Suqin He[4], Felix Gunkel[4], Ulrich Kentsch[1], Manfred Helm[1], and Shengqiang Zhou[1] — [1]Helmholtz-Zentrum-Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, D-01328 Dresden, Germany — [2]University of Electronic Science and Technology of China, State Key Laboratory of Electronic Thin Films and Integrated Device, Xiyuan Ave 2006, 611731 Chengdu, China — [3]Institute of Physics, Martin Luther University Halle-Wittenberg, Halle, 06120, Germany — [4]Peter Grünberg Institut (PGI-7), JARA-FIT, Forschungszentrum Jülich GmbH, Jülich, 52425, Germany

Perovskite oxides exhibits rich physics related to ionic defects. In particular, defect concentration and distribution alter the lattice parameters and affect the competitive interplay between strongly correlated electrons, enabling numerous applications, including sensors, catalysts, and memristive devices. In this work, helium-implantation is demonstrated as a fast, low temperature tool to modulate the vacancy profiles in epitaxial La0.6Sr0.4CoO3-δ thin films. Not only a significant lattice expansion solely along the out-of-plane direction is observed, but also a distinct change in physical properties is evidenced. By proper tuning of the implantation parameters, an enhanced resistivity up to several orders of magnitude is achieved at room temperature. These results offer a new playground for the optimization of oxide-based spintronic

and electronic devices.

HL 19.6 Thu 13:30 P

Electric-field-driven evolution of anti-Frenkel defects in ErMnO3 — •Jiali He[1], Ursula Ludacka[1], Donald Evans[1], Theodor Holstad[1], Erik Roede[1], Kasper Hunnestad[1], Konstantin Shapovalov[2], Zewu Yan[3,4], Edith Bourret[4], Antonius Van Helvoort[1], and Dennis Meier[1] — [1]Norwegian University of Science and Technology(NTNU), Trondheim, Norway. — [2]Institute of Materials Science of Barcelona, Bellaterra, Spain — [3]ETH Zurich, Zürich, Switzerland. — [4]Lawrence Berkeley National Laboratory, Berkeley, USA.

The electronic properties of complex oxides can readily be tuned via oxygen defects, offering intriguing opportunities for precisely controlling the conductivity of the materials. Recently, anti-Frenkel defects moved into focus for minimally invasive property engineering. Anti-Frenkel defects are charge-neutral interstitial-vacancy pairs, and their injection makes it possible to adjust the transport behavior in oxides without causing long-range ionic migration or changes in stoichiometry. Here, we present a detailed analysis of the electric-field-driven formation and response of anti-Frenkel defects in hexagonal ErMnO3. The defects are generated via an electrically biased nano-sized probe tip and imaged by cAFM and SEM. We investigate the spatio-temporal evolution of the written defects for different drive voltages, complemented by numerical simulations, which reveal a non-trivial evolution, allowing to separate the initially paired vacancies and interstitials. The results provide new insight into the local electronic properties of ErMnO3 and the nanoscale defect physics of functional oxides in general.

HL 19.7 Thu 13:30 P

Ammonia and Acetone Gas Sensor Based on Nanocomposites of Indium Oxide and Multiwalled Carbon Nanotubes — •Nipin Kohli — Technical University Berlin

This work reports the effect of introducing carbon nanotubes in indium oxide on structural, morphological, optical and ammonia sensing properties. Various characterization techniques such as X-ray diffraction, transmission electron microscopy, BET, Fourier transform infrared, UV-visible and Raman spectroscopy were employed to understand the structural, morphological and optical properties of the synthesized samples. The gas sensors were fabricated out of the synthesized samples to test their response towards ammonia and acetone at different operating temperatures and at different concentrations. The nanocomposite exhibits enhanced sensing performance and is capable of detecting concentration of acetone and ammonia as low as 10 ppm at optimum operable temperature of 300°C and 200°C, respectively.

HL 19.8 Thu 13:30 P

Förster-Type Energy Transfer Between Molecules and Atomically Thin Semiconductors — •Manuel Katzer[1], Malte Selig[1], Sviatoslav Kovalchuk[2], Kyrylo Greben[2], Kirill Bolotin[2], and Andreas Knorr[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Department of Physics, Quantum Nanoelectronics of 2D Materials, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Interfaces of dye molecules and two-dimensional transition metal dichalcogenides (TMDCs) are promising candidates for optoelectronic applications since they combine the large molecular optical amplitudes and spectral range with high carrier mobilities in the semiconductor [1]. In such interfaces, Förster energy transfer is a key mechanism due to the large dipole moments, and has many intriguing technical applications [2].
In a joint theory-experiment study, we report microscopic calculations of the Förster induced transition rate from dye molecules to a TMDC layer and provide the corresponding optical signatures, with excellent agreement to the experimental data. The theoretic approach is based on microscopic Bloch equations which are solved self-consistently together with Maxwells equations [3], incorporating the sample geometry within the Rytova-Keldysh framework.
[1] Jariwala et al. Nat. Mater. **16**, 170 (2017)
[2] Dagher et al. Nat. Nanotech. **13**, 925-932 (2018)
[3] Selig et al. Phys. Rev. B **99**, 035420 (2019)

HL 19.9 Thu 13:30 P

Atomic Structure of Antiphase Domains on GaP/Si(100):As — Dominik Bratek[1], •Peter Kleinschmidt[1], Manali Nandy[1], Oliver Supplie[1,2], Agnieszka Paszuk[1], and Thomas Hannappel[1] — [1]Institut für Physik, Grundlagen von Energiematerialien, Technische Universität Ilmenau, 98693 Ilmenau, Deutschland — [2]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin, Deutschland

We have investigated the atomic structure of antiphase domains on GaP(100) on As-terminated Si(100) by scanning tunneling microscopy (STM). Thin GaP layers of 5 nm and 10 nm thickness were deposited on predominately double atomic layer stepped, As-terminated Si(100)-substrates by metalorganic vapor phase epitaxy. Small residuals of the intermediate steps on the substrate lead to the formation of minority antiphase domains in the epitaxial GaP. We show that these antiphase domains extend parallel to the step edges of the substrate. In numerous locations, small residual antiphase domains are embedded in trenches parallel to these step edges, and in other locations only the trenches remain, suggesting that these trenches are residuals of overgrown antiphase domains. Our STM measurements reveal the atomic structure of the antiphase boundaries, which varies substantially: some of these boundaries are just characterized by a half bi-layer step, whereas deep trenches are also frequently observed.

HL 19.10 Thu 13:30 P

Ultrafast energy transfer triggers ionization energy offset dependent quantum yields in low-bandgap NFA solar cells — •Julien F. Gorenflot[1], Safakath Karuthedath[1], Yuliar Firdaus[1], Catherine S. De Castro[1], George Harrison[1], Anastasia Markina[2], Neha Chaturvedi[1], Jafar Khan[1], Ahmed H. Balawi[1], Sri H. K. Paleti[1], Thomas Anthopoulos[1], Derya Baran[1], Denis Andrienko[2], and Frédéric Laquai[1] — [1]KAUST Solar Center (KSC), Material Science and Engineering program (MSE), Physical Science and Engineering division (PSE), King Abdullah University of Science and Technology, Thuwal, Saudi Arabia. — [2]Max Planck Institute for Polymer Research, Mainz, Germany.

Organic solar cells associate an electron donor and an electron acceptor to drive exciton-to-charge conversion where the strong EA acceptor attracts electrons from donor excitons, and the low IE donor attracts holes from acceptor excitons. Recent studies however, claim efficient photocurrent generation in recent non-fullerene acceptor (NFA) based systems with close-to-zero IE or EA offsets. Here, we confirm that sizeable IE offsets are required to drive hole transfer from acceptor exciton. Further charge separation from the interface is however barrierless. Due to fast, Förster Resonant Energy Transfer to the low bandgap acceptor, charge transfer always occurs from the acceptor, making the EA offset unimportant. We model the IE offset dependence of hole transfer and find that two physical parameters are sufficient to describe it. Our model also explains barrierless charge separation and the high charge transfer states energies reported in NFA-based systems.

HL 19.11 Thu 13:30 P

Electronic properties of MoS_2 monolayer doped by donor, acceptor, and aromatic molecules — •Juan Pablo Guerrero[1,2], Ana M. Valencia[2,3], Jannis Krumland[2], and Caterina Cocchi[2,3] — [1]Department of Physics, Freie Universität Berlin (Germany) — [2]Department of Physics and IRIS Adlershof, Humboldt-Universität zu Berlin (Germany) — [3]Institute of Physics, Carl von Ossietzky Universität Oldenburg (Germany)

The electronic properties of hybrid inorganic-organic interfaces are critically influenced by the level alignment across the heterostructure and by possible hybridization effects that occur therein. In turn, these properties are determined by the nature of the molecular dopants and by their arrangements. In the framework of (hybrid) density functional theory, we investigate the electronic structure of a single sheet of MoS_2 covered by monolayers of planar molecules such as pyrene, tetrathiafulvalene, and bithiophene, which are known to act as donors, as well as with the acceptors 7,7,8,8-tetracyanoquinodimethane and its tetrafluorinated counterpart. Our results show that all considered heterostructures exhibit a type II level alignment with negligible charge transfer at the interface. However, in the electronic structure of the systems, the signatures of electron or hole doping to the MoS_2 can be identified.

HL 19.12 Thu 13:30 P

Coulomb Blockade at room temperature of self-assembled GaN quantum dot ensembles, measured via Capacitance-Voltage spectroscopy — •Carlo Alberto Sgroi[1], Julien Brault[2], Jean-Yves Duboz[2], Philippe Vennéguès[2], Sébastien Chenot[2], Arne Ludwig[1], and Andreas D. Wieck[1] — [1]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44780

Bochum, Germany — [2]CNRS - CRHEA, Rue Bernard Grégory, 06560 Valbonne, France

We present capacitance voltage (C(V)) measurements at room temperature of charge-tunable self-assembled wurtzite GaN quantum dots (QDs) in an $Al_xGa_{1-x}N$ matrix grown by MBE. GaN and its alloys have excellent properties such as their thermal stability, high thermal conductivity and wide bandgap energies which make them an ideal candidate for next-generation GaN-based power devices at elevated temperatures. Single-photon sources operating at up to 350 K are already possible1. Due to polarization and strain effects in wurtzite $GaN/Al_xGa_{1-x}N$ heterostructure layers, the band structure is different for the cross section with the GaN QDs and the GaN Wetting Layer (WL) on which the QDs are formed. Large electric fields and defect-assisted electron hopping promote charge transfer through the WL. Performing C(V) spectroscopy at 300 K on an AlGaN-Schottky diode structure with embedded GaN QDs, single-electron discharging in the C(V) spectrum and a Coulomb blockade energy of about 70 meV are measured.

[1] Holmes, M. J., et al. ACS Photonics **3**, 543-546 (2016).

HL 19.13 Thu 13:30 P

Exploration of the electrochemical Interface of InP under applied potentials with Reflection Anisotropy Spectroscopy — •Margot Guidat, Mario Löw, Vibhav Yadav, Jongmin Kim, and Matthias M. May — Universität Ulm, Institute of Theoretical Chemistry, Ulm, Germany

A possible way to achieve a low-carbon energy leads through hydrogen, which can be produced via photoelectrochemical water splitting, in which III-V semiconductors play an important role [1]. However, surface corrosion results in limited performance of photoelectrochemical solar cells.

Some studies have reported that surface functionalization is a way to protect the surface, achieved by etching processes. However, this faces fundamental challenges, especially in electrochemical environments [2]. In this work, we investigate photoelectrochemical etching of Indium Phosphide (100) in contact with hydrochloric acid controlled by Reflection Anisotropy Spectroscopy: an in situ optical probe of electrochemical interfaces with very high interface sensitivity.

The RA spectra show a reversible build-up of an optical anisotropy in cathodic potential ranges, which might account for the reduction of InP into phosphine and metallic In. The latter would further react with HCl to form InCl interfacial film.

[1] Wang, T. and Gong, J. Angew. Chem. Int. Ed. 54, 10718-10732 (2015).

[2] B. L. Pearce, S. J. Wilkins, T. Paskova, A. Ivanisevic. Journal of Materials Research 2015, 30, 2859-2870.

HL 19.14 Thu 13:30 P

Carrier effective masses in 2D halide perovskites from a first-principles approach — •Xiangzhou Zhu[1], Mateusz Dyksik[2,3], Jonas D. Ziegler[5], Matan Menahem[4], Jonas Zipfel[5], Barbara Meisinger[5], Michal Baranowski[3], Omer Yaffe[4], Alexey Chernikov[5,6], Paulina Plochocka[2,3], and David A. Egger[1] — [1]Technical University of Munich, Germany — [2]LNCMI CNRS, France — [3]Wroclaw University of Science and Technology, Poland — [4]Weizmann Institute of Science, Israel — [5]University of Regensburg, Germany — [6]Dresden University of Technology, Germany

Two-dimensional halide perovskites (2D HaPs) are attracting significant attention as promising optoelectronic materials. Effective masses of charge carriers are crucial parameters for device performance and exciton behavior. Here, we report first-principles calculations based on density functional theory (DFT) to investigate magnitudes, microscopic origins and consequences of carrier effective masses in 2D HaPs. We demonstrate that distortions due to organic spacers as well as orbital hybridization effects due to metal cations lead to a wide tunability of effectives mass in 2D HaPs[1]. Furthermore, it is shown that the knowledge of the DFT-computed electron and hole masses is key to capture efficient exciton diffusion, as measured by spatially-resolved optical spectroscopy[2].

[1] Dyksik, M, et al. ACS Energy Lett. 5, 3609 (2020)

[2] Ziegler, J. D., et al. Nano Lett. 20, 6674 (2020)

HL 19.15 Thu 13:30 P

The interfacial (electronic) structure of InP(001) in contact with electrolytes from computational spectroscopy — Vibhav Yadav, Margot Guidat, Mario Löw, •Jongmin Kim, and Matthias M. May — Institute of Theoretical Chemistry, Universität Ulm, Ulm, Germany

The relevance of controlling the electrochemical interface of InP derived materials for energy-conversion has already been established [1]. A tandem structure with the ternary compound, AlInP, in contact with the electrolyte showed 19%, solar-to-hydrogen efficiency [2]. In practical applications under operating conditions, a surface in contact with water oxidizes by insertion or substitution. This leads to surface polymerisation: formation of PO_x and In_2O_3. These species improve the stability of the surface and reduce surface charge-carrier recombination. Therefore, an investigation of the interfacial properties is crucial. In this computational work, we model the electrochemical interface, using first-principles calculations, in accordance with previous experimental studies. Using this model, we will probe the electrochemical double layer region to take into account the electric field fluctuations during a molecular dynamics simulation: simulating open circuit conditions. We develop a methodology, enabling the understanding of surface processes, by means of computational reflection anisotropy spectroscopy (RAS) results. Finally, we compare our results with experiments to derive a comprehensive understanding.

[1] O. Khaselev, et al. Science **280**, 425 (1998).

[2] M. M. May, et al. Nat. Commun. **6**, 8286 (2015).

HL 19.16 Thu 13:30 P

Reduction of crystal defects in GaP buffer layers grown on Si(100) by MOCVD — •Manali Nandy[1], Agnieszka Paszuk[1], Markus Feifel[2], Christian Koppka[1], Peter Kleinschmidt[1], Frank Dimroth[2], and Thomas Hannappel[1] — [1]TU Ilmenau, Gustav-Kirchhoff-Straße 5, 98693, Ilmenau — [2]Fraunhofer Institute for Solar Energy Systems ISE, Freiburg 79110, Germany

The performance of III-V-on-Si multijunction solar cells is still limited by a high density of defects at the GaP/Si heterointerface and in the III-V buffer layers. Here, in order to improve the crystal quality of the GaP(100) buffer layer, we modified the GaP pulse nucleation by substituting the first five TEGa pulses with TMAl. The influence of Al on the defect density in the GaP buffer layers is investigated by electron channeling contrast imaging. 60 nm thick GaP(100) buffer layers grown on GaP nucleation exhibit short misfit dislocations (MDs) and therefore, a high density of threading dislocations (TDs). In contrast, GaP(100) buffer layers grown on GaP/AlP nucleation exhibit less, but longer MDs, which result in a lower density of TDs. In addition, the density of stacking faults and stacking faults pyramids in the GaP layer grown on the AlGaP nucleation is significantly reduced. The surface morphology at the initial growth stage of GaP buffer layers grown on AlGaP nucleation, is smoother compared to buffer layer grown on the GaP nucleation. The application of Al in the GaP nucleation process provides a two-dimensional, smooth layer on which subsequent, high-quality GaP films could be grown, and therefore, shows a promising pathway for improving the performance of III-V-on-Si devices.

HL 19.17 Thu 13:30 P

Understanding surface properties of CsK_2Sb from first principles — •Richard Schier[1], Holger-Dietrich Sassnick[2], and Caterina Cocchi[2] — [1]Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, 12489 Berlin — [2]Carl von Ossietzky Universität Oldenburg, Institute of Physics, 26129 Oldenburg

Among the most promising compounds for next-generation photocathodes in particle accelerators, CsK_2Sb is regarded with particular interest. While first-principles calculations have recently contributed to gain insight into the bulk characteristics of this system [1], for most physical processes related to photoemission, surface properties are essential. To fill this gap, we use density functional theory to simulate and analyze the stability and the electronic properties of the low-Miller-index surfaces of CsK_2Sb. After assessing the formation energies, we calculate ionization potential (IP), band structure, and projected density of states (PDOS). Depending on the surface, we find IPs ranging from 2.2 eV to 3.4 eV. The computed band structures reveal that CsK_2Sb surfaces can exhibit either direct and indirect bandgaps, and in some specific cases they can even become metallic. The calculated PDOS offers insight into the atomic contributions to the bands around the Fermi energy.

[1] C. Cocchi et al., J. Phys: Condens. Matter 31, 014002 (2019)

HL 19.18 Thu 13:30 P

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

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

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

HL 19.19 Thu 13:30 P

Pump-probe measurements to detect ultra-fast carrier dynamics and carrier density saturation in GaN-based quantum wells — •Malte Schrader, Philipp Henning, Heiko Bremers, Uwe Rossow, and Andreas Hangleiter — Institut für Angewandte Physik & Laboratory for Emerging Nanometrology, Technische Universität Braunschweig, 38106 Braunschweig, Germany

The aim of our study is to understand the carrier dynamics in GaN-based quantum wells at high carrier densities. An accurate estimation of the excited charge carrier density in pulsed laser experiments by indirect fluence-to-charge-density conversion is flawed, because the available states for the excited electrons in the conduction band might already be completely filled by the high fluence laser pulse.

We therefore show in this contribution a direct approach by using two pulsed laser beams in quick succession in a pump-probe setup: a pump beam excites the carriers and a probe beam measures the transmission shortly thereafter, and therefore the occupation of the states above the band edge. A laser pulse duration of 35 fs at 5 kHz repetition rate is used in a degenerate setup, meaning pump and probe beam have the same wavelength. The decay of the excited carrier states is encoded in the transmitted probe beam as a function of the delay between pump and probe beam. To detect a saturation limit the fluence of the pump beam is increased. Besides two distinct decay times of around 10 ps and several 100 ps respectively, the ultra-fast intraband relaxation in the fs domain is of special interest.

HL 19.20 Thu 13:30 P

Tuning the electrochemical properties of multifunctional catalyst layers by plasma-enhanced atomic layer deposition — •Matthias Kuhl, Alex Henning, Lukas Haller, Laura Wagner, Chang-Ming Jiang, Verena Streibel, Ian D. Sharp, and Johanna Eichhorn — Walter Schottky Institut, Technische Universität München

Major challenges in photoelectrochemical (PEC) energy conversion systems are the poor efficiency and material instability of semiconductor photoelectrodes under the harsh operating conditions. Recently, it was demonstrated that plasma-enhanced atomic layer deposition (PE-ALD) can be used to fabricate conformal, biphasic $Co_3O_4/Co(OH)_2$ catalyst layers on semiconductor photoelectrodes, which are simultaneously robust and electrochemically active. The nanocrystalline Co_3O_4 layer forms a durable interface to the substrate and the disordered $Co(OH)_2$ surface layer significantly improves the electrocatalytic oxygen evolution reaction (OER) activity.

Here, we leverage the precise control of PE-ALD to further tailor the thickness ratio of the surface and interface layers of the $Co_3O_4/Co(OH)_2$ bilayer by tuning the plasma exposure time during growth. Short pulses lead to the formation of porous, unstable, catalytically active $Co(OH)_2$ layers due to an incomplete precursor decomposition, while long pulses result in denser films and form stable, inactive Co_3O_4 layers. More generally, this work highlights the power of PE-ALD for engineering catalyst/semiconductor interfaces simultaneously exhibiting multiple functionalities.

HL 19.21 Thu 13:30 P

Effect of hydrogen in low temperature GaN underlayer on the effective carrier lifetime in GaInN/GaN single quantum wells — •Rodrigo De Vasconcellos Lourenço[1,2], Philipp Henning[1,2], Samar Hagag[1,2], Uwe Rossow[1], Heiko Bremers[1,2], and Andreas Hangleiter[1,2] — [1]Institute of Applied Physics, Technische Universität Braunschweig, Germany — [2]Laboratory for Emerging Nanometrology, Braunschweig, Germany

The luminescence efficiency of GaInN single quantum well (SQW) structures is affected by the growth conditions of all the layers grown before it and especially those ones directly before the quantum well - the so-called underlayer (UL). Usually, nitrogen is used as carrier gas during low temperature UL growth in low-pressure MOVPE. In this work, molecular hydrogen was added to the carrier gas during pure GaN UL growth and its supply was closed well before the QW is grown. Time-resolved photoluminescence measurements of SQWs with UL containing hydrogen and intentional Si doping suggest that they have better internal quantum efficiency at low temperature compared to the reference sample. Additionally, those showed longer radiative lifetime and longer emission wavelengths at low temperature compared to SQWs with doped UL and without hydrogen. This may indicate that hydrogen reduces the free carriers density by partly compensating the Si doping. Comparing SQWs with UL not intentionally doped, the one containing hydrogen showed shorter effective lifetime at low temperature, which could suggest that hydrogen acts as a donor or that hydrogen induces non-radiative centers.

HL 19.22 Thu 13:30 P

Transient Dielectric Function of Ge, Si, and InP from Femtosecond Pump-Probe Ellipsometry — •Carola Emminger[1,2], Shirly Espinoza[3], Steffen Richter[3,4], Oliver Herrfurth[5,6], Mateusz Rebarz[3], Martin Zahradník[3], Rüdiger Schmidt-Grund[6,7], Jakob Andreasson[3], and Stefan Zollner[1] — [1]New Mexico State University — [2]Masaryk University — [3]ELI Beamlines — [4]Linköpings universitet — [5]Active Fiber Systems — [6]Universität Leipzig — [7]Technische Universität Ilmenau

Structures in the dielectric function (DF), known as critical points (CPs), depend on temperature, strain, composition, and doping. We investigate CPs in the transient DF of Ge, Si, and InP measured with femtosecond pump-probe spectroscopic ellipsometry by calculating the second derivatives of the DF with respect to energy using a linear filter technique, which combines interpolation, noise reduction, scale change, and differentiation. From fitting an n-dimensional CP lineshape to the second derivatives, we find the amplitude, excitonic phase angle, threshold energy, and broadening as functions of delay time. A distinctive change of the CP parameters occurs within the first couple of picoseconds after the pump pulse. In the case of Ge, the CP energies red-shift due to band gap renormalization and an increase in temperature due to laser heating. After about 4 ps, the DF and CP parameters start to recover. Up to about 30 ps, coherent acoustic phonon oscillations are observed in the temporal evolution of the CP parameters. The period of these oscillations is approximately 11 ps, which is in good agreement with theory.

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X-ray absorption fingerprints in $LiCoO_2$ and CoO_2 — •Daniel Duarte Ruiz and Caterina Cocchi — Carl von Ossietzky Universität Oldenburg, Institut für Physik, Oldenburg, Deutschland

$LiCoO_2$ is a popular cathode material for Li-ion batteries, whereby X-ray absorption near-edge structure (XANES) is typically used to characterize electrodes in operando conditions. Identifying the spectral fingerprints of this compound and of its delithiated counterpart is therefore essential to provide references for the interpretation of the experimental spectra. In an *ab initio* work based on all-electron density functional theory and many-body perturbation theory (Bethe-Salpeter equation)[1], the XANES spectra of LiCoO2 and CoO2 are computed and analized for O K-edge as well as for the Co K- and $L_{2,3}$-edges. With the adopted approach, we are able to assess that in all spectra, excitonic effects manifest themselves only via a red-shift on the absorption peaks. Clear signatures distinguishing binary and ternary compounds in the O K-edge and Co $L_{2,3}$-edges spectra can be identified.

[1] C. Vorwerk et al. *Electron. Struc.* 1, 037001 (2019).

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RF beat note analysis of a semiconductor optical frequency comb — •Duc Nam Nguyen[1], Dominik Auth[1], Quentin Gaimard[2], Abderrahim Ramdane[2], and Stefan Breuer[1,3] — [1]Institute of Applied Physics, TU Darmstadt, Darmstadt, Germany — [2]Centre de Nanosciences et Nanotechnologies, Palaiseau, France —

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We experimentally study the RF beat note and optical spectra evolution of a frequency-modulated near-infrared semiconductor comb laser. We show and explain a transition towards stable optical frequency comb generation in dependence on the electrical biasing conditions.

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Contactless Measurement of the Sheet Resistance of two-dimensional Electron Gases — •Timo A. Kurschat, Arne Ludwig, and Andreas D. Wieck — Angewandte Festkörperphysik, Ruhr-Universität Bochum, Universitätsstraße 150, D-44780 Bochum

The aim of this work is to measure the sheet resistance of two-dimensional electron gases in GaAs without the need for built-in contacts. Thus a characterization is possible without destroying the wafer. This method can be used to create spatially resolved maps of whole wafers to evaluate quality and homogeneity prior to further processing.

The sheet resistance is measured by placing two electrodes (round metal plates) close to the sample. These electrodes form capacitances C with the conductive layer. With a high-frequency alternating voltage applied to one electrode, the transmitted power can be measured at the other one. The measured amplitude depends on the sample resistance and the impedance of the capacitances, which are proportional to $1/\omega C$.

The electrodes have a diameter of 3 mm and 6 mm center-to-center distance. The measurement range starts at about 300 Ω/□ and goes up to 50 kΩ/□. The sheet resistance is determined by sweeping the frequency between 1 MHz and 400 MHz and then applying a fit.

Besides the measurements of samples with known sheet resistance, maps of complete wafers are shown. The lateral resolution of about 5 mm depends on the size of the electrodes and was estimated by etching a structure on a wafer.

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

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

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

HL 19.27 Thu 13:30 P

Contact Preparation and Thermoelectric Properties of Bismuth Nanowires — •Mahni Müller[1], Rüdiger Mitdank[1], Hoda Moosavi[2], Michael Kröner[2], Peter Woias[2], Jeongmin Kim[3], Wooyoung Lee[3], Adnan Hammoud[4], Thomas Lunkenbein[4], and Saskia Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Laboratory of Design of Microsystems, University of Freiburg, IMTEK, 79110 Freiburg, Germany — [3]Department of Material Science and Engineering, Yonsei University, 03722 Seoul, Repuplic of Korea — [4]Fritz Haber Institute of the Max Planck Society, 14195 Berlin, Germany

Bismuth-based thermoelectric materials have always been promising for improving the thermoelectric figure of merit [1]. Those properties can strongly be modified through nanostructuring and additionally a high surface-to-volume-ratio is obtained with nanowires [2].

However, due to air exposure, a native oxide shell forms around the bismuth core, which leads to non-ohmic contact resistances. To achieve ohmic contacts for low temperature measurements, we present a preparation method with focused-ion-beam-induced deposition (fibid). Measurements of the electrical and thermal conductivity and of the Seebeck coefficient of bismuth nanowires with fibid-contacts between 10 K and 300 K were performed and compared to bulk. We discuss the change in properties and the possible influence of the contacting method.

[1] M. S. Dresselhaus *et al.*, Phys. Solid State **41**, 679-682 (1999).
[2] T. E. Huber *et al.*, Phys. Rev. B **83**, 2354414 (2011).

HL 19.28 Thu 13:30 P

Nonlinear down-conversion in a single quantum dot — •Björn Jonas, Dirk Heinze, Eva Schöll, Patricia Kallert, Timo Langer, Sebastian Krehs, Alex Widhalm, Klaus D. Jöns, Dirk Reuter, Stefan Schumacher, and Artur Zrenner — Paderborn University, Physics Department, Warburger Straße 100, 33098 Paderborn, Germany

In our work we study an all optical approach based on nonlinear principles, to tune the emission of the biexciton state in a single quantum dot[1]. After preparation of the biexciton state via phonon-assisted two-photon excitation, we introduce a control-laser which enables a nonlinear down-conversion via a virtual state. Previous theoretical work suggests that the spectral and polarization properties of this stimulated emission can be fully controled by adjusting the respetive properties of the control-laser[2]. In this work we show the first experimental demonstration of this process. The stimulated down-conversion works best if the virtual state is tuned close to the exciton energy and we can achieve a tuning range of about 0.5 meV around the exciton and biexciton emission. We furthermore make use of the spin conservation in the system to demonstrate control of the polarization of the emitted photon.

[1] http://arxiv.org/abs/2105.12393
[2] D. Heinze et al., Nature Communications **6**, 8473 (2015)

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Spin lasing in bimodal quantum dot micropillar cavities — •Niels Heermeier[1], Tobias Heuser[1], Jan Grosse[1], Natalie Jung[2], Markus Lindemann[2], Nils Gerhard[2], Martin Hofmann[2], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universiät Berlin, D-10623 Berlin, Germany — [2]Lehrstuhl für Photonik und Terahertztechnologie, Fakulktät für Elektrotechik und Informationstechnik, Ruhr-Universität Bochum, D-44780 Bochum

Spin-controlled lasers are highly interesting photonic devices and have been shown to provide ultra-fast polarization dynamics in excess of 200 GHz. In contrast to conventional semiconductor lasers their temporal properties are not limited by the intensity dynamics, but are governed primarily by the birefringent mode splitting that determines the polarization oscillation frequency. Another class of modern semiconductor lasers are high-beta emitters which benefit from enhanced light-matter interaction due to strong mode confinement in low-mode-volume microcavities. In such structures, the emission properties can be tailored by the resonator geometry to realize for instance bimodal emission behavior in slightly elliptical micropillar cavities. We utilize this attractive feature to demonstrate and explore spin-lasing effects in bimodal high-beta quantum dot micropillar lasers. The studied microlasers show spin laser effects with polarization oscillation frequencies up to 15 GHz which is controlled by the ellipticity of the resonator. Our results reveal appealing prospects for very compact and energy-efficient spin lasers and can pave the way for future purely electrically injected spin lasers enabled by short injection path lengths.

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Non-integer high-harmonic generation in a topological insulator — Christoph P. Schmid[1], Leonard Weigl[1], Patrick Grössing[2], Vanessa Junk[2], Cosimo Gorini[2], Stefan Schlauderer[1], Suguru Ito[3], •Manuel Meierhofer[1], Niklas Hofmann[1], Dmytro Afanasiev[1], Jack Crewse[2], Konstantin A. Kokh[4,5], Oleg E. Tereshchenko[5,6], Jens Güdde[3], Ferdinand Evers[2], Jan Wilhelm[2], Klaus Richter[2], Ulrich Höfer[3], and Rupert Huber[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, Germany — [2]Institute of Theoretical Physics, University of Regensburg, Germany — [3]Department of Physics, Philipps-University of Marburg, Germany — [4]V.S. Sobolev Institute of Geology and Mineralogy SB RAS, Novosibirsk, Russia — [5]Novosibirsk State University, Russia — [6]A.V. Rzhanov Institute of Semiconductor Physics SB RAS, Novosibirsk, Russia

We demonstrate multi-THz high-harmonic generation (HHG) in the

topological insulator bismuth telluride. The frequency of the driving field discriminates between HHG from the bulk and the topological surface, where long scattering times and the quasi-relativistic dispersion enable unusually efficient HHG. All observed orders, generated in the surface state, can be continuously shifted to arbitrary non-integer multiples of the driving frequency by varying the carrier-envelope phase of the driving field. The anomalous Berry curvature enforces meandering ballistic trajectories of the Dirac fermions, causing a hallmark HH polarization pattern. Our study provides a fascinating new platform to explore topology and relativistic strong-field quantum physics.

HL 19.31 Thu 13:30 P

Exciton-phonon coupling in transition metal dichalcogenides revealed by ultrafast electron diffraction. — •Ahmed Hassanien, Arne Ungeheuer, Mashood Tarek Mir, Lukas Nöding, Arne Senftleben, and Thomas Baumert — Institute of Physics and CINSaT, University of Kassel, Heinrich-Plett-Strasse 40, D-34132 Kassel, Germany

Exciton-phonon coupling (EXPC) is responsible in principle for the temperature-dependence of optoelectronic and transport properties of transition metal dichalcogenides (TMDCs). The signatures of EXPC are usually observed in resonance Raman scattering [1], time-resolved transmission measurements [2], in optical absorption [3] or recently in two-dimensional electronic spectroscopy (2DES) [4]. Using a highly compact femtosecond electron diffractometer developed in our group [5], we were able to probe a polarization-dependent lattice dynamics in mechanically exfoliated few-layers ReS2. These anisotropic structural dynamics followed the photoexcitation by femtosecond laser pulses spectrally in resonance with the lowest excitonic transitions in ReS2 [6].

References:

[1] Yang, Jinho, et al. FlatChem 3 (2017): 64-70. [2] Jeong, Tae Young, et al. Acs Nano 10.5 (2016): 5560-5566. [3] Christiansen, Dominik, et al. Physical review letters 119.18 (2017): 187402. [4] Li, Donghai, et al. Nature communications 12.1 (2021): 1-9. [5] Gerbig, C., et al. New J. Phys. 17.4 (2015):043050. [6] Sim, Sangwan, et al. Nature communications 7 (2016): 13569.