

## HL 13: Heterostructures, Interfaces and Surfaces

Time: Monday 16:45–18:30

Location: H17

HL 13.1 Mon 16:45 H17

**reducing waste through substrate reuse: a pathway to cost-effective iii-v optoelectronics** — ●RADOUANE ENNADIR — 3IT, Sherbrooke University, Sherbrooke, QC, Canada

III-V materials, such as Gallium Arsenide (GaAs), are widely used in optoelectronic devices due to their superior electronic and optical properties. However, the high cost of III-V substrates, primarily made from Ge or other expensive materials, represents a significant barrier to the widespread adoption of these technologies. Our research focuses on reducing waste in the production of III-V optoelectronics through the reuse of Germanium (Ge) substrates. In this study, we propose a novel approach to mitigate substrate waste by reusing Ge substrates in the fabrication of III-V optoelectronics. By carefully optimizing the recycling process, including substrate cleaning, surface treatment, and the integration of new III-V layers, we aim to significantly reduce material costs without compromising device performance. This approach not only enhances the sustainability of optoelectronic manufacturing but also provides a cost-effective pathway to large-scale production of III-V-based devices. The findings of this study contribute to both environmental sustainability and economic viability in the growing field of optoelectronics, opening up new opportunities for the development of advanced, cost-effective optoelectronic devices.

HL 13.2 Mon 17:00 H17

**Understanding local charge transfer processes in nanostructured photosystems** — ●NINA MILLER, SVEN DOLL, SERGEJ LEVASHOV, LUKAS WOLZ, MATTHIAS KUHLE, and JOHANNA EICHHORN — Physics Department, School of Natural Sciences, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany

Photoelectrochemical energy conversion offers a promising approach for directly converting solar energy into storable chemical fuels. For scalability, photoelectrodes are often fabricated using thin film technologies yielding material architectures with complex micro- and nanoscale structures. One challenge in this context is that the characteristics of these nanostructured material architectures often deviate from the properties of idealized model systems. To understand energy conversion processes at surfaces and interfaces of nanostructured material systems, novel atomic force microscopy methods have emerged recently, such as AFM-based scanning electrochemical microscopy, to resolve local chemical transformations, charge transport, and material changes under operation conditions. By correlating nanoscale and macroscale properties, we will establish the link between nanoscale processes and macroscopic performance, advancing the design of efficient semiconductor/catalyst systems for PEC applications.

HL 13.3 Mon 17:15 H17

**Simulation of charge and excitation dynamics across nanostructured organic-organic interfaces** — ●GIACOMO COTELLI<sup>1,2</sup>, ENGIN TORUN<sup>2</sup>, STEFANO GOTTARDI<sup>2</sup>, and ANNA KÖHLER<sup>1</sup> — <sup>1</sup>Soft Matter Optoelectronics (EP II), University of Bayreuth, Bayreuth 95440, Germany — <sup>2</sup>Simbeyond B.V., Eindhoven, The Netherlands

The deposition of organic layers via solution processing may lead to rough interfaces or intermixed regions between layers. To investigate the impact of roughness at organic-organic interfaces on the performances of OLEDs, we performed 3D kinetic Monte Carlo simulations of symmetrical bi- and three-layer devices. Our results reveal that the macroscopic behaviour of a device can be significantly affected by the shape and size of roughness at the organic interfaces, influencing both charge and exciton dynamics.

Namely, we introduced interfaces with periodic corrugation and either triangular or rectangular cross-section. In presence of charge accumulation at an interface with triangular cross-section, bilayer devices exhibit strong inhomogeneity in the spatial distribution of charge carriers, excitons and excitonic losses. Comparison to a flat-interface device reveals an increment in current density by a factor from 2 to 10<sup>3</sup>, depending on the height of the energy barrier at the interface. This current density boost was successfully applied to improve charge injection towards a central emissive layer (EML) in simulated three-layer devices; the size and configuration of the interfaces can also be leveraged to fine-tune the recombination zone inside the EML. Nevertheless, we raise our concerns in terms of increased local material degradation.

HL 13.4 Mon 17:30 H17

**Strain gradients in bent GaAs nanowires as a new way of engineering electronic transitions** — ●FRANCISCA MARÍN<sup>1</sup>, YIANNIS HADJIMICHAEL<sup>2</sup>, CHRISTIAN MERDON<sup>2</sup>, PATRICIO FARRELL<sup>2</sup>, CONSTANZA MANGANELLI<sup>3</sup>, OLIVER BRANDT<sup>1</sup>, and LUTZ GEELHAAR<sup>1</sup> — <sup>1</sup>Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e. V. Berlin, Germany — <sup>2</sup>Weierstraß-Institut für angewandte Analysis und Stochastik. Berlin, Germany — <sup>3</sup>Institut für Halbleiterphysik, Leibniz-Institut für innovative Mikroelektronik. Frankfurt (Oder), Germany

Strain gradients open up a new degree of freedom in strain engineering, enabling polarization in all dielectric materials through the flexoelectric effect. However, flexoelectric coefficients remain unknown for many inorganic semiconductors, including GaAs, leaving this phenomenon unexplored in this material system.

Here, we exploit the pronounced strain gradient in bent GaAs nanowires grown by molecular beam epitaxy to study this effect using photoluminescence spectroscopy. Strain and strain gradients in these nanowires influence the bandgap and generate electric fields from piezoelectric and flexoelectric effects. By combining experiments with a simple one-dimensional model to calculate the expected shift of the electronic transitions, and finite element simulations of piezoelectricity, we provide new insights into flexoelectricity in GaAs.

HL 13.5 Mon 17:45 H17

**Understanding Local Charge Transport Using Advanced Kelvin Probe Force Microscopy** — ●SVEN ERIK DOLL, SERGEJ LEVASHOV, NINA MILLER, and JOHANNA EICHHORN — Department of Physics, TUM School of Natural Sciences, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany

Efficient photosystems for solar-to-chemical energy conversion are often based on nanostructured semiconductor architectures. In these material systems, the nanoscale properties frequently dominate the performance at the macroscale. Therefore, local understanding of their charge transfer and transport properties is decisive for optimizing their efficiency and stability.

To this end, we use Kelvin probe force microscopy (KPFM) in a controlled atmosphere to spatially resolve band bending, charge accumulation, and local variations of the generated surface photovoltage. However, analyzing nanostructured materials with complex morphologies is not trivial since topographic crosstalk can dominate the results. To overcome these limitations, we combine a commercial AFM with an external Lock-In amplifier to enable dual-frequency and heterodyne KPFM measurements with improved resolution and sensitivity compared to conventionally frequency-modulated and amplitude-modulated KPFM modes. Here, we compare different KPFM modes and highlight the importance of careful imaging and data analysis to reveal insights into local semiconductor material properties at grain boundaries or different facets.

HL 13.6 Mon 18:00 H17

**Topological Phase Diagram of Mercury Cadmium Telluride Quantum Wells** — ●LEONID BOVKUN<sup>1,2</sup>, LENA FÜRST<sup>1,2</sup>, CHRISTOPHER FUCHS<sup>1,2</sup>, VLADIMIR MARKOVIĆ<sup>1,2</sup>, MAXIMILIAN HOFER<sup>1,2</sup>, MORITZ SIEBERT<sup>1,2</sup>, CHRISTIAN BERGER<sup>1,2</sup>, FLORIAN BAYER<sup>1,2</sup>, WOUTER BEUGELING<sup>1,2</sup>, STEFFEN SCHREYECK<sup>1,2</sup>, HARTMUT BUHMANN<sup>1,2</sup>, LAURENS W. MOLENKAMP<sup>1,2</sup>, and TOBIAS KIESSLING<sup>1,2</sup> — <sup>1</sup>Physikalisches Institut (EP3), Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — <sup>2</sup>Institute for Topological Insulators, Am Hubland, 97074 Würzburg, Germany

The key ingredient for the formation of a topological insulator phase in Mercury Cadmium Telluride is the inversion of the energetic positions of the electronic  $\Gamma_6$  and  $\Gamma_8$  bulk bands, that can be controlled by alloying with Cd to get within reach of electronic tunability.

We present a systematic experimental study of the topological phase transition in a series of  $\sim 10$  nm thick  $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$  quantum wells by tuning the Cd content  $x$ . We provide detailed structural and magnetooptical spectroscopic characterization measurements and establish a comprehensive picture of the alloy structural and energetic properties.

Using these as input, we employ  $\mathbf{k}\cdot\mathbf{p}$  modeling to establish the topological phase diagram of  $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$  in dependence of the Cd content and quantum well thickness for thin films which are pseudomorphically

strained to the lattice constant of pure CdTe.

HL 13.7 Mon 18:15 H17

**Electrostatic control of the band structure in HgTe heterostructures** — ●MORITZ SIEBERT<sup>1,2</sup>, MAXIMILIAN HOFER<sup>1,2</sup>, LEONID BOVKUN<sup>1,2</sup>, VLADIMIR MARKOVIĆ<sup>1,2</sup>, CHRISTIAN BERGER<sup>1,2</sup>, FLORIAN BAYER<sup>1,2</sup>, JULIAN KUTHER<sup>1,2</sup>, DANIEL MICHEL<sup>1,2</sup>, LENA FÜRST<sup>1,2</sup>, CHRISTOPHER FUCHS<sup>1,2</sup>, WOUTER BEUGELING<sup>1,2</sup>, STEFFEN SCHREYECK<sup>1,2</sup>, HARTMUT BUHMANN<sup>1,2</sup>, LAURENS W. MOLENKAMP<sup>1,2</sup>, and TOBIAS KIESSLING<sup>1,2</sup> — <sup>1</sup>Physikalisches Institut (EP3), Universität Würzburg, Am Hubland, 97074 Würzburg, Ger-

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We investigate the band structure of topologically inverted thick HgTe quantum wells employing magneto-optical THz- and IR-spectroscopy. The lithographic fabrication of a semi-transparent gate enables control of the charge carrier density in the quantum well. Our magnetic field dependent self-consistent  $\mathbf{k} \cdot \mathbf{p}$  band structure calculations give insights into the physical origin of the observed spectral signatures. In this talk, I present how the electrostatic gating not only sets the number of free charge carriers in the HgTe quantum well - but also modifies the electronic dispersion - and explain the observed features.