# HL 48: Heterostructures, Interfaces and Surfaces: Fabrication and Structure

Time: Thursday 15:00–17:15 Location: POT/0251

HL 48.1 Thu 15:00 POT/0251

**Cross-sectional scanning tunneling microscopy (XSTM) study of nearly lattice-matched III-V semiconductor heterostructures** — •Hitesh Kumar[1], Rüdiger Schott[2], Zijin Lei[2], Werner Wegscheider[2], and Stefan Fölsch[1] — [1]Paul Drude Institute for Solid State Electronics, Berlin, Germany — [2]Laboratory for Solid State Physics, ETH Zürich, Zürich, Switzerland

XSTM is a powerful technique for investigating the structural and electronic properties of III-V semiconductor heterostructures. These heterostructures are grown along the [001] direction by molecular beam epitaxy and accessible in cross-sectional view by cleaving the sample in ultrahigh vacuum to expose the (110) cleavage surface. We used this approach to study a GaSb-InAs-AlGaSb-InAs-InAsSb layered heterostructure grown on a Te-doped GaSb substrate. Voltage-dependent chemical contrast in STM imaging allows differentiation between anions and cations in the III-V semiconductors. Using this capability, we analyzed the degree of homogeneity in the ternary materials (Al-Ga mixing in the AlGaSb layer and As-Sb mixing in the InAsSb layer). With the help of scanning tunneling spectroscopy, we precisely determined the band gaps of the individual layers and locally probed the band lineup across the entire heterostructure. This allowed us to investigate the behavior of charge carriers governed by the band lineup. Specifically, we studied the spatial confinement and quantization of conduction band states in the InAs layer and their decay into the gap region of the adjacent layers.

HL 48.2 Thu 15:15 POT/0251

**Theoretical Exploration of the Electronic Structure at Group-III Nitride Interfaces** — •Maximilian Lauer[1,2], Christian Maas[1,2], Jan M. Waack[1,2], Michael Czerner[1,2], and Christian Heiliger[1,2] — [1]Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Germany — [2]Zentrum für Materialforschung (ZfM), Justus-Liebig-Universität Gießen, Germany

Group-III nitrides are an essential group of materials at the forefront of modern optoelectronics. Recently, the metastable zincblende (In,Ga)N system emerged as a promising material for optoelectronic devices. Heterojunctions play a central role in device design, making a precise understanding of their electronic structure essential. Determining the band alignment at the interface is crucial for understanding its electronic properties.

Here, we show that the zb-GaN/zb-InN heterojunction exhibits a Type-I alignment with no states forming within the band gap at the interface. We performed KKR calculations with LDA-1/2 band gap corrections on coherently strained supercells. We report values for the band offset parameters and explore the microscopic electronic structure at the interface. Our calculations demonstrate the importance of band corrections for calculating electronic structure parameters, such as band offsets, and provide a basis for further investigations into the (Ga,In)N alloy system using the CPA.

HL 48.3 Thu 15:30 POT/0251

**GaPN growth on As-Modified Si(100) for defect-reduced heteroepitaxy** — •Hitha Haridas[1], Kai Daniel Hanke[1], Agnieszka Paszuk[1,2], and Thomas Hannappel[1] — [1]Technische Universität Ilmenau, Fundamentals of Energy Materials, Ilmenau,Germany — [2]BMFTR Junior Research Group PARASOL, Technische Universität Ilmenau, Germany

The Monolithic integration of III-V semiconductors with Si(100) offers a promising route toward high-efficiency,low-cost optoelectronic devices. Among these materials, GaPN is a promising candidate for III-V/Si integration because it can be grown lattice-matched to silicon, thereby minimizing strain and reducing the formation of misfit dislocations. However, structural defects generated during the earliest stages of growth can propagate into subsequent epitaxial layers, ultimately limiting device performance. In this study, we investigate the nucleation and early-stage growth behavior of GaPN on As-modified Si(100) surfaces by combining ex situ surface morphology analysis,electron channeling contrast imaging, and in situ optical spectroscopy.This integrated approach allows us to systematically evaluate how variations in the initial growth conditions influence defect formation. The insights gained provide broader guidance for improving interface quality and advancing III-V/Si heteroepitaxy through more precise control over the initial growth phases.

HL 48.4 Thu 15:45 POT/0251

**Acoustoelectric effect in organic-inorganic semiconductor systems** — •Paromita Bhattacharjee[1], Patrick Ganswindt[2], Alexander S. Urban[2], and Hubert Krenner[1] — [1]Institute of Physics, University of Münster, Germany — [2]Faculty of Physics, Ludwig-Maximilians-Universität München, Germany

Surface acoustic waves (SAWs) are elastic waves propagating on the surface of a piezoelectric solid and while interacting with a semiconductor, its strain and piezoelectric fields modulate the band-gap. Strain-induced field imposes an acoustoelectric (AE) drag on the charges in the direction of SAW propaga-tion, and in a photoconductive semiconductor, excitons get ionized by piezoelectric field into separate elec-trons and holes, captured and transported by SAW [1]. Utilizing these effects, we present first study of SAW-induced charge transport in hybrid organic-inorganic semiconductor system of organic polymer, poly(3-hexylthiophene) (P3HT) and halide perovskite (CsPbBr3 and CsPb(IxBr1-x)3) nanowires (HPNWs). In samples with only HPNWs the total AE current nearly vanishes due to comparable electron-hole mobilities in these materials [2]. However, in hybrid layers, weak AE effect is observed with CsPb(IxBr1-x)3 NWs and a hole dominated AE transport with CsPbBr3 NWs. The band realignment at the heterojunction explains that while for CsPb(IxBr1-x)3 -P3HT ambipolar electron-hole transport occurs via the NWs, for CsPbBr3-P3HT, electrons are limited by low electron mobility in P3HT. References: [1] J. Phys. D: Appl. Phys. 57, 423001 (2024). [2] Nano Lett., 19, 8701-8707 (2019).

**15 min. break**

HL 48.5 Thu 16:15 POT/0251

**Ultra-high vacuum exfoliation method for the preparation of large-area single layer TMDC films** — •Zhiying Dan[1], Ronak Sarmasti Emami[1], Antonija Antonija Grubisic-Cabo[1], Petra Rudolf[1], Deepnarayan Biswas[2], and Tien-Lin Lee[2] — [1]Zernike Institute for Advanced Materials, University of Groningen, 9747 AG Groningen, The Netherlands — [2]Diamond Light Source Ltd., Harwell Science and Innovation Campus, Didcot, Oxfordshire, OX11 0DE, UK

Two-dimensional transition metal dichalcogenides (2D TMDCs) are promising candidates for next-generation electronic, optical, and spintronic devices. While mechanical exfoliation yields high-quality 2D flakes, their lateral size is typically limited to tens of micrometers. Here, we report the preparation of 2D WS2 and WSe2 using a recently developed kinetic in situ single-layer synthesis (KISS) method, performed in ultra-high vacuum and tailored for surface science studies. We examine how substrate choice and chalcogen species affect film size and quality using X-ray photoelectron spectroscopy, low-energy electron diffraction, atomic force microscopy, and X-ray standing waves (XSW). Our results show that the quality of the bulk TMDC crystal is crucial for successful KISS exfoliation. Moreover, preliminary XSW data suggest that KISS does not degrade the underlying substrate, highlighting its potential as a non-destructive approach for 2D material synthesis.

HL 48.6 Thu 16:30 POT/0251

**Electrical conduction and sensing properties of contacted CNTs after MOF synthesis** — •Marvin J. Dzinnik[1], Adrian Hannebauer[2], Feriel Friha[1], Andreas Schaate[2], and Rolf J. Haug[1,3] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hanover, Germany — [2]Institut für Anorganische Chemie, Leibniz Universität Hannover, 30167 Hanover, Germany — [3]Laboratorium für Nano- und Quantenengineering, Leibniz Universität Hannover, 30167 Hanover, Germany

Metal-organic frameworks (MOFs) are a versatile sensor material: they are tunable, highly porous, and can be precisely grown on carbon nanotubes (CNTs).[1]

Here, we investigate how UiO-66 MOF growth affects single nanotubes. We performed DC measurements on contacted multi-walled carbon nanotubes (MWCNTs) before and after UiO-66 synthesis. We observe pronounced changes in both magnitude and character of the electrical response, indicating a strong interaction between MWCNT

and MOF. AC measurements show a linear response to ethanol vapor up to 40 000 ppm, suggesting that single MWCNT-MOF hybrids are promising, tunable gas-sensing elements.

[1] Dzinnik, M. J. et al. Commun Mater 5, 38 (2024).

HL 48.7 Thu 16:45 POT/0251

**Nucleation behavior for remote epitaxy of GaAs and AlAs on carbon-covered GaAs substrates** — •Binamra Shrestha, Tobias Henksmeier, and Dirk Reuter — Paderborn University, Paderborn, Germany

Recently, remote epitaxy was proposed as a method that enables the growth of free-standing single-crystal layers and substrate reuse by using atomically thin 2D materials as release layers. In this work, we investigate the epitaxial growth behavior of GaAs and AlAs on ultrathin amorphous carbon layers deposited by PECVD on GaAs substrates. The amorphous carbon exhibits a graphene-like structure consisting predominantly of in-plane $sp^2$ bonding, thereby serving as a quasi-2D template capable of transmitting the substrate's electrostatic potential for remote epitaxial growth.

We performed controlled nucleation studies using molecular beam epitaxy (MBE). First, a GaAs buffer layer is grown on the bare GaAs to planarize the substrate surface, then the sample is covered with amorphous carbon. Subsequently, ultrathin GaAs layers ranging from 0.25 nm to 2 nm are deposited on the graphene/GaAs template at 300 °C, and the resulting nuclei are examined via atomic force microscopy (AFM). Nucleation is first observed at approximately 0.37 nm deposition thickness, with nuclei predominantly aligned along atomic steps. This strong step-edge preference indicates that remote epitaxy is the dominant mechanism, compared to pinhole-initiated nucleation. These results highlight the suitability of PECVD-deposited amorphous carbon as an effective 2D interlayer for remote epitaxy.

HL 48.8 Thu 17:00 POT/0251

**Quantum confinement in semiconductor random alloys: a case study on Si/SiGe/Si** — •Daniel Dick[1,2,3,4], Florian Fuchs[1,2,3], Sibylle Gemming[2,4], and Jörg Schuster[1,2,3] — [1]Center for Micro- and Nanotechnology, TU Chemnitz, Germany — [2]Center for Materials, Architecture and Integration of Nanomembranes, TU Chemnitz, Germany — [3]Fraunhofer Institute for Electronic Nanosystems (ENAS), Chemnitz, Germany — [4]Institute of Physics, TU Chemnitz, Germany

When the size of random alloys is reduced, local fluctuations of alloy composition become more influential. Using extended Hückel theory, we study the semiconductor alloy SiGe sandwiched between Si due to its relevance in semiconductor devices. We evaluate the effects of the alloy composition, layer thickness, and local fluctuations of the Ge concentration on band alignment and the band gap. Results are compared to the finite quantum well model. This model captures the essenial physics and can act as a computationally faster surrogate model.