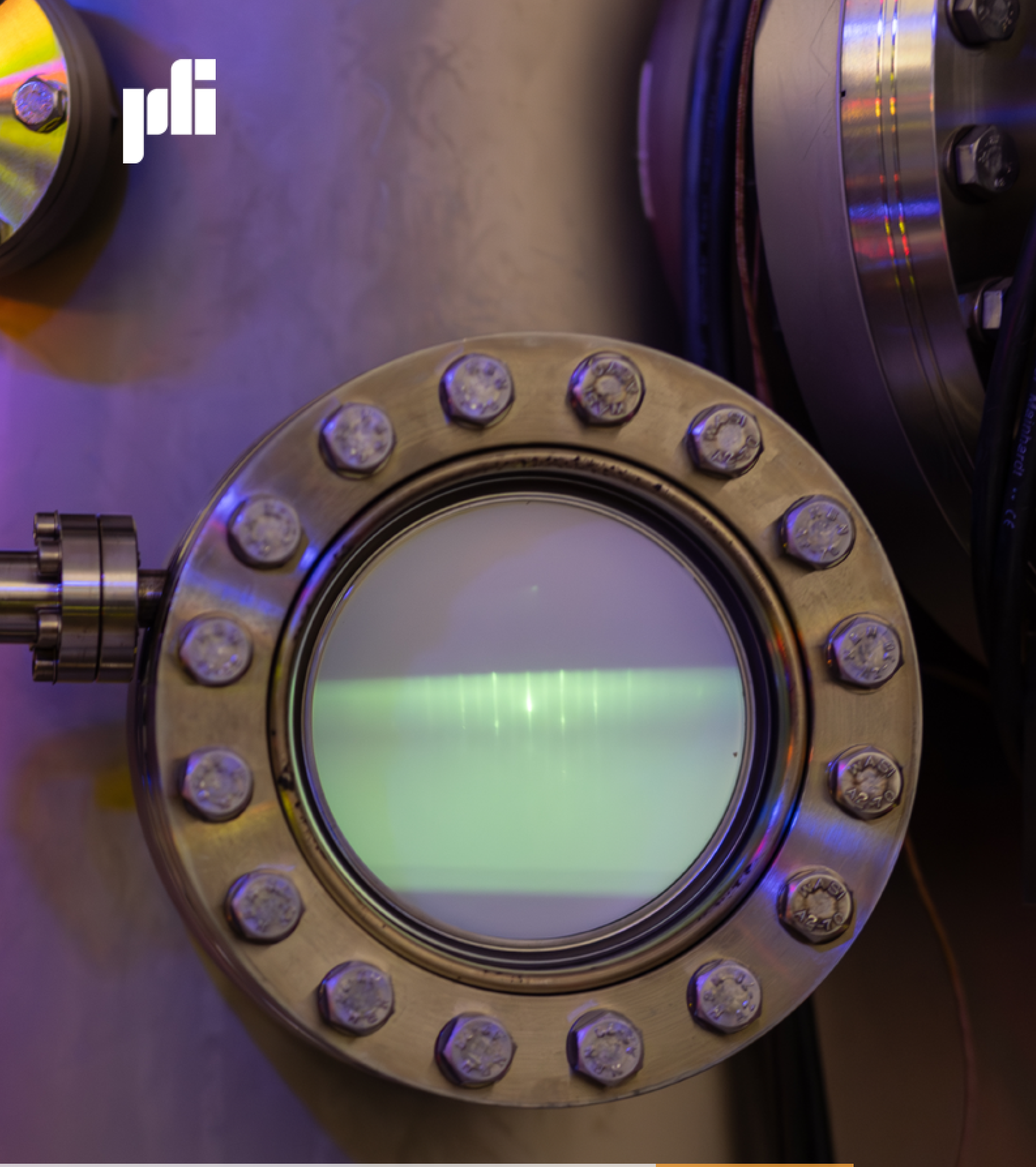

PDI ANNUAL REPORT
PDI JAHRESBERICHT

Paul-Drude-Institut für Festkörperelektronik (PDI)
Leibniz-Institut im Forschungsverbund Berlin e.V.

2025

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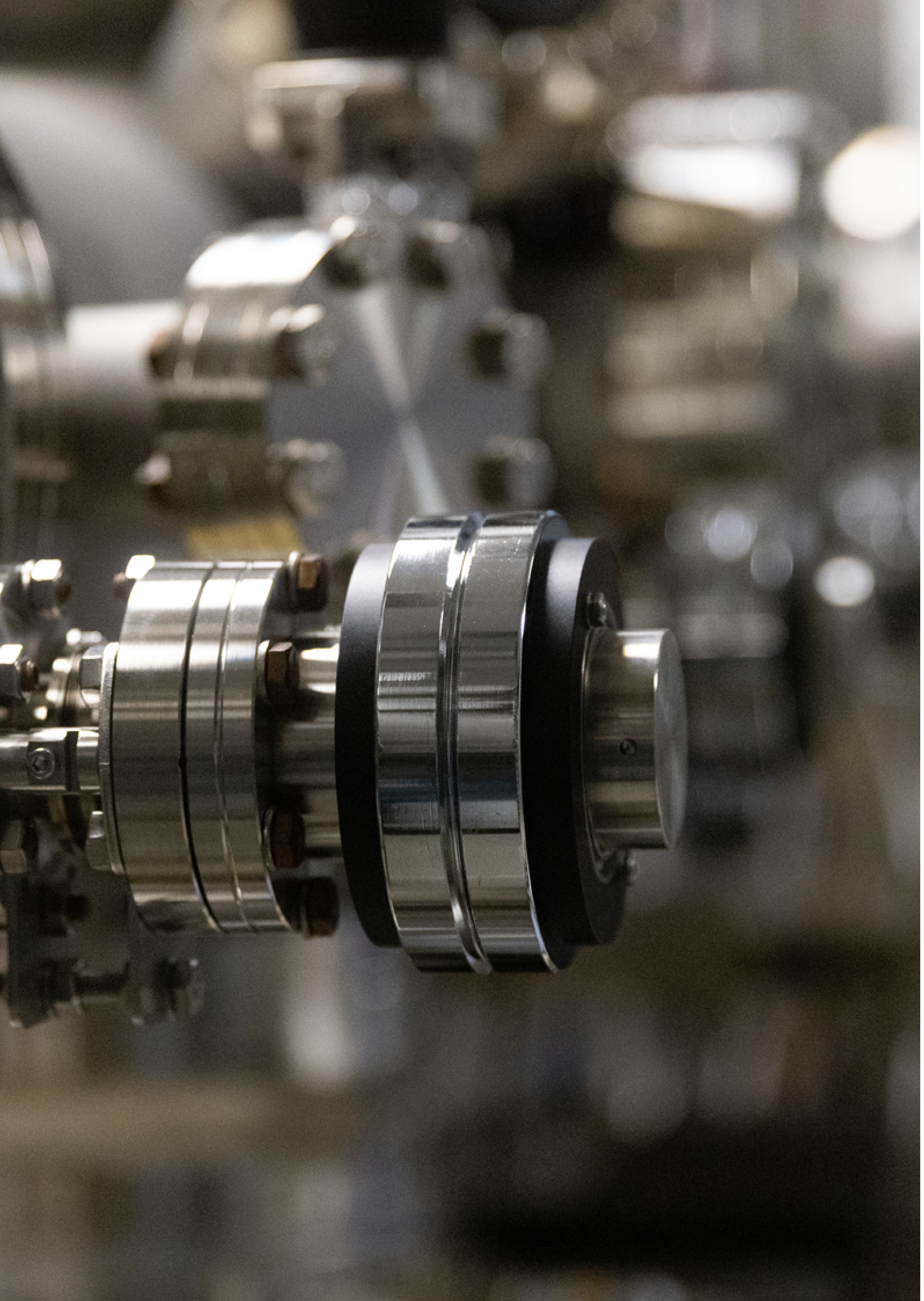

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Research Highlights

Forschungs-Highlights

Rational Computational Design of Metal-Organic Precursors for Complex Oxide Thin Film Growth via Multi-Physics Modeling: Titanium(IV)-Isopropoxide Thermolysis as a Case Study

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Metalorganic molecules play a crucial role in thin film growth and the coating industry, offering a low-temperature deposition route through thermal decomposition by releasing organic ligands. Yet, despite their widespread use, we still don't fully understand how these molecules break down at the atomic level—especially under ultra-high vacuum conditions like those adopted in both conventional and hybrid MBE experimental setups at our institute, PDI. In this talk, I'll walk you through our newly developed multiscale modeling approach to tackle this knowledge gap, using the most widely studied metalorganic precursor, *Titanium(IV)-Isopropoxide (TTIP)*, as a case study [1]. There's been ongoing debate in the community about how *TTIP* decomposes—most assume it's mainly via ß-hydride elimination through C–O bond dissociation [2-3].

Our work challenges that assumption. Using a combination of quantum chemistry, reactive molecular dynamics and metadynamics simulations, we show that while via ß-hydride elimination is prominent, it's only part of the picture. We've identified additional, previously underemphasized reactions—what we call via ß-X eliminations—that also play a major role in the overall decomposition mechanism. I'll show how this combined modeling approach not only gives us a clearer picture of the chemistry involved but also helps correct for the temperature bias in reactive molecular dynamics simulations. More importantly, it opens the door to computationally guided design of untapped precursor chemistries—ones with tailored decomposition pathways optimized for specific thin film growth applications. While we focus on *TTIP*, the methodology is general and can be applied to other metalorganic systems to accelerate precursor development across a range of materials and technologies.

[1] Fazlioglu et al. Npj. Comput. Mater.
[2] Chaukulkar et al. J. Vac. Sci. Technol. A: Vac. Surf. Films, 31, 031509 (2013).
[3] Anderson et al. J. Vac. Sci. Technol. A: Vac. Surf. Films 32, 01A114 (2014).

Rationales computergestütztes Design metallorganischer Vorstufen für das Wachstum komplexer Oxid-Dünnschichten mittels Multiphysik-Modellierung: Thermolyse von Titan(IV)-isopropoxid als Fallstudie

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Metallorganische Moleküle spielen eine entscheidende Rolle beim Dünnschichtwachstum und in der Beschichtungsindustrie, da sie durch thermische Zersetzung unter Freisetzung organischer Liganden einen Niedertemperatur-Abscheidungsweg ermöglichen. Trotz ihrer weiten Verbreitung ist jedoch noch immer nicht vollständig verstanden, wie diese Moleküle auf atomarer Ebene zerfallen – insbesondere unter Ultrahochvakuum-Bedingungen, wie sie sowohl bei konventionellen als auch bei hybriden MBE-Anlagen an unserem Institut, dem PDI, eingesetzt werden. In diesem Beitrag stellen wir unseren neu entwickelten Multiskalen-Modellierungsansatz vor, mit dem wir diese Wissenslücke am Beispiel des am häufigsten untersuchten metallorganischen Precursors, *Titan(IV)-isopropoxid (TTIP)*, schließen [1]. In der Fachwelt wird seit langem diskutiert, wie *TTIP* zerfällt – die meisten gehen davon aus, dass dies überwiegend durch ß-Hydrid-Eliminierung über die Dissoziation der C–O-Bindung geschieht [2–3].

Unsere Arbeit stellt diese Annahme infrage. Mithilfe einer Kombination aus Quantenchemie, reaktiver Molekulardynamik und Metadynamik-Simulationen zeigen wir, dass die ß-Hydrid-Eliminierung zwar dominant, aber nur ein Teil des Bildes ist. Wir haben zusätzliche, bislang unterschätzte Reaktionen identifiziert – sogenannte ß-X-Eliminierungen –, die ebenfalls eine wesentliche Rolle im gesamten Zersetzungsmechanismus spielen. Wir zeigen, wie dieser kombinierte Modellierungsansatz nicht nur ein klareres Bild der beteiligten Chemie liefert, sondern auch hilft, die Temperaturverzerrung in reaktiven Molekulardynamik-Simulationen zu korrigieren. Vor allem aber eröffnet er die Möglichkeit, bislang ungenutzte Precursor-Chemien computergestützt zu entwerfen – mit maßgeschneiderten Zersetzungspfaden, die auf spezifische Anwendungen im Dünnschichtwachstum optimiert sind. Obwohl der Fokus auf *TTIP* liegt, ist die Methodik allgemein anwendbar und kann auf andere metallorganische Systeme übertragen werden, um die Entwicklung von Precursoren für eine Vielzahl von Materialien und Technologien zu beschleunigen.

[1] Fazlioglu et al. Npj. Comput. Mater.
[2] Chaukulkar et al. J. Vac. Sci. Technol. A: Vac. Surf. Films, 31, 031509 (2013).
[3] Anderson et al. J. Vac. Sci. Technol. A: Vac. Surf. Films 32, 01A114 (2014).

Cross-sectional scanning tunneling microscopy study of nearly lattice-matched III–V semiconductor heterostructures

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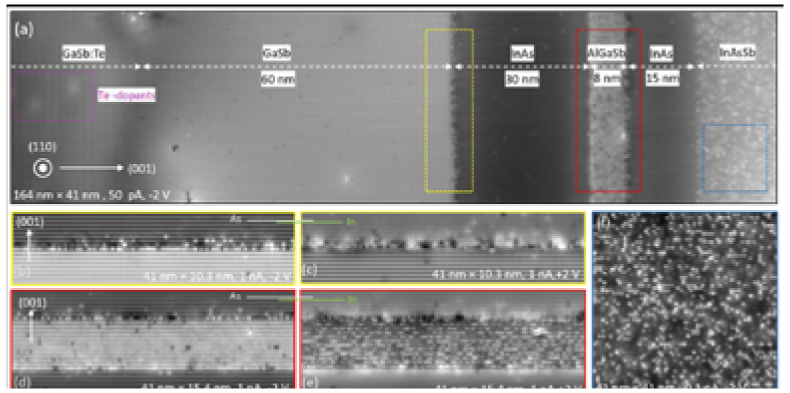
Cross-sectional scanning tunneling microscopy (X-STM) is a powerful technique for investigating the atomic and electronic properties of materials. III-V semiconductor heterostructures grown along the (001) direction by molecular beam epitaxy are accessible in cross-sectional view by cleaving the sample 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. We examined its topography, layered and interfacial properties, including roughness, composition, and electronic properties, using scanning tunneling microscopy and spectroscopy.



The figure shows constant-current topography images of the entire heterostructure (a) and selected areas (b-f), highlighting the interfaces, the degree of homogeneity in the ternary AlGaSb layer, and the As-Sb mixing in the InAsSb capping layer. The interface roughness was deduced from atomically resolved images, revealing, for example, asymmetries in interface roughness along the growth direction (d). For tunneling into unoccupied sample states, we obtained chemical contrast in the AlGaSb layer [protrusions in (e)], showing that the intermixing between Al and Ga is not perfect; the Ga content is found to be approximately ~65%. Also, in the InAsSb region (f), our data reveal chemical contrast between As and Sb, yielding an As:Sb ratio of approximately 10:1, in close agreement with the growth parameters.

X-STM of III-V semiconductor materials provides valuable information for optimizing the epitaxial growth process: it ensures controlled layer thickness and helps to elucidate defect densities, interface roughness, and the degree of homogeneity in ternary materials. These improvements are vital for the fabrication of high-performance quantum cascade lasers (QCLs), multi-junction solar cells, and high-speed optoelectronic devices.

Querschnitts-Rastertunnelmikroskopie-Untersuchung nahezu gitterangepasster III-V-Halbleiter-Heterostrukturen

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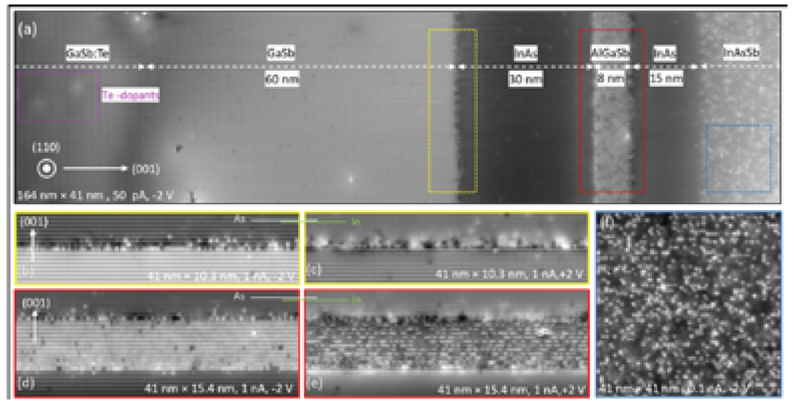
Die Querschnitts-Rastertunnelmikroskopie (X-STM) ist eine leistungsfähige Methode zur Untersuchung der atomaren und elektronischen Eigenschaften von Materialien. III-V-Halbleiter-Heterostrukturen, die entlang der (001)-Richtung mittels Molekularstrahlepitaxie gewachsen wurden, sind im Querschnitt zugänglich, indem die Probe im Ultrahochvakuum gespalten wird, um die (110)-Spaltfläche freizulegen. Mit diesem Ansatz untersuchten wir eine geschichtete GaSb-InAs-AlGaSb-InAs-InAsSb-Heterostruktur, die auf einem Te-dotierten GaSb-Substrat gewachsen wurde. Wir analysierten deren Topographie sowie Schicht- und Grenzflächeneigenschaften – einschließlich Rauheit, Zusammensetzung und elektronischer Eigenschaften – mittels Rastertunnelmikroskopie und -spektroskopie.



Die Abbildung zeigt Topographiebilder der gesamten Heterostruktur bei konstantem Strom (a) sowie ausgewählter Bereiche (b–f), die die Grenzflächen, den Grad der Homogenität in der ternären AlGaSb-Schicht sowie die As-Sb-Durchmischung in der InAsSb-Deckschicht hervorheben. Die Grenzflächenrauheit wurde aus atomar aufgelösten Bildern abgeleitet und zeigt beispielsweise Asymmetrien in der Grenzflächenrauheit entlang der Wachstumsrichtung (d). Beim Tunneln in unbesetzte Probenzustände ergab sich chemischer Kontrast in der AlGaSb-Schicht [Erhebungen in (e)], der zeigt, dass die Durchmischung von Al und Ga nicht vollständig ist; der Ga-Gehalt liegt bei etwa 65 %. Auch im InAsSb-Bereich (f) zeigen unsere Daten chemischen Kontrast zwischen As und Sb, mit einem As:Sb-Verhältnis von etwa 10:1, was gut mit den Wachstumsparametern übereinstimmt.

X-STM an III-V-Halbleitermaterialien liefert wertvolle Informationen zur Optimierung des Epitaxieprozesses: Es ermöglicht eine kontrollierte Schichtdicke und hilft, Defektdichten, Grenzflächenrauheit und den Homogenitätsgrad in ternären Materialien aufzuklären. Diese Verbesserungen sind für die Herstellung leistungsstarker Quantenkaskadenlaser (QCLs), Mehrfachsolarzellen und schneller optoelektronischer Bauelemente von wesentlicher Bedeutung.

Self-assembled $Al_{1-x}Sc_xN$ nanowires: a strain-free model system to investigate fundamental materials properties

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The incorporation of Sc into wurtzite AlN is an effective way to extend the functionalities of the group III-nitride semiconductors. Ternary metastable $Al_{1-x}Sc_xN$ alloys are strongly piezoelectric, ferroelectric and exhibit promising non-linear optical properties, which are already being exploited in novel device applications. However, studying the fundamental physical behavior of $Al_{1-x}Sc_xN$ remains challenging due to the absence of bulk material. In particular, residual strain in currently available epilayers – resulting from the lattice and thermal expansion mismatch to the underlying substrate – can significantly affect its properties.

We use molecular beam epitaxy to grow ≈ 500 nm long wurtzite $Al_{1-x}Sc_xN$ nanowire segments with $0 \le x \le 0.38$ on self-assembled AlN nanowire stems. The nanowire sidewalls facilitate elastic strain relaxation, thus enabling an accurate determination of both lattice parameters and phonon energies of bulk-like $Al_{1-x}Sc_xN$ in the entire compositional range. Our nanowires show a non-monotonic variation in the c-lattice constant as a function of Sc content, with a maximum value at $x \approx 0.2$, in agreement with *ab-initio* calculations [1] and previous experimental reports [2]. Raman spectroscopy reveals a monotonic red-shift of the E_1(TO), E_2^h and A_1(TO) modes as a function of Sc content. Thanks to the absence of strain, the peak positions directly reflect the energy variation of these modes with composition. The broadening of both the $Al_{1-x}Sc_xN$(0002) reflection and the Raman peaks with increasing Sc content reflects the strong compositional disorder induced by the incorporation of Sc in the ternary alloy.

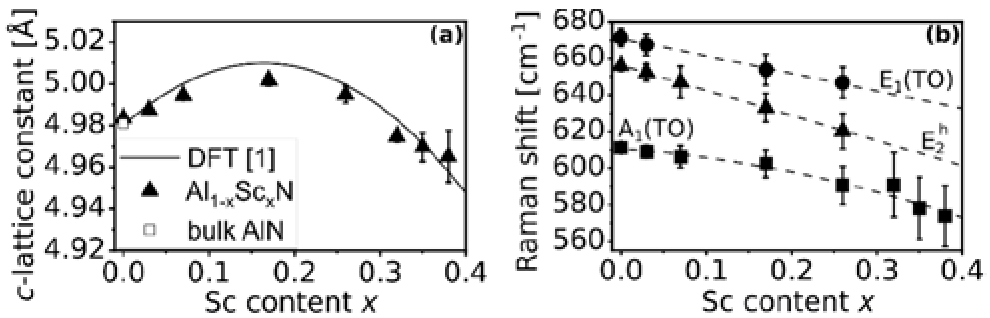

Figure 1. (a) c-lattice constant and (b) E_1(TO), E_2^h and A_1(TO) Raman modes of $Al_{1-x}Sc_xN$ nanowires with varying Sc content (excitation at 473 nm). Dashed lines are guides to the eye.

[1] D. Urban, O. Ambacher, and C. Elsässer: Physical Review B 11, 115204 (2021).
[2] O. Ambacher, B. Christian, N. Feil, D. Urban, C. Elsässer, M. Prescher, and L. Kriste: Journal of Applied Physics 130, 045102 (2021).

Selbstorganisierte $Al_{1-x}Sc_xN$-Nanodrähte: ein spannungsfreies Modellsystem zur Untersuchung grundlegender Materialeigenschaften

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Der Einbau von Sc in wurtzitisches AlN ist ein wirksamer Weg, um die Funktionalität von Gruppe-III-Nitrid-Halbleitern zu erweitern. Ternäre, metastabile $Al_{1-x}Sc_xN$-Legierungen sind stark piezoelektrisch, ferroelektrisch und weisen vielversprechende nichtlineare optische Eigenschaften auf, die bereits in neuartigen Bauelementen genutzt werden. Die Untersuchung des grundlegenden physikalischen Verhaltens von $Al_{1-x}Sc_xN$ bleibt jedoch aufgrund des Fehlens von Volumenmaterial eine Herausforderung. Insbesondere kann Restverspannung in derzeit verfügbaren Epischichten – bedingt durch die Gitter- und Wärmeausdehnungsfehlanpassung zum darunterliegenden Substrat – die Eigenschaften erheblich beeinflussen.

Wir nutzen Molekularstrahlepitaxie, um ≈ 500 nm lange, wurtzitische $Al_{1-x}Sc_xN$-Nanodrahtsegmente mit $0 \le x \le 0{,}38$ auf selbstorganisierten AlN-Nanodrahtstämmen zu wachsen. Die Seitenflächen der Nanodrähte ermöglichen eine elastische Spannungsrelaxation und erlauben so eine präzise Bestimmung sowohl der Gitterparameter als auch der Phononenenergien von volumenartigem $Al_{1-x}Sc_xN$ über den gesamten Zusammensetzungsbereich. Unsere Nanodrähte zeigen eine nicht-monotone Variation der c-Gitterkonstante in Abhängigkeit vom Sc-Gehalt, mit einem Maximum bei $x \approx 0{,}2$, in Übereinstimmung mit *Ab-initio*-Rechnungen [1] und früheren experimentellen Berichten [2]. Raman-Spektroskopie zeigt eine monotone Rotverschiebung der E_1(TO)-, E_2^h- und A_1(TO)-Moden in Abhängigkeit vom Sc-Gehalt. Dank der Abwesenheit von Verspannung spiegeln die Peak-Positionen direkt die Energievariation dieser Moden mit der Zusammensetzung wider. Die Verbreiterung sowohl der $Al_{1-x}Sc_xN$(0002)-Reflexion als auch der Raman-Peaks mit zunehmendem Sc-Gehalt spiegelt die starke kompositionelle Unordnung wider, die durch den Einbau von Sc in die ternäre Legierung verursacht wird.

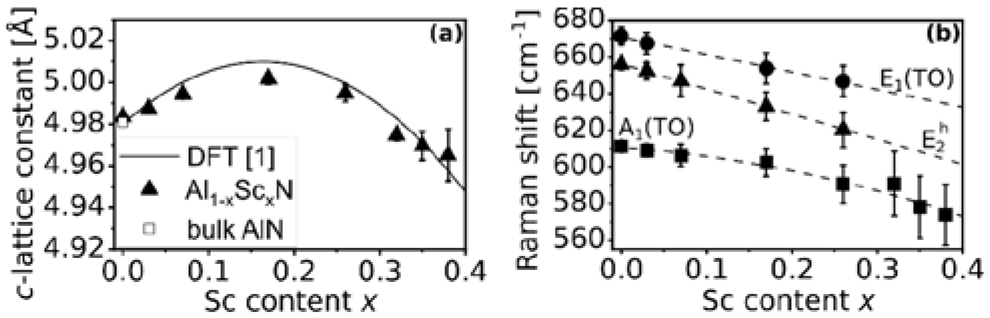

Abbildung 1. (a) c-Gitterkonstante und (b) E_1(TO)-, E_2^h- und A_1(TO)-Raman-Moden von $Al_{1-x}Sc_xN$-Nanodrähten mit variierendem Sc-Gehalt (Anregung bei 473 nm). Gestrichelte Linien dienen der Orientierung.

[1] D. Urban, O. Ambacher, und C. Elsässer: Physical Review B 11, 115204 (2021).
[2] O. Ambacher, B. Christian, N. Feil, D. Urban, C. Elsässer, M. Prescher, und L. Kriste: Journal of Applied Physics 130, 045102 (2021).

PDI Annual Report 2025

2D Magnetic Materials and Heterostructures at the PDI: Current Status and Prospects

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Two-dimensional (2D) magnetic materials are promising building blocks for the realization of novel devices for spintronics and quantum technologies with low-power consumption. Moreover, combining them with other 2D crystals such as graphene and transition metal dichalcogenides to form van der Waals heterostructures is a very attractive route to obtain hybrid systems exhibiting integrated electronic, optical, and magnetic functionalities [1]. So far, most of the research on 2D magnets and related heterostructures has been conducted on flakes exfoliated from bulk single crystals. However, the implementation of these materials in various technologies depends strongly on the development of large-scale epitaxial growth.

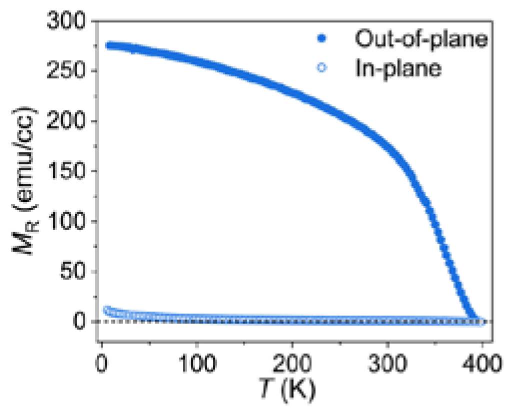

Figure 1. Remanent magnetization (M_R) measured by SQUID as a function of temperature in out-of-plane and in-plane configurations for a 10 nm thick Fe_3GaTe_2 film on graphene/SiC(0001).

This contribution will present an overview of our achievements in the MBE growth and characterization of the 2D ferromagnetic metals $Fe_{5-x}GeTe_2$ [2] and Fe_3GaTe_2 [3] on single crystalline graphene and WSe_2 templates. These ternary compounds are particularly promising among different 2D magnets due to their relatively high Curie temperature at or above 300 K [1]. We will show that our MBE films exhibit high crystalline quality and sharp interfaces to the underlying templates. Remarkably, magnetic characterization utilizing different methods reveals that, depending on the composition and crystalline phase, ferromagnetic order persisting up to 400 K with a predominant out-of-plane anisotropy can be achieved (e.g., see Fig. 1).

These findings will be discussed by considering the correlation between structure and magnetism, with a focus on the effects of compositional tuning and formation of metastable phases. We will also present a comparison of our results with those reported for state-of-the-art bulk crystals and flakes of the same materials, to highlight the importance of our research in terms of further material development and applications. Finally, the main prospects and future research directions on 2D magnets at the PDI will be presented.

[1] A. Grubisic-Cabo et al., 2D Materials 12, 031501 (2025).
[2] H. Lv et al., Small 19, 2302387 (2023); IEEE Transactions on Magnetics 60, 4100505 (2024). [3] T. Shinwari et al., arXiv:2505.06128 (2025).

2D-Magnetische Materialien und Heterostrukturen am PDI: Aktueller Stand und Perspektiven

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Zweidimensionale (2D) magnetische Materialien sind vielversprechende Bausteine für die Realisierung neuartiger Bauelemente für Spintronik und Quantentechnologien mit geringem Energieverbrauch. Darüber hinaus stellt ihre Kombination mit anderen 2D-Kristallen wie Graphen und Übergangsmetalldichalkogeniden zu Van-der-Waals-Heterostrukturen einen äußerst attraktiven Weg dar, um Hybridsysteme mit integrierten elektronischen, optischen und magnetischen Funktionalitäten zu erhalten [1]. Bisher wurde der Großteil der Forschung an 2D-Magneten und verwandten Heterostrukturen an aus Volumenkristallen exfolierten Flakes durchgeführt. Die Anwendung dieser Materialien in verschiedenen Technologien hängt jedoch entscheidend von der Entwicklung großflächiger epitaktischer Wachstumsverfahren ab.

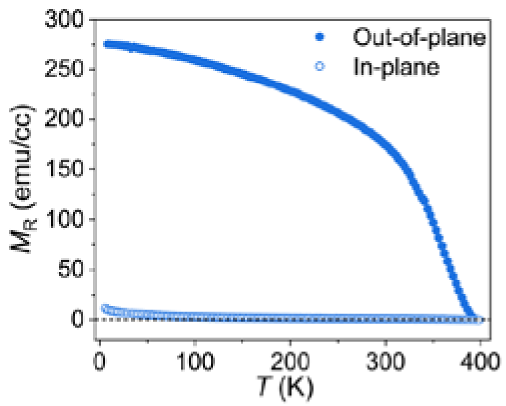

Abbildung 1. Remanente Magnetisierung (M_R), gemessen mittels SQUID als Funktion der Temperatur, in Out-of-Plane- und In-Plane-Konfiguration für eine 10 nm dicke Fe_3GaTe_2-Schicht auf Graphen/SiC(0001).

Dieser Beitrag gibt einen Überblick über unsere Fortschritte beim MBE-Wachstum und der Charakterisierung der 2D-ferromagnetischen Metalle $Fe_{5-x}GeTe_2$ [2] und Fe_3GaTe_2 [3] auf einkristallinen Graphen- und WSe_2-Templaten. Diese ternären Verbindungen sind aufgrund ihrer vergleichsweise hohen Curie-Temperatur von 300 K oder darüber [1] unter den verschiedenen 2D-Magneten besonders vielversprechend. Wir zeigen, dass unsere MBE-Schichten eine hohe kristalline Qualität und scharfe Grenzflächen zu den darunterliegenden Templaten aufweisen. Bemerkenswerterweise zeigt die magnetische Charakterisierung mittels verschiedener Methoden, dass je nach Zusammensetzung und Kristallphase eine ferromagnetische Ordnung bis zu 400 K mit vorwiegend Out-of-Plane-Anisotropie erreicht werden kann (siehe z. B. Abb. 1).

Diese Ergebnisse werden im Hinblick auf die Korrelation zwischen Struktur und Magnetismus diskutiert, mit besonderem Fokus auf die Effekte der kompositionellen Abstimmung und der Bildung metastabiler Phasen. Zudem vergleichen wir unsere Ergebnisse mit denen aktueller Volumenkristalle und Flakes derselben Materialien, um die Bedeutung unserer Forschung für die weitere Materialentwicklung und Anwendungen hervorzuheben. Abschließend werden die wichtigsten Perspektiven und zukünftigen Forschungsrichtungen zu 2D-Magneten am PDI vorgestellt.

[1] A. Grubisic-Cabo et al., 2D Materials 12, 031501 (2025).
[2] H. Lv et al., Small 19, 2302387 (2023); IEEE Transactions on Magnetics 60, 4100505 (2024).
[3] T. Shinwari et al., arXiv:2505.06128 (2025).

Core Research Areas
Forschungsschwer-punkte

Control of Elementary Excitations by Acoustic Fields
Kontrolle elementarer Anregungen durch akustische Felder

Solid-state excitations—electrons, excitons, magnons—are highly sensitive to strain, and acoustic phonons offer a dynamic way to control them. This CReA uses surface and bulk acoustic waves, generated by piezoelectric transducers at frequencies up to 20 GHz, to manipulate excitations in semiconductor and magnetic nanostructures. Applications span telecommunications, quantum information processing, and hybrid acousto-opto-electronic systems, with future potential for coherent microwave-to-optical transduction.

Anregungen in Festkörpern – Elektronen, Exzitonen, Magnonen – reagieren empfindlich auf Verspannung, und akustische Phononen bieten einen dynamischen Weg, sie zu kontrollieren. Dieses CReA nutzt akustische Oberflächen- und Volumenwellen, erzeugt durch piezoelektrische Wandler bei Frequenzen bis zu 20 GHz, um Anregungen in Halbleiter- und magnetischen Nanostrukturen zu manipulieren. Anwendungen reichen von der Telekommunikation über Quanteninformationsverarbeitung bis zu hybriden akusto-opto-elektronischen Systemen, mit Zukunftspotenzial für kohärente Mikrowellen-Optik-Umwandlung.

Reports

MEMBERS

Senior Scientists: A. Hernández-Mínguez, K. Biermann, P. V. Santos
Postdocs: A. S. Kuznetsov, M. Yuan
PhD Students: M. Saeedi, N. Ashurbekov
Visiting scientists: P. W. Matrone (PhD), R. Rachmandran (PhD), J. Gordon, I. Carraro Haddad (PhD), Prof. M. Msall, Prof. A. Pitanti

FACTS & FIGURES

Publications: 4
Talks & Seminars: 10
Third-party Funding: Nanoscale optomechanical interactions in semiconductor microcavities: DFG, Coherent GHz electro-optomechanics with polaromechanical crystals: DFG, High-frequency SAW resonators on SiC: EU, Nitrides4Future

Disordered Semiconductors
Ungeordnete Halbleiter

Organic semiconductors offer tunable electronic properties, mechanical flexibility, and sustainability, but structural disorder and instability limit their performance. This CReA uses epitaxial growth to bring order to organic semiconductors, combined with advanced spectroscopy and modeling. Focus areas include epitaxial photoactive layers for solar cells, device physics of organic/hybrid solar cells, and room-temperature spin transport for future spintronic applications.

Organische Halbleiter bieten anpassbare elektronische Eigenschaften, mechanische Flexibilität und Nachhaltigkeit, doch strukturelle Unordnung und Instabilität begrenzen ihre Leistungsfähigkeit. Dieses CReA nutzt epitaktisches Wachstum, um Ordnung in organische Halbleiter zu bringen, kombiniert mit fortschrittlicher Spektroskopie und Modellierung. Schwerpunkte sind epitaktische photoaktive Schichten für Solarzellen, die Bauelementphysik organischer/hybrider Solarzellen sowie Raumtemperatur-Spintransport für künftige spintronische Anwendungen.

Reports

MEMBERS

Senior Scientists: S. Shoaee

Postdocs: N. Tokmoldin, K. Stavrou

PhD Students: F. Ashtari Mahini, Y. Cao, J. Langentepe-Kong, D. Sun

FACTS & FIGURES

Publications: 2

Third-party Funding:
• Sinfonia: Leibniz,
• OPVStability: EU MSCA,
• DFG: Pushing the FF of Non-Fullerene Acceptors Based Solar Cells Above 80% (Fabulous II)

PDI Annual Report 2025

III-V Nanowires for Optoelectronics
III-V-Nanodrähte für die Optoelektronik

When III-V semiconductors are shaped into nanowires, their properties change fundamentally, opening new optoelectronic possibilities. This CReA grows III-nitride and III-arsenide nanowires by molecular beam epitaxy and top-down methods, studying properties intrinsic to their wire-like geometry and testing them in demonstrator devices. Applications range from photoelectrochemical CO_2 conversion to pseudo-substrates and piezoelectric power generation.

Werden III-V-Halbleiter zu Nanodrähten geformt, verändern sich ihre Eigenschaften grundlegend – das eröffnet neue optoelektronische Möglichkeiten. Dieses CReA wächst Gruppe-III-Nitrid- und Gruppe-III-Arsenid-Nanodrähte mittels Molekularstrahlepitaxie sowie Top-down-Verfahren und untersucht Eigenschaften, die sich direkt aus ihrer drahtförmigen Geometrie ergeben, sowie deren Einsatz in Demonstrator-Bauelementen. Anwendungen reichen von der photoelektrochemischen CO_2-Umwandlung bis zu Pseudo-Substraten und piezoelektrischer Energiegewinnung.

Reports

MEMBERS

Senior Scientists: O. Brandt, L. Geelhaar, J. Lähnemann

Postdocs: P. John, J. Kang, M. Gómez Ruiz, Franscisca Marín Largo

PhD Students: A. Campbell, A. Notarangelo, H. Zhang

FACTS & FIGURES

Publications: 3

Collaborations 2025: Weierstraß-Institut, Helmholtz-Zentrum Berlin, U Potsdam, Walter-Schottky-Institut, CNRS-Institut Néel, CEA/PHELIQS, CNRS-CHREA, Cambridge University, NIST, U Berkeley, McMaster University

Intersubband Emitters: GaAs-based Quantum-Cascade Lasers

Intersubband-Emitter: GaAs-basierte Quantenkaskadenlaser

Quantum-cascade lasers generate terahertz light through engineered intersubband transitions in GaAs-based heterostructures, making them powerful sources for high-resolution spectroscopy. This CReA designs, grows, and characterizes THz QCLs by molecular beam epitaxy, aiming to improve operating temperature and efficiency. Applications include molecular and atomic spectroscopy, atmospheric and astronomical research—such as detecting atomic oxygen—and plasma diagnostics.

Quantenkaskadenlaser erzeugen Terahertz-Licht durch gezielt konstruierte Intersubband-Übergänge in GaAs-basierten Heterostrukturen und sind damit leistungsstarke Quellen für die hochauflösende Spektroskopie. Dieses CReA entwirft, wächst und charakterisiert THz-QCLs mittels Molekularstrahlepitaxie mit dem Ziel, Betriebstemperatur und Effizienz zu verbessern. Anwendungen umfassen molekulare und atomare Spektroskopie, Atmosphären- und Astronomieforschung – etwa den Nachweis von atomarem Sauerstoff – sowie die Plasmadiagnostik.

Reports

MEMBERS

Senior Scientists: K. Biermann, X. Lü, E. Luna Garcia de la Infanta

Postdocs: V. Pistore, S. Ghayeb Zamharir

FACTS & FIGURES

Publications: 1

Third-party Funding:
- Micro-QCL: DFG (2023-2026)
- iQCT: DFG (2025-2027
- UTC4QCL: DFG (2025-2027)

PDI Annual Report 2025

Magnetic Materials for Spintronics and Magnetoacoustics

Magnetische Materialien für Spintronik und Magnetoakustik

Magnetic materials enable new ways to control electronic and magnetic properties for spintronic and magnetoacoustic technologies. Building on PDI's expertise in ferromagnet/semiconductor and 2D magnetic heterostructures, this CReA studies spin-dependent transport, epitaxial growth of 2D ferromagnets, hybrid heterostructures, and magnetoacoustic coupling between surface acoustic waves and magnetization—advancing next-generation spintronic and quantum technologies.

Magnetische Materialien eröffnen neue Wege zur Steuerung elektronischer und magnetischer Eigenschaften für spintronische und magnetoakustische Technologien. Aufbauend auf der Expertise des PDI in Ferromagnet/Halbleiter- und 2D-magnetischen Heterostrukturen untersucht dieses CReA spinabhängigen Transport, das epitaktische Wachstum von 2D-Ferromagneten, hybride Heterostrukturen sowie die magnetoakustische Kopplung zwischen akustischen Oberflächenwellen und Magnetisierung – als Grundlage für spintronische und Quantentechnologien der nächsten Generation.

Reports

MEMBERS

Senior Scientists: J. Herfort, J.M.J. Lopes, A. Hernández-Mínguez, A. Trampert, M. Hanke

Postdocs: H. Lv, T. Shinwari, K.I.A. Khan, H. Tornatzky

PhD Students: M. Hansemann, J.P.L. Gomes

FACTS & FIGURES

Publications: 2

Talks & Seminars: 14

Third-party Funding:
- EU Flagera (2024 – 2027)
- DFG SPP 2244 (2024 – 2027)

Nanoanalytics
Nanoanalytik

As devices shrink to the nanoscale, understanding atomic-scale structure and composition becomes essential to material performance. This CReA develops high-sensitivity characterization and modeling tools to clarify structure-property relationships in nanomaterials. Focus areas include epitaxial interfaces and 2D layers, strain and defect characterization, phase stability, and artificial quantum structures—supported by PDI's electron tomography, synchrotron, and low-temperature STM facilities.

Mit zunehmender Miniaturisierung von Bauelementen wird das Verständnis atomarer Struktur und Zusammensetzung für die Materialleistung entscheidend. Dieses CReA entwickelt hochempfindliche Charakterisierungs- und Modellierungswerkzeuge zur Klärung von Struktur-Eigenschafts-Beziehungen in Nanomaterialien. Schwerpunkte sind epitaktische Grenzflächen und 2D-Schichten, Verspannungs- und Defektcharakterisierung, Phasenstabilität sowie künstliche Quantenstrukturen – unterstützt durch die Elektronentomographie-, Synchrotron- und Tieftemperatur-STM-Einrichtungen des PDI.

Reports

MEMBERS

Senior Scientists: S. Fölsch, M. Hanke, E. Luna Garcia de la Infanta, A. Trampert
PhD Students: A. Reis, E. Paysen, K. Graser, H. Kumar
Master Student: M. Karadag
Visiting scientists: K. Hagen (U Strassbourg), A. McMinn (Arizona State U)

FACTS & FIGURES

Publications: 12
Third-party Funding: BALET: EFRE, Artificial quantum states on semiconductor surfaces created and probed by cryogenic scanning tunneling microscopy: DFG (2024-2027), New strategies for reducing dislocation density in monolithic III/V epitaxy on Si: DFG (2021-2025) DFG

PDI Annual Report 2025

Nanoelectronics
Nanoelektronik

Quantum effects are increasingly central to next-generation data processing, communication, and storage. This CReA investigates quantum transport and coherent coupling in artificial hetero- and nanostructures fabricated by electron-beam lithography, using low-temperature, high-field transport spectroscopy. A current focus is the coherent coupling of electrons or holes with lattice vibrations (phonons) as a route toward solid-state quantum bits.

Quanteneffekte gewinnen für Datenverarbeitung, Kommunikation und Speicherung zunehmend an Bedeutung. Dieses CReA untersucht Quantentransport und kohärente Kopplung in künstlichen Hetero- und Nanostrukturen, die mittels Elektronenstrahllithographie hergestellt werden, mit Transportspektroskopie bei tiefen Temperaturen und hohen Magnetfeldern. Ein aktueller Schwerpunkt ist die kohärente Kopplung von Elektronen oder Löchern mit Gitterschwingungen (Phononen) als Weg zu Festkörper-Quantenbits.

MEMBERS

Senior Scientists: S. Ludwig

PhD Students: S. Sirt

FACTS & FIGURES

Publications: 9

Collaborators 2025: ETH Zürich, National Research Council, Canada, İstanbul ATLAS University, Weizmann Institute, Israel, Universität Bochum, Freie Universität Berlin, Instituto de Ciencia de Materiales de Madrid (CSIC)

Nitride Semiconductors
Nitrid-Halbleiter

Nitride semiconductors—indium, gallium, and aluminum nitride and their alloys—underpin LEDs and power electronics, making them the second most economically important semiconductor class after silicon. PDI grows high-quality nitride epilayers by molecular beam epitaxy and characterizes them via luminescence spectroscopy. Current focus areas include AlN-based high electron mobility transistors, novel nitride alloys with transition metals for ferroelectric and ferromagnetic functionality, and charge-carrier recombination studies supported by the new ZALKAL cathodoluminescence laboratory.

Nitrid-Halbleiter – Indium-, Gallium- und Aluminiumnitrid sowie ihre Legierungen – bilden die Grundlage für LEDs und Leistungselektronik und sind damit nach Silizium die wirtschaftlich bedeutendste Halbleiterklasse. Das PDI wächst hochwertige Nitrid-Epischichten mittels Molekularstrahlepitaxie und charakterisiert sie mittels Lumineszenzspektroskopie. Aktuelle Schwerpunkte sind AlN-basierte High-Electron-Mobility-Transistoren, neuartige Nitridlegierungen mit Übergangsmetallen für ferroelektrische und ferromagnetische Funktionalität sowie Untersuchungen zur Ladungsträgerrekombination, unterstützt durch das neue Kathodolumineszenz-Anwendungslabor ZALKAL.

Reports

MEMBERS

Senior Scientists: Y. Cho, J. Lähnemann, O. Brandt, J.M.J Lopes, M. Wagner, L. Geelhaar
Postdocs: H. Yazdani, K. Loeto, D. Dinh, A. Gilbert, M. Yuan
PhD Students: X. Du, A. Campbell, D. Spallek, P. Vierck, N. Bernhardt, H. Zhang, A. Notarangelo, M. Blonski
MSc Students: N. Hajizadeh

FACTS & FIGURES

Publications: 7
Third-party Funding: ENGRAVE: Leibniz, ZALKAL: EFRE, ATLAS: EFRE, 2D-Charm: DFG-ANR, Integrated acousto-NEMS on monolithic new-nitride thin films: DFG-Nitrides4Future, Transition-metal nitride based heterostructures for integrated thermoelectrics: DFGitrides4Future

Novel Functional Oxide Materials
Neuartige funktionale Oxidmaterialien

Oxides span an exceptional range of properties—from insulators to superconductors to magnets—making them promising for next-generation electronics. This CReA uses molecular beam epitaxy, which offers higher material quality than conventional oxide growth methods, to synthesize novel oxide systems. Focus areas include high-quality epitaxial synthesis, in-house structural and electronic characterization, prototype device demonstration, and integration with existing semiconductor platforms—supporting applications in memory, logic, sensing, and quantum information processing.

Oxide decken ein außergewöhnlich breites Eigenschaftsspektrum ab – von Isolatoren über Supraleiter bis zu Magneten – und sind damit vielversprechend für die Elektronik der nächsten Generation. Dieses CReA nutzt Molekularstrahlepitaxie, die im Vergleich zu konventionellen Methoden eine höhere Materialqualität ermöglicht, zur Synthese neuartiger Oxidsysteme. Schwerpunkte sind hochwertige epitaktische Synthese, umfassende hausinterne strukturelle und elektronische Charakterisierung, prototypische Bauelementdemonstration sowie die Integration mit bestehenden Halbleiterplattformen – mit Anwendungen in Speicher-, Logik- und Sensortechnologien sowie der Quanteninformationsverarbeitung.

Reports

MEMBERS

Senior Scientists: O. Bierwagen, R. Engel-Herbert, M. R. Wagner, M. Hanke, J. Lähnemann, E. Luna, N. Nayir, A. Tahraoui
Postdocs: G. Hoffmann, H. Tornatzky, K. Loeto
PhD Students: A. Ardenghi, W. Chen, N. Gutmann, S.-H. Liu, S. Sirt, C. Sanga
L. Choi

FACTS & FIGURES

Publications: 14
Third-party Funding: DFG, Leibniz Association, EU
2025 Collaborators: IKZ, FBH, HU, TU, FHI, U Leipzig, FAU, RWTH Aachen U, DESY, ICMAB, ITU, CNRS, PSI, U Oxford, U Parma, U Oslo, Penn State, Seoul U, MAGLAB, Elettra Sincrotrone Trieste

Brief Reports

Stress-induced reconstruction in two-dimensional silver intercalated between graphene and SiC

V. D. PHAM*, B. ZHENG[1], A. JAIN[1], Z. HENSHAW[2], W. BLADES[2], J. A. ROBINSON[1], V. H. CRESPI[1], A. TRAMPERT, R. ENGEL-HERBERT

[1] 2D Crystal Consortium, Materials Research Institute, Penn State University, USA
[2] Department of Physics & Engineering Physics, Juniata College, Huntingdon, USA

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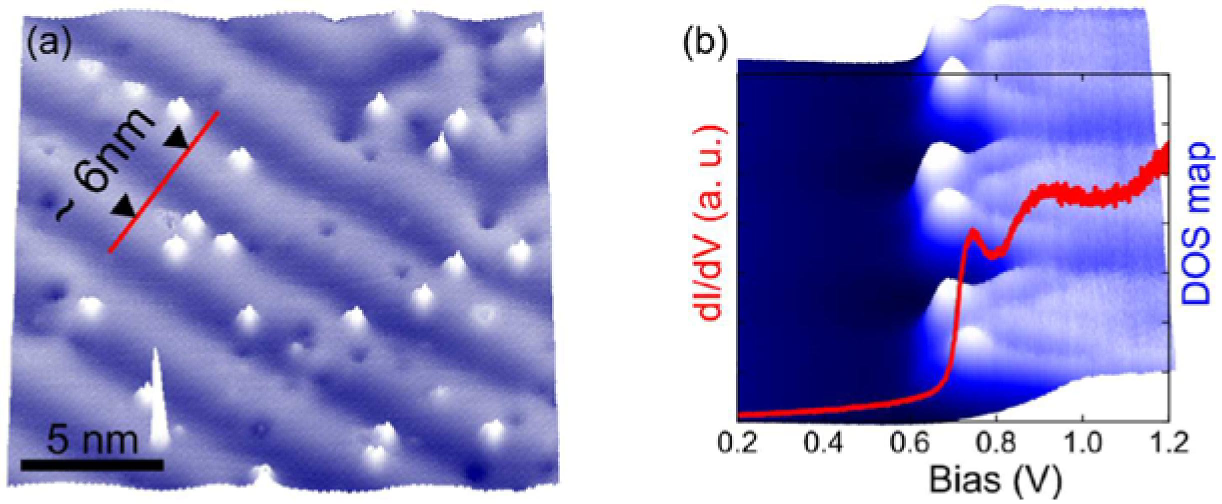
Two-dimensional (2D) metals intercalated at the interface between graphene and SiC emerge as an intriguing platform for quantum technologies [1–3] with new quantum phenomena. However, the interplay between metal layer and SiC which support the stability of 2D metal has not deeply been explored. Here we identify that stress within a monolayer silver induces a long-range reconstruction identified by scanning tunneling microscopy (STM) in combination with DFT. This reconstruction is formed as a result of registry competition between the silver-SiC and silver-to-silver interatomic force in a closed-packed (111) monolayer. Considering a 1:1 matching between silver and SiC, we found that a 21×√3 one-dimensional silver supercell must be reconstructed in order to fit 20 lattice sites of SiC and relax. This registry reduces the in-plane tensile stress, giving rise to periodic potential charge modulation, reminiscent of herringbone reconstruction in Au(111), and a localized state at the edge of the silver monolayer conduction band. Our finding unveils exciting structures and electronic properties of intercalated metals imposed by the SiC substrate and graphene, which sheds new light on fundamental and application investigations.



(a) Monolayer silver intercalated between graphene and SiC exhibiting reconstruction stripes. (b) dI/dV spectroscopy (red) and the dI/dV map revealing a localized state.

[1] S. Forti, S. Link, A. Stöhr, Y. Niu, A. A. Zakharov, C. Coletti, and U. Starke, Nat. Commun. 11, 2236 (2020).
[2] N. Briggs et al., Nat. Mater. 19, 637 (2020).
[3] C. Schmitt et al., Nat. Commun. 15, 1486 (2024).

Absence of exciton localization by isolated twin boundaries in GaAs nanowires

M. GÓMEZ RUIZ[1],* O. BRANDT[1], J. HERRANZ[1,2], R. B. LEWIS[1,3], L. GEELHAAR[1], V. KAGANER[1], J. LÄHNEMANN[1]

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[2] Present Address: Microsoft Quantum Materials Lab, Lyngby, Denmark
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GaAs and its ternary alloys have long served as materials of choice for a wide range of optoelectronic applications, with their fundamental properties exhaustively investigated. Over the past decades, polytypism has been observed as an almost universal feature in GaAs nanowires (NWs)—as stacking faults in the wurtzite phase or twin boundaries in the zincblende phase. Prior investigations of GaAs NWs—proposed for monolithic integration on silicon photonic platforms—demonstrate that bundles of twin boundaries (TBs) notably influence their optoelectronic properties [1]. In this work, we combine electron backscatter diffraction (EBSD) and cathodoluminescence spectroscopy (CL) for investigating highly phase-pure GaAs NWs with a passivating $Al_{0.3}Ga_{0.7}As$ shell. In Ref. [2], the lack of signatures of polytypism in these NWs has been reported by photoluminescence spectroscopy.

EBSD reveals the presence of isolated TBs in these GaAs NWs with typical densities below 1 μm^{-1}. To elucidate the role of these isolated twin boundaries in exciton recombination, we recorded CL linescans on the same single NWs previously characterized by EBSD. In these linescans, we do not observe any bound exciton states at the locations of twin boundaries. Therefore, we discuss the possibility of twin boundaries to localize holes and the related capture efficiency, as well as the role of the excitation conditions.

To investigate carrier transport is in these phase-pure NWs, intensity profiles of the freee exciton emission extracted from the CL linescans are analyzed using a diffusion model, which yields a record diffusion length for GaAs NWs of 1.32 µm at 10 K.

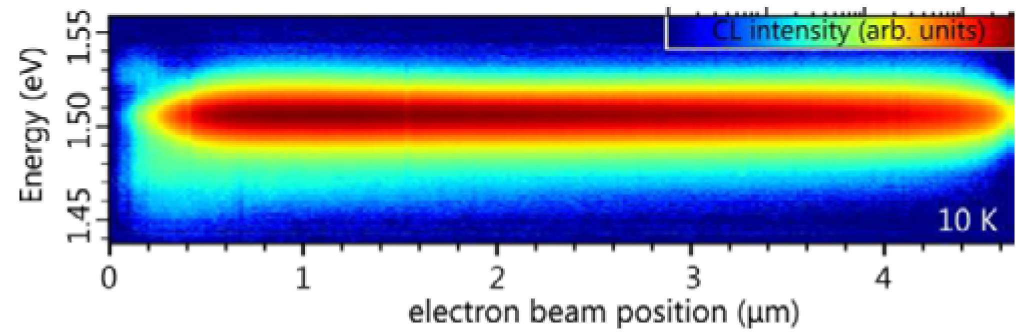

Figure 1: Hyperspectral CL linescan measured along the NW axis showing the absence of any additional emission peaks along the length of the NW, which contains a twin boundary at approximately 2 µm.

[1] Heiss et al., Phys. Rev. B 83, 45303 (2011); Spirkoska et al., Phys. Rev. B 80, 245325 (2009); Lin et al., Nanotechnology 28, 415703 (2017); Jahn et al., Phys. Rev. B 85, 045323 (2012).
[2] Oliva et al., ACS Appl. Nano Mater. 6, 15278 (2023)

Piezo-electrically driven GHz Helical Acoustic Waves

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[1] Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany
[2] University of Pisa, Dipartimento di Fisica E. Fermi, Italy
[3] Department of Physics and Astronomy, Bowdoin College, USA

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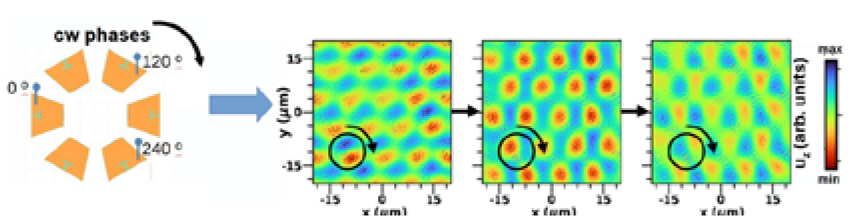
The dynamic control of circular polarization in light has enabled groundbreaking advancements in both fundamental research and applied technologies including optical wireless communication, microscopy and sensing of biological samples, as well as the transfer of optical chirality to mechanical systems. Such a control can be realized at GHz frequencies exploiting the interaction of light with helical surface acoustic waves (SAWs) and bulk acoustic waves (BAWs) in solid-state systems. Mechanical vibrations provide a versatile platform for coupling to electrons via piezoelectric and deformation potential mechanisms, as well as for controlling photons and magnetic excitations through the photoelastic effect or direct geometric deformation of materials.

In this work, we aim at the opto-mechanical control of light, achieving the simultaneous modulation of both the light amplitude and orbital angular momentum (OAM). Our strategy is based on the transfer of the angular momentum of a piezoelectrically driven helical mechanical wave to the optical field. A key challenge lies in the precise generation and detection of helical acoustic waves, which requires fully tunable manipulation of the mechanical field [1]. We have investigated two types of structures for generating helical acoustic waves. The first is a ring-shaped bulk acoustic wave resonator (BAWR) for the GHz frequency range consisting of three independent sectors [2]. By applying RF signals with phases differing by 0° or 120°, we generate transversal waves with circular or spiral-like wavefronts, respectively.



3 SAW cavities formed by 6 planar IDTs are excited piezo-electrically with clockwise phase delays of 0o, 120o, and 240o for f_{RF} = 610.5 MHz. The resulting interference is an array of surface acoustic vortices and is recorded using interferometric techniques.

The second structure comprises six planar interdigital transducers (IDTs) for surface acoustic waves arranged in a circular configuration, forming three SAW delay rotated by 120° relative to each other. By applying phase-delayed excitations to corresponding IDT pairs, we generate surface acoustic vortices with tunable rotational directions, which are mapped using interferometric and AFM techniques at frequencies in the hundreds of MHz. In particular, the interferometric measurements directly prove the transfer of the mechanical angular momentum to the optical field. Finite Element Method (FEM) simulations are used to validate and interpret the experimental results. Current experiments are performed on sapphire substrates due to their low acoustic transmission losses. Future work will focus on fabricating devices on GaAs-based microcavities to explore light OAM control in integrated opto-mechanical systems.

[1] A. Pitanti et al., https://doi.org/10.48550/arXiv.2410.17877
[2] N. Ashurbekov et al., https://doi.org/10.48550/arXiv.2502.20899

New platform for high-purity single photons at GHz rates

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[2] National Institute of Standards and Technology, Boulder, Colorado 80305, USA

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Single-photon sources (SPSs) are a key component in quantum communication. Solid state epitaxial III-V quantum dots (QDs) are near-perfect SPSs in terms of reaching 99.999% SP emission [1]. The efficiency of SPS-based applications depends strongly on the SP emission rates (γ_{SP}). In the technologically-relevant monolithic QD SPSs, the maximum γ_{SP} values are limited to the MHz-range. A typically employed strategy to enhance γ_{SP} is via the Purcell-effect by embedding QDs in optical microcavities (MC), which requires static field or temperature tuning of the energy matching between MC optical mode and QD energies. Here, we propose a new platform for ultra-bright SPSs using InAs QDs [2] embedded into the spacer of a patterned hybrid photon-phonon AlGaAs MC [3], see Fig. 1(a), where the strain of the piezoelectrically generated GHz-frequency bulk acoustic wave modulates the energy of the QD and, hence, the SP emission rate via the dynamical Purcell effect. Our preliminary data shows that the energy of a QD can be modulated at frequency up to 14 GHz, Fig. 1(b). The platform is promising for SP generation with rates γ_{SP} > 20 GHz.

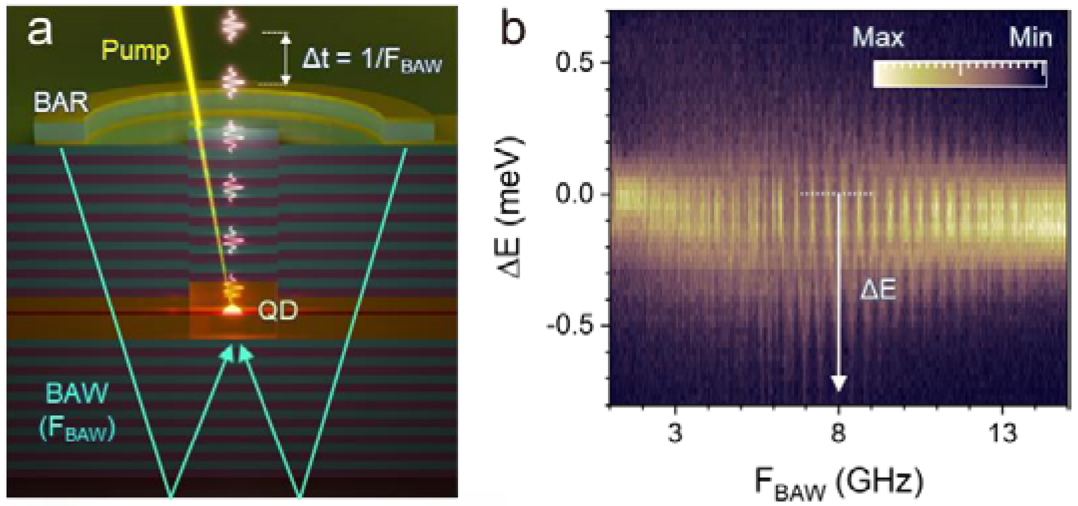

Fig. 1: (a) A sketch of the device for the regulated single photon emission based on the patterned high-Q (Al,Ga)As microcavity with a InAs QD embedded in its spacer. The single photon emission rate of the optically pumped QD is regulated via dynamical Purcell-effect induced by the GHz-frequency (F_{BAW}) bulk acoustic wave (BAW) generated piezoelectrically by a bulk acoustic resonator (BAR). (b) Spectrum of a QD as the function of F_{BAW} recorded at 5 K. Strong modulation of the QD energy (ΔE, referenced to 1286.7 meV) is observed at well-defined acoustic resonances of the microcavity up to 14 GHz.

[1] P. Senellart, G. Solomon & A. White: Nature Nanotechnology 12, 1026 (2017).
[2] Z. Wang, ... and K. Silverman: Optica 32(22), 38384 (2024).
[3] A. Kuznetsov et al.: Nature Communications 14, 5470 (2023).

Imaging surface acoustic waves in transferred and epitaxial 2D materials using atomic-force microscopy

M. YUAN[1],* A. HERNÁNDEZ-MÍNGUEZ[1], J. M. J. LOPES[1], I. AHARANOVICH[2], Y-T LIOU[1], N. ASHURBEKOV[1], P. V. SANTOS[1]

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[2] School of Mathematical and Physical Sciences, University of Technology Sydney, Ultimo, Australia

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The visualization of sound has fascinated researchers and the public alike, dating back to Chladni's study in the 19th century. Recently, coupling surface acoustic waves (SAWs) to 2D-material based nanostructures has been gaining momentum, aiming at e.g. the acoustic manipulation of their electronic and optoelectronic properties with the dynamic strain provided by the SAWs. While optical properties in 2D materials can be conveniently probed by photoluminescence spectroscopy, mapping of mechanical properties remains challenging. This task can, however, be accomplished by high-frequency (GHz) SAWs, which are particularly suitable for probing very thin layers thanks to their micron-size wavelengths and the confinement in the vicinity of the surface.

Here, we present the imaging of GHz SAWs coupled to two different types of 2D material nanostructures using atomic-force microscopy (AFM). The first is a multilayer hexagonal Boron Nitride (hBN) flake, irradiated with Ar ions for spin center creation, stamped on piezoelectric LiNbO3. The second is an embedded monolayer graphene epitaxially grown on SiC and covered with piezoelectric ZnO thin film. Standing SAWs are excited in the piezoelectric materials using resonators formed by interdigital transducers. In the former, we observe spatial inhomogeneities, revealing that the strain transferred to stamped 2D materials can exhibit large spatial fluctuations, depending on the adhesion quality. In the latter, in contrast, we observe a near perfect strain transfer. Rich acoustic patterns arise in the graphene structure that forms a phononic cavity. Furthermore, the enhanced acoustic intensity in the graphene region indicates a waveguiding effect, with graphene serving as an atomically thin, embedded shorting layer. Effects such as strain transfer and phonon scattering are quantitatively analyzed by performing fast Fourier transform. The high spatial resolution of AFM enables us to investigate the SAW strain transferred onto 2D materials with high precision. Our result demonstrates an effective way to determine the dynamic strain fields in hybrid SAW-2D material systems, which can illuminate the path towards acoustic control of the optoelectronic properties.

Multivariate optimization of THz QCL cavity parameters via a unified design approach

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The performance of terahertz (THz) quantum cascade lasers (QCLs) is highly dependent on the resonator geometry, which influences key metrics such as output power, operating temperature, and efficiency. Here we present a model that systematically optimizes Fabry–Pérot resonator dimensions by accounting for the interplay between optical and thermal effects under real-world constraints like limited cooling and electrical power. Using temperature-dependent measurements [Fig. 1(a)] [1] and electromagnetic simulations, the model identifies geometries that maximize output power or practical operating temperature, while ensuring compatibility with thermal dissipation limits. As shown in Fig. 1(b), the model captures the impact of geometrical parameters across different operating conditions and duty cycles, offering clear design guidance. This integrated approach enables the development of high-performance QCLs tailored to specific applications, eliminating the need for exhaustive experimental testing. It also reconciles previous efforts focused on optimizing individual parameters [2,3] and is adaptable to various waveguide structures and operating modes. By addressing practical limitations, this model supports the advancement of efficient, application-ready THz QCLs for spectroscopy, imaging, sensing, and resource-constrained environments like satellite-based systems.

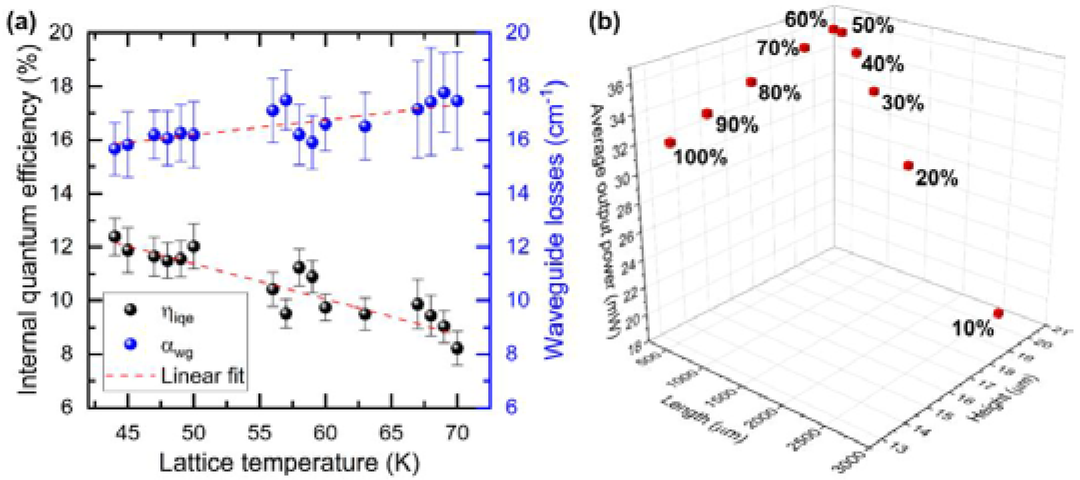

Fig. 1: (a) Internal quantum efficiency η_{iqe} (black) and waveguide losses α_{wg} (blue) vs. lattice temperature for a 3.5 THz QCL. (b) Simulated average output power as a function of optimized cavity length and active region thickness for various duty cycles (labels).

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Toward bandstructure engineering of THz QCLs using GHz acoustic strain

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Active frequency comb generation and waveform control are central challenges in the terahertz (THz) domain. In THz quantum cascade lasers (QCLs), these functions have typically been achieved through active bias modulation, which alters the operating point of the device and imposes strong limitations on its flexibility [1]. Here, we propose a novel approach based on the direct modulation of the QCL bandstructure using GHz-frequency bulk acoustic waves (BAWs), promising direct and localized control of the optical gain and chromatic dispersion [Fig. 1(a)]. To implement this concept, we integrate piezoelectric transducers [2] directly onto the QCL top contact. Initial results [Fig. 1(b)] demonstrate acoustic modulation of the GaAs bandgap and active region energies [3]: the central panel displays photoluminescence (PL) spectra under different BAW frequencies, revealing Fabry–Pérot resonances from acoustic echoes (top panel). Spectral shifts between on- and off-resonance conditions (right panel) confirm dynamic modulation of the bandstructure by up to 5 meV. These results mark the first demonstration of dynamic bandstructure modulation in a THz QCL using GHz acoustic strain, introducing a fundamentally new paradigm that establishes a powerful synergy between QCLs and BAWs toward coherent control and frequency comb engineering.

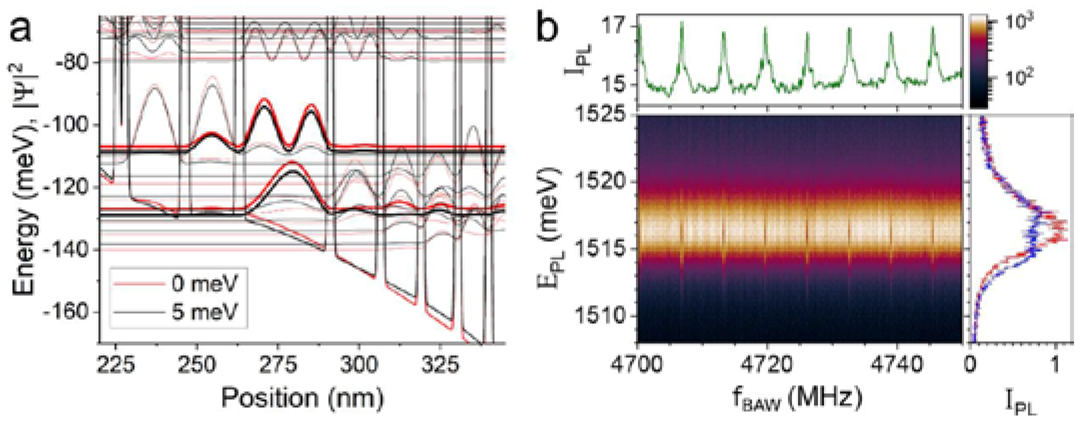

Fig. 1: (a) Simulated QCL bandstructure without (0 meV) and with GHz BAW modulation (5 meV). Laser levels are highlighted. (b) Central panel: PL spectra of the QCL active region under varying BAW frequencies at 10 K, showing Fabry–Pérot resonances (top panel). Right panel: comparison of PL spectra on (blue) and off (red) BAW resonance.

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Solid Phase Epitaxy of r-GeO_2 on r-TiO_2 Substrate

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Rutile GeO_2 (r-GeO_2) is a promising ultra-wide bandgap semiconductor (UWBG) with superior thermal conductivity, high carrier mobility, and potential ambipolar doping—making it attractive for next-generation power electronics. However, epitaxial growth of r-GeO_2 remains challenging due to (1) the presence of competing polymorphs (amorphous and quartz-type), (2) volatility of GeO species in vacuum, and (3) the lack of a commercial available lattice-matched substrate.

To address these challenges, we demonstrate solid-phase epitaxy (SPE) of r-GeO_2 thin films on r-TiO_2 substrates using molecular beam epitaxy (MBE). A 5 nm amorphous GeO_2 layer was first deposited, followed by *in-situ* annealing in a plasma-activated oxygen atmosphere at varying temperatures. The aim is to establish a r-GeO_2 template suitable for quasi-homoepitaxial growth.

We find that the annealing temperature critically infl uences the resulting fi lm morphology. At 900°C, discrete crystalline islands of r-$(Ge_xTi_{1-x})O_2$ are formed, suggesting a potential Stranski–Krastanov growth mode driven by strain accumulation and accompanied by some Ti diffusion. In contrast, the GeO_2 layer remains amorphous at 800°C and fully desorbs at 1000°C. Annealing at 850°C yields a continuous and uniform layer. Characterization by XPS, AFM, and RHEED indicates the formation of a homogeneous crystalline surface at this temperature, although further analysis is needed to conclusively determine the crystallinity throughout the entire film.

Transmission electron microscopy (TEM) analysis is ongoing to examine the substrate alignment and layer composition to gain deeper insight into the mechanisms governing epitaxial crystallization. These results point toward a promising pathway for engineering r-GeO_2 templates to enable controlled growth of the epitaxial thin film, advancing its potential as an UWBG oxide semiconductor.

FAIR data management approach for MBE growth using NOMAD

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Data-driven material science has the potential to transform the way we design and develop materials. This emerging field represents a significant departure from traditional trial-and-error methods and empirical approaches that have characterized materials science for decades. Finding predictive empirical relations that allow for precise control over various aspects of the growth process has posed a challenge to human cognitive abilities alone. This becomes even more complex when combining datasets from different labs or from different scientists due to the lack of established standards for data models, including elaborate workflows and a large diversity of instruments. Here, a radical shift is required in how information is handled and research is performed. In contrast to traditional experimental descriptions and data provided in publications, laboratory notebooks, and on file servers, growth and characterization data must be complemented with its rich metadata context, also covering ontologies and workflows according to the FAIR (findable, accessible, interoperable, reusable) principles [1]. Opening new perspectives towards finding correlations between materials' growth process and is intimately connected to the challenge of integrating growth and characterization information into a FAIR data infrastructure [2].

We present the initial implementation of this use case in NOMAD (nomad-lab.eu) [3] and discuss the functionalities developed to digitize the entire data lifecycle in MBE growth, with in-situ- and ex-situ characterization. A NOMAD based Electronic Laboratory Notebook (ELN) is structured according to the following guiding principles: It contains fill-in schemas for every entity (e.g. users, equipment, samples) and activity (e.g. sample processing, growth, characterization), it uses automatic timestamping of all data, and it automates the data collection and processing to minimize errors by users. The resulting structured FAIR data opens up the potential to create tools that facilitate and automate data management, and the sustainable application of AI-based analytics, dedicated to optimization in MBE growth.

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Formation of two-dimensional electron gases at $SrTiO_3$ interfaces via redox reactions

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Strontium titanate ($SrTiO_3$) has been the workhorse for emergent phenomena in perovskite oxides for decades, hosting many fundamental physics phenomena ranging from quantum paraelectric over superconductivity to magnetic order phenomena, thus playing a central role in this research field and bringing widespread attention to this class of complex oxides. Despite its long history, $SrTiO_3$ remains a key subject of current research, particularly in the study of two-dimensional electron gases (2DEGs) exhibiting sizeable electron correlation effects.
These 2DEGs can be created via two main routes: (1) through polar discontinuity when interfacing non-polar $SrTiO_3$ with polar perovskites such as $LaAlO_3$, and (2) via redox reaction by oxidizing reactive metals like aluminum deposited on $SrTiO_3$ surfaces [1,2] via oxygen scavenging, and oxygen vacancy formation in the proximity of the interfaces, making them highly conductive.

In this work, amorphous aluminum layers of varying thicknesses between 0.5 and 2.5 nm were deposited on TiO_2-terminated $SrTiO_3$ (001) substrates using molecular beam epitaxy (MBE). The presence of interfacial redox reaction and a spatially confined conducting channel near the interface were identified using X-ray photoelectron spectroscopy (XPS) and capacitance-voltage (CV) measurements, respectively. Further, mobility values of 4 cm^2/Vs at room temperature and 196 cm^2/Vs at 4 K were determined using van der Pauw measurements. Using the complimentary approach of XPS, transport and CV measurements optimal conditions were identified, where redox-oxidation of Al has enabled the formation of a spatially confined conducting layer, while the subsequent alumina oxygen diffusion cap was thick enough to stabilize and preserve the 2DEG long term in air.

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Electrical properties of semiconducting CrN layers grown by molecular beam epitaxy

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CrN is an emerging group-IIIB transition-metal nitride semiconductor, notable for its unique combination of mechanical, electronic, thermoelectric, and magnetic properties. The electronic structure of CrN, particularly its bandgap, is the subject of ongoing debate, with reported values ranging from 0.02 to 0.09 eV [1,2]. These values are usually derived from the thermally activated electrical conductivity. However, temperature-dependent Hall-effect measurements, which can shed light on the underlying transport mechanisms, have not yet been performed, thus impeding a comprehensive understanding of the electronic properties of CrN.

Here we investigate the electrical properties of 75-nm-thick nominally undoped CrN(111 and CrN(113) layers grown simultaneously on AlN(0001) and AlN(11$\bar{2}$2) templates using plasma-assisted molecular beam epitaxy, respectively. Temperature-dependent Hall-effect measurements, performed using the van der Pauw configuration, from 4 to 400 K show that both layers exhibit n-type semiconducting behavior. Additionally, these measurements clearly reveal a Néel temperature of about 280 K, reflecting the antiferromagnetic nature of the CrN layers.

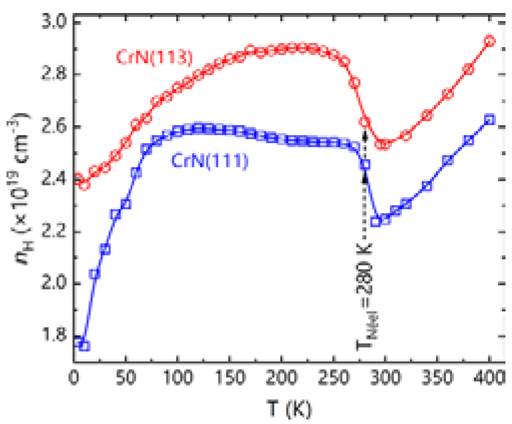

Figure 1: Temperature-dependent effective carrier concentrations of the layers.

Leveraging knowledge from another transition-metal nitride, ScN [3], we thoroughly analyze the electrical properties of the layers. We found that the layers exhibit a two-band conduction mechanism, characterized by a metallic-like impurity band conduction at low temperatures, and thermally activated conduction at high temperatures. Whether the latter is due to the activation of electrons from the impurity band or across the actual band gap of the material requires measurements at even higher temperatures.

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Growth of highly relaxed (In,Ga)N pseudo-substrates without ex-situ patterning

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(In,Ga)N alloys can be employed as active region for light-emitting diodes (LEDs) with wavelengths across the entire visible spectrum. Notably, blue (In,Ga)N LEDs (≈15% In) achieve external quantum efficiencies (EQEs) exceeding 90%. However, the EQE of red (In,Ga)N LEDs (≈40% In) is much lower, primarily due to the effects of the large lattice mismatch with the GaN template that is typically used as substrate. The established material for red LEDs is (Al,Ga,In)P. Nevertheless, for red micro-LEDs in display applications, (In,Ga)N shows promise thanks to the lower susceptibility to etching damage and slower non-radiative surface recombination compared to phosphides. In order to mitigate the effects of the lattice mismatch between high-In-content (In,Ga)N and GaN, various approaches have been proposed. Here, we introduce a novel fabrication scheme for highly relaxed (In,Ga)N layers that offer attractive properties for the use as pseudo-substrates for red (In,Ga)N LEDs.

The growth of (In,Ga)N layers was performed by plasma-assisted molecular beam epitaxy on GaN templates. The basic idea of our approach is to tune the III/V flux ratio from N-rich to metal-rich conditions to impede or enhance lateral growth, respectively. The first N-rich step gives rise to three-dimensional growth promoting strain relaxation and the filtering of dislocations, while the subsequent metal-rich conditions establish a smooth layer via lateral growth and eventually complete coalescence. Importantly, this strategy does not require any ex-situ patterning.

Two variants of the growth protocol, which differed in the Ga/In flux ratio under N-rich conditions, produced different three-dimensional structures. Yet, both resulted in a similar final layer after coalescence, with a root-mean-square roughness of about 2 nm (as determined by atomic force microscopy), a high degree of strain relaxation (≈80%) and an In content controllable in the range of 15-35% (as determined by X-ray diffractometry). Photoluminescence spectra re- vealed a significant red shift and narrower linewidths for pseudo-substrates compared to a reference sample which was grown directly on GaN. Also, the reference sample exhibited only ≈50% strain relaxation. Furthermore, panchromatic cathodoluminescence mapping showed a larger fraction of non-radiative surface area compared to the pseudo-substrates.

Our straightforward, cost-efficient approach is compatible with large-scale production and may pave the way towards highly efficient red (In,Ga)N micro-LEDs.

High-resolution luminescence spectroscopy of excitonic transitions in homoepitaxial AlN layers

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Over the past decade, AlN has emerged as a promising material for high power electronics and deep-ultraviolet emitters owing to its ultrawide bandgap and the recent availability of bulk substrates. The emergence of high-quality material has facilitated detailed spectroscopic studies of the near band-edge emission [1,2]. Previous studies have focused on categorizing excitonic emission lines by their selection rules in angle-dependent measurements, but these experiments alone cannot distinguish between intrinsic (free exciton) and extrinsic (bound exciton) transitions.

In this contribution, continuous-beam and time-resolved (TR) cathodoluminescence (CL) and photoluminescence (PL) spectroscopy are utilized to identify criteria for the unambigious attribution of the near band-edge emission lines to either free or bound exciton states. Two high-quality, homoepitaxial AlN layers are investigated, where one was grown by molecular beam epitaxy and the other by metal-organic vapor-phase epitaxy. Both show a variety of excitonic lines near the band edge, whose origin (free or bound exciton) is as yet unknown.

We utilize temperature-dependent PL and CL measurements with high spectral resolution (0.28 and 1 meV, respectively) to determine the characteristic thermal broadening and quenching of the excitonic lines. In addition, TRCL and TRPL at low temperatures allow the determination of the rise and decay times of each line. Bound excitons can be identified by their narrower linewidth ($< k_BT$), stronger quenching, and longer rise and decay times as compared to free excitons. Lineshape fits allow us to extract accurate values for all these quantities. We will discuss the nature and assignment of the excitonic emission lines based on the above criteria. In particular, we will present data identifying a controversially discussed line as bound exciton. Moreover, we have discovered a peculiar bound exciton state with exceptionally long lifetime (≈ 2 ns), but very low activation energy of ≈ 4 meV.

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Tailoring Structure and Magnetism in Large-Area Epitaxial Fe_3GeTe_2 via Ni-Doping

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The two dimensional (2D) magnetic crystal Fe3GeTe2 (FGT) exhibits various promising features such as large anomalous Hall effect, current-induced magnetization switching, and magnetic skyrmions, which are highly beneficial in spintronic devices for memory application [1-2]. However, most of the experimental studies on 2D magnetic materials are limited to micrometer-sized flakes exfoliated from bulk single crystals, which are not scalable, not uniform, and difficult to integrate into conventional device fabrication schemes [3]. Thus, it is essential to develop large-scale epitaxial growth of these 2D magnets, including the realization of controlled doping with elements such as Ni, which is known to be an effective approach for tailoring magnetism [4]. In this work, we demonstrate the large-area epitaxial growth of Ni- doped FGT films via molecular beam epitaxy. X-ray diffraction and Scanning Transmission Electron Microscopy measurements suggest the formation of high-quality epitaxial films of pure and Ni-doped FGT phases on graphene/SiC(0001) substrates. Superconducting Quantum Interference Device, Hall, and X-ray magnetic circular dichroism measurements unveils the ferromagnetic nature of the films, with strong perpendicular magnetic anisotropy for both pure FGT and Ni-doped films. We found that both Fe and Ni intercalate into the van der Waals gaps, shrinking both the in-plane and out-of-plane lattice parameters. This leads to a dilution of FGT's ferromagnetic properties including the suppression of perpendicular magnetic anisotropy and reduction the Curie temperature (TC) to below 50 K. Our results demonstrate the significant role of Ni incorporation in modulating the ferromagnetic behavior of FGT films, which is crucial for designing future spintronic devices.

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Formation of [111]-Ge Domains in layered α-$FeGe_2$ synthesized by MBE and solid phase epitaxy

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Layered magnets can be seen as ideal platforms for exploring magnetism in the 2D limit Previously, we have successfully synthesized at wafer-scale a metastable polytype of $FeGe_2$ using a combination of MBE and solid-phase epitaxy (SPE)[1]. The layered structure of this α-$FeGe_2$ (not observed as a bulk) as well as an antiferromagnetic to ferromagnetic phase transition observed by vertical spin-valve measurements and predicted by DFT [2], make it a promising candidate for the study of 2D-magnetism and spintronics applications, which recently have attracted a great interest. In previous work [3,4] we were also able to synthesize single-crystalline, layered α-$FeGe_2$ films with very high structural and interface perfection on GaAs(001). In this work we investigate the limits of the SPE as we find residual layers of Fe_3Si and parasitic formation of [111]-Ge domains in thicker layers of α-$FeGe_2$. Through comprehensive structural characterization by XRD, XRR, AFM and TEM/STEM of layers with thicknesses between 4 nm and 18 nm, we show residual layers of Fe_3Si on the GaAs interface, independent from the layer thickness.

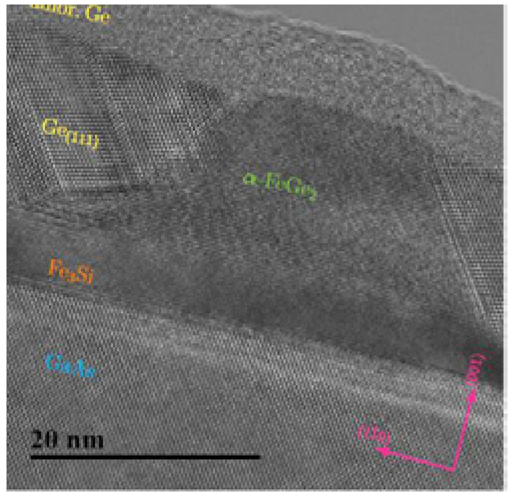

Figure 1: TEM micrograph of α-$FeGe_2$-layer taken along the [110] zone axis, showing a layer with 15 nm nominal thickness. The α-$FeGe_2$ is broken up by [111]-Ge domains.

Additionally we find agglomerates on the surface, that we can link to the Germanium content in the layer. In the TEM micrographs we see layers with very few crystalline defects and homogeneity over long distances. The layers are occasionally interrupted by small Germanium domains, in which the [111] crystal direction is aligned with the [001] growth direction. These grow in a competing manor to the α-$FeGe_2$ in the SPE and are a known problem of the solid phase epitaxy process [5].

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PDI Annual Report 2025

Probing excited state kinetics in organic photovoltaic cells

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Organic photovoltaic cells (OPVs) have a different modus operandi to conventional inorganic photovoltaics. The high exciton binding energy of these materials coupled with the significantly lower mobilities underscores the importance of the processes relating to generation, decay and dissociation of intramolecular localised excitons, the subsequent formation and fate of interfacial charge-transfer states, as well as the interplay of these processes with the encounter and recombination of spatially separated electrons and holes in determining overall device efficiency [1]. All of these processes occur on different timescales, ranging from femtoseconds to microseconds. Therefore, building a detailed physical understanding requires a multifaceted experimental investigation using complementary techniques that span these diverse timescales. Our work demonstrates the utilization of a suite of optoelectronic methods to build a detailed kinetic picture of free carrier generation, recombination and transport in non-fullerene-acceptor-based organic solar cells, providing a foundation for further device optimization [2, 3].

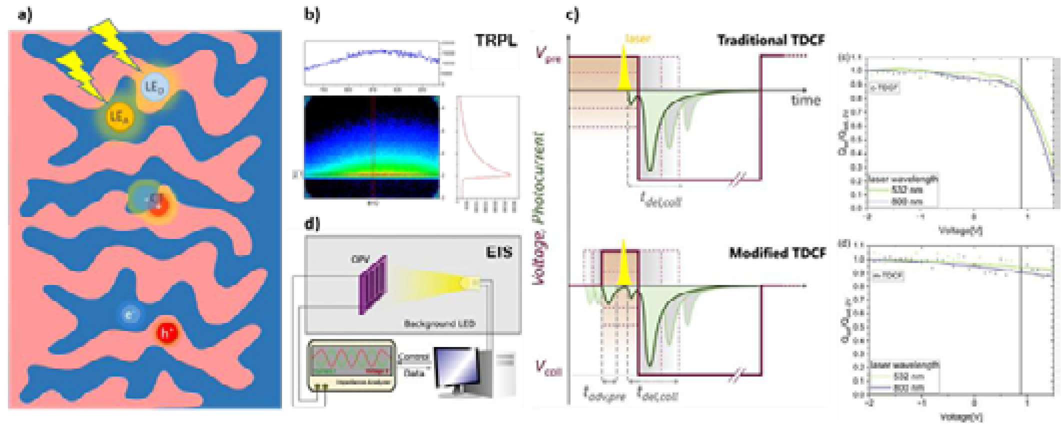

Figure 1. Photogeneration in an OPV (a) and investigation techniques: b) time-resolved photoluminescence (TRPL) to study decay of localized excitons (LE); c) time-delayed collection field (TDCF) to study generation of free carriers; d) electrochemical impedance spectroscopy (EIS) to study free carrier recombination.

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Research on 2D Material Synthesis, Theory, and Properties at the PDI: Current Status and Future Prospects

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Two-dimensional (2D) materials, such as graphene, hexagonal boron nitride and transition metal dichalcogenides, have attracted significant attention due to their unique properties, which typically differ from those of their bulk counterparts [1]. This has opened up new possibilities for scientific exploration and the development of novel, ultra-compact devices for a wide range of applications. Although significant progress has been made in this field since graphene was first isolated around 20 years ago, there are still many challenges associated with the synthesis of 2D materials and the development of an in-depth understanding of their properties. This is particularly true considering that the library of 2D crystals is constantly growing, with many novel single phases and van der Waals heterostructures that display distinct properties and functionalities remaining to be investigated.

PDI has been actively advancing research in the field of 2D materials, cultivating interdisciplinary expertise across multiple fronts, including synthesis and advanced characterization, exploration of fundamental properties, and theoretical modeling [2–7]. In this contribution, we will provide an overview of these core competencies, highlight recent achievements involving various types of 2D materials and their heterostructures, and discuss future prospects. More importantly, we will present our concept for establishing a new core research area dedicated to 2D materials. This initiative aims to enhance synergy among existing activities within the institute and drive more impactful research outcomes in the field. It will also allow us to define and pursue strategic research directions, particularly regarding epitaxially grown 2D systems — an area where PDI is uniquely positioned to contribute. This is essential, not only for advancing fundamental understanding, but also for enabling future technological applications based on this class of materials.

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Facts & Figures

Data as of 31.07.2025 | Finance as of 13.08.2025

PDI Publications
PDI-Publikationen

Computational Thin Films Group

Aghamohammadi, P., F. Karakaya Mert, E. T. Akgul, N. Aghabalapoor Keshtiban, O. C. Altıncı, A. Gelir, C. Sanga, N. Nayir, H. Aydın, and M. Demir
Synthesis, characterization, and theoretical modeling of 2D molybdenum boride (MBene) for all solid-state flexible interdigitated supercapacitor application
ACS Omega 10, 8202 (2025).
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Students
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Mikel Gómez Ruiz
Humboldt University Berlin
Cathodoluminescence spectroscopy and correlated chemical and structural analysis of core/shell III-V nanowires

Wenshan Chen
Technische Universität Berlin
(Ge,Sn)O_2-based Ultra-wide Bandgap Semiconductor Thin Films for Power Electronics

BACHELOR STUDENTS WORKING ON THEIR THESIS / BACHELORSTUDIERENDE IN DER ABSCHLUSSARBEIT

Jakob Schadow
HTW Berlin
Optimierung von Zink-Oxid-Schichten inklusive Kontaktierungen und s-Parameter-Messungen

MASTER STUDENTS WORKING ON THEIR THESIS / MASTERSTUDIERENDE IN DER ABSCHLUSSARBEIT

Murat Karadag
Technische Universität Berlin
Monte Carlo Simulations for resolution determination in electron tomography

Budget Summary
Haushaltsübersicht

FISCAL YEAR	2024 (ACTUAL AMOUNT) K€	2025 (13.08.2025) K€
Revenues		
Allocations	12,408.5	11,827.9
Earnings	13.0	60.0
Sum	12,421.5	11,887.9
Expenditures		
Staff	7,154.6	7,446.6
Administrative expenses	2,648.8	2,996.4
Equipment investment funds	1,691.3	1,444.9
Sum	11,494.7	11,887.9
External funding through projects		
Granted funds	3,825.3	1,752.0*
Spent funds	2,954.0	877.6

Summary of External Funding
Übersicht der Drittmittelförderung

AGENCY	PERIOD	TITLE	PROJECT LEADER	FST
AvH	01.05.2025 – 30.04.2027	Humboldt Research Fellowship for Postdocs – Dr. Kagiso Loeto	Dr. Jonas Lähnemann	9245
DAAD	01.01.2025 – 31.12.2026	Complementary Electron Microscopy Techniques for Efficient AlGaN Optoelectronics	Dr. Jonas Lähnemann	9244
DFG	01.04.2021 – 30.09.2025	Nanoscale optomechanical interactions in semiconductor microcavities	Dr. Paulo V. Santos	9208
DFG	01.03.2021 – 31.05.2025	Point defects control in Ga2O3 thin films grown via molecular beam epitaxy	Dr. Oliver Bierwagen	9217
DFG	01.09.2021 – 31.01.2025	New strategies for dislocation density reduction in monolithic III/V epitaxy on Si	Dr. Achim Trampert	9218
DFG	01.02.2022 – 31.04.2025	Lead-free piezoelectric nanowire-nanocellulose hybrids for flexible energy harvesters	Dr. Lutz Geelhaar	9219
DFG	01.05.2022 – 31.12.2025	Coherent GHz electro-optomechanics with polarmechanical crystals	Dr. Alexander Kuznetsov	9223
DFG	01.05.2022 – 31.12.2025	Coherent GHz electro-optomechanics with polarmechanical crystals	Dr. Paulo V. Santos	9224
DFG	01.02.2024 – 31.01.2027	Artificial quantum states on semiconductor surfaces created and probed by cryogenic scanning tunneling microscopy	Dr. Stefan Fölsch	9231
DFG	01.03.2024 – 28.02.2027	"Magic Tune" - Enabling large tunnel magnetoresistance at room temperature in scalable epitaxial van der Waals magnet heterostructures	Dr. J. Marcelo J. Lopes	9232
DFG	01.07.2025 – 30.06.2028	"2d CHARM" - MBE growth and advanced characterization of large-scale van der Waals heterostructures	Dr. J. Marcelo J. Lopes	9239
DFG	01.05.2025 – 30.04.2028	"NOBLESSE" - New oxide-based two-dimensional electron and hole gases for spin-orbitronics	Prof. Dr. Roman Engel-Herbert	9240
DFG	Bewilligung vom 23.10.2024	Pushing the FF of Non-Fullerene Acceptors Based Solar Cells Above 80 %: Relating Order to Reduced Recombination to Device Performance II (Fabulous II)	Prof. Dr. Safa Shoaee	9242

AGENCY	PERIOD	TITLE	PROJECT LEADER	FST
DFG	01.05.2025 – 30.04.2028	Heterogeneous Integration of novel ultra-wide band gap oxides on silicon	Prof. Dr. Roman Engel-Herbert	9243
DFG (SPP)	01.03.2023 – 28.02.2026	Priority Programme "INtegrated TERahErtz sySTems Enabling Novel Functionality (INTEREST)" (SPP 2314) Micro-integrated terahertz quantum-cascade laser for high-resolution spectroscopy (Micro- QCL)	Dr. Klaus Biermann	9222
DFG (SPP)	01.04.2025 – 31.03.2028	Integrated terahertz quantum-cascade transceiver for high-resolution spectroscopy and space applications (iQCT)	Dr. Klaus Biermann	9237
DFG (SPP)	Bewilligung vom 29.08.2024	Terahertz Injection Locking of Quantum Cascade Lasers using Modified Uni-Travelling Carrier Photodiodes (UTC4QCL)	Dr. Xiang Lü	9238
DFG (OAK)	01.01.2023 – 31.12.2025	Open-Access-Publikationskosten	Anne Timm	9226
EFRE	01.01.2023 – 31.12.2025	ZALKAL – Application laboratory time-resolved cathodoluminescence spectroscopy	Dr. Jonas Lähnemann	9225
EFRE	01.07.2025 – 30.06.2028	ATLAS – Application Laboratory Thermal Laser Epitaxy	Dr. Lutz Geelhaar	9247
EU	01.09.2023 – 31.08.2027	Understanding, Predicting and Enhancing the Stability of Organic Photovoltaics (OPVStability)	Prof. Dr. Safa Shoaee	9234
EU	01.11.2024 – 31.10.2028	HINA - Hybrid INtegration of Alkaline niobate - tantalate films for advanced photonic and piezoelectric devices	Dr. Alberto Hernandez-Minguez	9241

Seminars of Visitors
Gastseminare

14.07.2025
Yusuke Hayashi, National Institute for Materials Science (NIMS), Tsukuba, Ibaraki, Japan
Nanobeam X-ray diffraction for wide bandgap materials/devices

01.07.2025
Mike Scarpulla, The University of Utah, Salt Lake City, USA
Ga_2O_3 defects and devices

12.06.2025
Manuel Bibes, Laboratoire Albert Fert, CNRS, Thales, Université Paris-Saclay, Palaiseau, France
Redox engineering of quantum oxide materials

04.06.2025
Saroj P. Dash, Chalmers University of Technology, Sweden
Spin Dynamics in 2D Quantum Material Devices

02.06.2025
Saskia Fiedler, Institute for Atomic and Molecular Physics (NWO-I AMOLF), Amsterdam, The Netherlands
Incoherent and coherent cathodoluminescence spectroscopy - a versatile tool to study nanoscale light distribution

29.04.2025
Hannah Nerl, Humboldt-Universität zu Berlin, Germany
Measuring transport properties and hybrid quasiparticles in the electron microscope

07.04.2025
Bárbara Rosa, University of Campinas, Brazil
2D semiconductors: A promising platform for optoelectronic applications and quantum technologies

28.03.2025
Robert Martin, Strathclyde University, Glasgow, Scotland, UK
CL-EBSD: Combining cathodoluminesence and electron backscatter diffraction to learn about frontier semiconductor materials and devices

24.03.2025
Frank Schreiber, Tübingen University, Institute of Applied Physics, Germany
Growth of Functional Molecular Thin Films

27.01.2025
Alexander Tselev, CICECO-Aveiro Institute of Materials, University of Aveiro, Portugal
Scanning Probe Microscopy of Functional Materials

07.01.2025
Jit Sarkar, Fritz Haber Institute of Max-Planck Society, Germany
Coherent Light Control of the Metastable Hidden Phase in TaS2: Controlling phase-transition at ultrashort timescale

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Visiting scientists
Gastwissenschaftler:innen

NAME	INSTITUTE	PERIOD	TOPIC	COUNTRY
Ignacio Carraro Haddad	Centro Atomico Bariloche	02.08.2025-16.08.2024	Phonon-induced coherent dynamics of confined polariton condensates	Argentina
Prof.Dr. Stefano Cecchi	Università degli Studi di Milano-Bicocca	01.04.2025 – 31.03.2026	Conclusion of studies related to Ge-Sb-Te alloys	Italy
Giuditta Cicconi	Universität Parma	21.07.2025 – 19.08.2025	Growth and characterization of r-GeO2 thin films on r-TiO2	Italy
Dr. Kagiso Loeto	Stipendiat der Alexander von Humboldt-Stiftung	01.03.2025 – 30.04.2027	Hochauflösende Kathodolumineszenzkartierung von einzelnen Punktdefekten in AlGaN-LEDs	Germany
Allison McMinn	Arizona State University	13.06.2025 – 14.07.2025	Timeframe on interface analysis of Antimonide-based type II superlattices	USA
Prof. Dr. Madeleine Elizabeth Msall	Bowdoin College, USA	02.06.2025 – 03.08.2025	Optimierung des Designs von Interdigitalwandlern für die Anregung von hochfrequenten Oberflächenwellen(SAWs)	USA
Hai Nguyen	TU Berlin	28.04.2025 – 31.05.2025	Messungen an Strontiumtitanat mit Hilfe der Ramanspektroskopie	Germany
Maria Chiara Paolozzi	Sapienza University of Rome	15.05.2025 – 15.07.2025	Growth of Teluride Thin Films by Molecular Beam Epitaxy	Italy
Suyoung Park	Seoul National University	01.07.2025 – 31.08.2025	Implementation of optoelectronic devices on ultra wide band gap oxide semiconductors heterojunction with Si substrates	South Kore
Alessandro Pitanti	Consiglio Nazionale delle Richerche (CNR)	25.07.2025 – 10.08.2025	Acoustic chirality and polarization in solid- state systems	Italy
Marc Rovirola	Universitat de Barcelona	23.06.2025 – 25.07.2025	Acoustic chirality and polarization in solid- state systems	Spain
Dr. Lutz Schrottke	Senior Scientist im Bereich THz QCL	01.04.2025 – 31.03.2026	Simulation and design of terahertz quantum-cascade lasers	Germany
Dr. Alexander Tselev	CICECO-Aveiro Institute of Materials/ University of Aveiro	27.01.2025 – 31.01.2025	Scanning-probe microscopy/near-field microwave microscopy	Portugal
Jonathan Ernesto Valenzuela	Lehigh University, Pennsylvania	09.06.2025 – 30.06.2025	Spectrally and time-resolved cathodoluminescence measurements of hBN crystals	USA
Pedro Winckler Matrone	Gleb Wataghin Physics Institute (IFGW), University of Campinas (UNICAMP)	06.05.2025 – 31.01.2026	Acoustic modulation of excitonic complexes in transition metal dichalcogenide heterostructures	Brazil
Minwook Yoon	Seoul National University	01.07.2025 – 31.08.2025	Implementation of optoelectronic devices with GeO_2 heterojunction on Si substrates using TiO_2 nanomembrane	South Korea

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Scientific Staff
Wissenschaftliches Personal

Scientific staff: including Ph. D. students (D) and externally funded personnel (P)
Wissenschaftliches Personal: einschließlich Doktorandinnen und Doktoranden (D) sowie drittmittelfinanziertes Personal (P)

Adeli, Narges (D)	Electron tomography of epitaxially strained heterostructures
Ashtari Mahini, Faezeh (D, P)	Stability, understanding, predicting and enhancing stability of organic solar cells
Ashurbekov, Nazim (D, P)	Radio-frequency phonon resonators for coherent electron-phonon coupling
Biermann, Klaus	Molecular beam epitaxy of GaAs-based advanced heterostructures
Bierwagen, Oliver	Molecular beam epitaxy of oxides
Brandt, Oliver	Group-III nitrides and semiconductor nanowires
Campbell, Aidan (D)	Characterization of an ultra-fast time-resolved cathodoluminescence spectroscopy setup and application to semiconductor nanowires
Cao, Yonglin (D, P))	Probing spin in disordered semiconductors
Chen, Wenshan (D, P)	Growth and doping of (Si,Ge,Sn)O2-based materials
Cho, YongJin	Molecular beam epitaxy of nitrides
Dinh, Duc Van (P)	Growth of (Sc,Al)N thin films
Du, Xin (D)	Molecular Beam Epitaxy of AlN-Based Ultrawide-Bandgap Semiconductor Heterostructures
Engel-Herbert, Roman	Director
Flissikowski, Timur	Ultrafast dynamics of semiconductor structures
Fölsch, Stefan	Low-temperature scanning tunneling microscopy and spectroscopy
Geelhaar, Lutz	Molecular beam epitaxy and semiconductor nanowires
Ghayeb Zamharir, Sara (P)	Weiterentwicklung/Optimierung von Schichtaufbau und Prozessierung von THz-QCLs
Gilbert, Audrey Muriel (P)	ENGRAVE - Tailoring h-BN/graphen heterostr. (Defect-engineering in graphene via focused ion beam for tailored van der Waals epitaxy of h-BN)
Gómez Ruiz, Mikel	Cathodoluminescence spectroscopy and correlated chemical and structural analysis of core/shell III-V nanowires
Gordon, Jonathan Edward Ryan (P)	Imaging nano-earthquakes on a chip
Graser, Karl (D, P)	Transmission electron microscopy on dislocation reduction in III-V on Si heterostructures
Gutmann, Nicola (D)	2D hole gas at the interface LaInO3/BaSnO3
Hanke, Michael	Synchrotron x-ray diffraction
Hansemann, Moritz (D)	Synthesis of FeGe2 layers
Henn, Sebastian (P)	"Integrierter Terahertz Quantenkaskaden-Transceiver für hochauflösende Spektroskopie und Weltraumanwendungen (iQCT)" im Rahmen des Schwerpunktprogramms „Integrierte Terahertz- Systeme mit neuartiger Funktionalität (INTEREST) “
Herfort, Jens	Ferromagnet-semiconductor heterostructures Chairman Works Council
Hernández Mínguez, Alberto	Manipulation of optical and electronic properties of low-dimensional structures using surface acoustic waves
Hoffmann, Georg	2D electron gas at the interface LaInO3/BaSnO3
Hucho, Carsten	Technology and transfer
John, Philipp (P)	Epitaxy and materials science of (Al,Sc)N nanowires
Jordão Lopes, João Marcelo	Epitaxy of two-dimensional materials
Kaganer, Vladimir	Theories of molecular-beam-epitaxial growth and x-ray scattering
Kang, Jingxuan (D, P)	Top-down synthesis and optical properties of ordered (In,Ga)N nanowire arrays
Karadag, Murat	Master student - Monte Carlo Simulations
Khan, Kacho Imtiyaz Ali	Molecular beam epitaxy of layered magnetic materials
Kumar, Hitesh (D, P)	Cryogenic scanning tunneling microscopy and atom manipulation on III-V semiconductor surfaces
Kuznetsov, Alexander (P)	Coherent electro-optomechanics at GHz frequencies with confined microcavity exciton-polaritons
Lähnemann, Jonas	Spatially resolved optical spectroscopy and structural as well as compositional analysis of nanostructures
Langentepe-Kong, Jonathan (D)	Triplets, solar cells and beyond
Leite Gomes, João Pedro (D)	Acoustically-driven magnomics
Liu, Shi-Hui (D)	Molecular-beam epitaxy of superconducting oxide heterostructures
Loeto, Kagiso	Time-resolved cathodoluminescence spectroscopy on various semiconductor materials
Lü, Xiang	Terahertz quantum-cascade lasers
Ludwig, Stefan	Quantum transport in nanoelectronic systems
Luna Garcia de la Infanta, Esperanza	Transmission electron microscopy of heterointerfaces
Lv, Hua	Spin-transport phenomena in layered and two-dimensional magnetic materials
Marín Largo, Francisca (D, P)	Growth and luminescence analysis of bent GaAs nanowires
Meißner, Moritz	Student assistant: Quantum efficiencies of micro LEDs
Nayir, Nadire	Junior Research Group Leader Computational Materials Science
Nguyen, Hai	Bachelor student - Bestimmung von relativen Ramantensorelementen
Paulo-Wach, Daniel Ramesh (D, P)	"Time-Resolved Variable-Temperature Cathodoluminescence of Gallium Sulfide Telluride Layered Nanowires"
Pham, Van Dong	Scanning tunneling microscopy on 2D metal intercalation and magnetic layered materials
Pistore, Valentino (P)	Micro- integrated terahertz quantum cascade laser for ultrahigh- resolution spectroscopic
Rose, Jonas (D)	Optical investigation of hybrid ferromagnetic / semiconducting 2D-heterostructures
Saeedi, Meysam (D)	Optomechanical exciton-polariton metamaterials
Sarkar, Jit	Optical pump-probe spectroscopy of epitaxial films and heterostructures
Schadow, Jakob	Bachelor student - Optimierung von Zink-Oxid-Schichten inklusive Kontaktierungen und s-Parameter-Messungen
Shinwari, Tauqir (P)	Epitaxial growth of 2D ferromagnetic materials
Shoaee, Safa	Junior Research Group Leader Heterostructure Semiconductor Physics
Sırt, Serkan (D, P)	Interplay between the quantum Hall and Aharonov-Bohm effects in mesoscopic circuits
Spallek, Domenik (D)	Cathodoluminescence of ultrawide bandgap semiconductors
Sun, Doyoung (D)	Role of energetic disorder for industrial fabrication of organic solar cells
Tahraoui, Abbes	Comprehensive semiconductor technology

Takagaki, Yukihiko	Electric properties of nanometer-scale materials
Tokmoldin, Nurlan	Reducing recombination loss process in relation to organic solar cells
Tornatzky, Hans	Raman spectroscopy of binary and complex oxides
Trampert, Achim	Microstructure and electron microscopy
Ventura Santos, Paulo	Abschlussarbeiten an laufenden Forschungsvorhaben/ Abschluss der laufenden Betreuungsverhältnisse
Vierck, Paula Lotte (D)	Epitaxial growth h-BN films on single crystal metal templates
Wagner, Markus	Semiconductor Spectroscopy
Yazmaciyan, Aren (P)	Understanding, controlling and optimising organic solar cell performance as a function of preparation conditions
Yuan, Mingyun	GHz acoustic control in semiconductor nanostructures
Zhang, Huaide (D)	(In,Ga)N nano-epitaxy for amber LEDs

Non-Scientific Staff
Nichtwissenschaftliches Personal

Anders, Walid	Technology	Rauwerdink, Sander	Technology
Arnhold, Kerstin	Finances/Purchasing	Sawert, Susanne	Technology
Baumann, René	Head of Workshop	Schönherr, Hans-Peter	HR Manager
Behnke, Steffen	Technician	Sieg, Michael	Technician
Bluhm, Anne-Kathrin	Technician	Steffen, Doreen	Workshop
Bruen, Eimear	Communications / EOO	Stemmler, Carsten	Technician
Ehrensack, Kerstin	Technician / Deputy EOO	Suchilina, Ekaterina	Office Assistant / Travel Management
Ferber, Thomas	Workshop	Szegedy, Erika (P)	Administrative Coordinator (Project)
Garcia Gomez, Sokrates	IT	Timm, Anne Susanne	Library / Deputy Chairperson Work Council
Heinitz, Sebastian	Electrician	Venohr, Thomas	Workshop
Herrmann, Claudia	Technician	Volkmer, Nicole	Technology
Litschauer, Maximilian	Technician	Wendt, Christian	Head of IT
Matzeck, Christopher	Technician	Wirsig, Arno	Technology
Morgenroth, Katrin	Technician	Wirt-Brunnckow, Andreas	IT
Prüfer, Evan	HR / Diversity Officer		

PDI Annual Report 2025

Equal Opportunity & Diversity
Chancengleichheit und Vielfalt

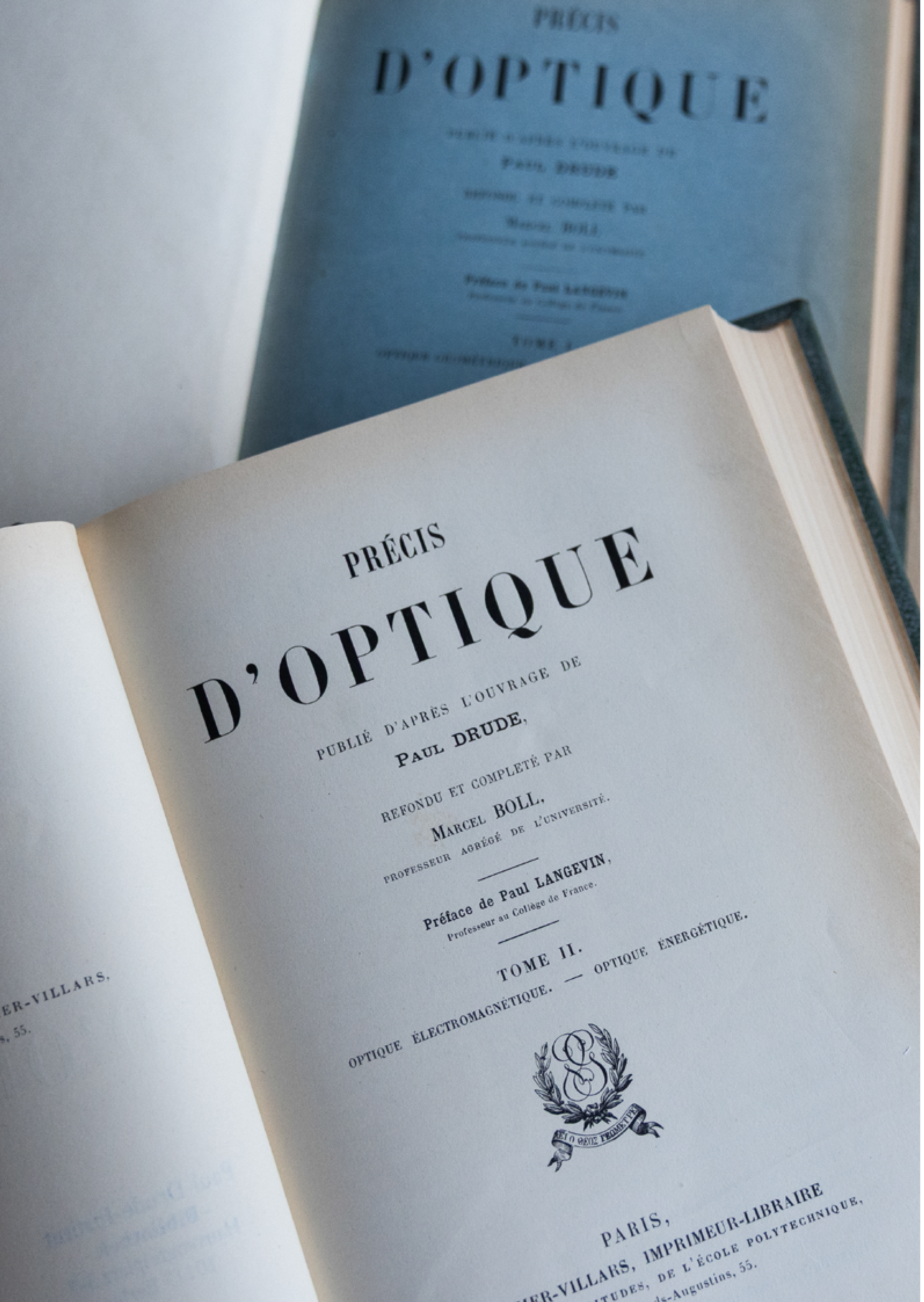
Our work is guided by PDI's Equal Opportunity Plan (Gleichstellungsplan), the FVB Diversity & Inclusion Strategy, and the Diversity Charter (Charta der Vielfalt), and aligned with the standards of the Leibniz Association and Forschungsverbund Berlin (FVB). Together, these frameworks define our approach to diversity and set the goals and principles for a culture of equity, transparency, and accountability.

- Dedicated Equal Opportunity and Diversity Officers, each with a deputy
- 2025 targets (Kaskadenmodell): met or exceeded for group leaders (100%) and doctoral researchers (29.2%); gaps remain at postdoc/senior scientist level (10.5% vs. 33.3%) and department head level (0% vs. 25%)
- Engagement through Girls' Day, Sendung mit der Maus, lab outreach, and Diversity Day 2025 ("Excellence Through Inclusion")
- Certified by berufundfamilie as a family- and life-phase-conscious employer, audited annually
- Represented in management meetings and on the Scientific Advisory Board

Unsere Arbeit orientiert sich am Gleichstellungsplan des PDI, der FVB-Diversity-&-Inclusion-Strategie sowie der Charta der Vielfalt und folgt den Standards der Leibniz-Gemeinschaft und des Forschungsverbunds Berlin (FVB). Gemeinsam definieren diese Rahmenwerke unseren Ansatz für Diversität und legen die Ziele und Grundsätze für eine Kultur der Gleichstellung, Transparenz und Verantwortlichkeit fest.

- Eigene Gleichstellungs- und Diversitätsbeauftragte, jeweils mit Stellvertretung
- Zielvorgaben 2025 (Kaskadenmodell): erreicht bzw. übertroffen bei Gruppenleitungen (100 %) und Promovierenden (29,2 %); Lücken bestehen auf Postdoc-/Senior-Scientist-Ebene (10,5 % vs. 33,3 %) und auf Abteilungsleitungsebene (0 % vs. 25 %)
- Engagement durch Girls' Day, Sendung mit der Maus, Laborbesuche und den Diversity Day 2025 ("Excellence Through Inclusion")
- Zertifiziert durch berufundfamilie als familien- und lebensphasenbewusster Arbeitgeber, jährlich auditiert
- Vertreten in Leitungssitzungen und im Wissenschaftlichen Beirat

	% WOMEN / FRAUEN		
Career Level Karrierestufe	2020	2025	Goal Ziel 2025
Director Direktor*in	0,0%	0,0%	0,0%
Department Heads Abteilungsleitungen	0,0%	0,0%	25%
Group Leaders Gruppenleitungen	0,0%	100%	100%
PhD Scientists without Leadership Role, incl. Postdocs Promovierte Wissenschaftler*innen ohne Leitungsfunktion inkl. Postdocs	6,9%	10,5%	33,3%
Doctoral Researchers Doktorand*innen	35,7%	29,2%	28,6%
Salary Group Tarifgruppe			
W3 / C4	0%	0%	0%
W2/C3	0%	100%	100%
E15/E15Ü/AT-B	0%	0%	28,6%
E14	7,1%	12,5%	28,6%
E13	23,1%	22,2%	30,8%



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