Leibniz
Gemeinschaft

Der Senat

16. November 2021

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

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Vorbemerkung

Die Einrichtungen der Forschung und der wissenschaftlichen Infrastruktur, die sich in der Leibniz-Gemeinschaft zusammengeschlossen haben, werden von Bund und Ländern wegen ihrer überregionalen Bedeutung und eines gesamtstaatlichen wissenschaftspolitischen Interesses gemeinsam gefördert. Turnusmäßig, spätestens alle sieben Jahre, überprüfen Bund und Länder, ob die Voraussetzungen für die gemeinsame Förderung einer Leibniz-Einrichtung noch erfüllt sind.[1]

Die wesentliche Grundlage für die Überprüfung in der Gemeinsamen Wissenschaftskonferenz ist regelmäßig eine unabhängige Evaluierung durch den Senat der Leibniz-Gemeinschaft. Die Stellungnahmen des Senats bereitet der Senatsausschuss Evaluierung vor.

Für die Bewertung einer Einrichtung setzt der Ausschuss Bewertungsgruppen mit unabhängigen, fachlich einschlägigen Sachverständigen ein. Der für das PDI zuständigen Gruppe stand eine von der Einrichtung erstellte Evaluierungsunterlage zur Verfügung. Die wesentlichen Aussagen dieser Unterlage sind in der Darstellung (Anlage A dieser Stellungnahme) zusammengefasst.

Wegen der Corona-Pandemie musste der für den 23. und 24. Februar 2021 vorgesehene Evaluierungsbesuch am PDI in Berlin entfallen. Die Bewertung erfolgte im Rahmen eines Ersatzverfahrens, das der Senatsausschuss Evaluierung (SAE) in Umsetzung eines Grundsatzbeschlusses des Senats vom 31. März 2020 eingerichtet hat. Der Senat hält in diesem Grundsatzbeschluss fest, dass das Ersatzverfahren ein Notbehelf ist und ausschließlich auf Einrichtungen angewendet wird, die im Regelturnus von sieben Jahren evaluiert werden. Die Bewertungen, auf deren Grundlage der Senat Stellung nimmt, sind auf zentrale Kernfragen der Entwicklung und Perspektive einer Leibniz-Einrichtung fokussiert. Ausführliche Einschätzungen und Schlussvoten zu Teilbereichen und Planungen für „kleine strategische Sondertatbestände“ müssen regelmäßig entfallen.

Die Bewertungsgruppe erstellte den Bewertungsbericht (Anlage B). Das PDI nahm dazu Stellung (Anlage C). Der Senat der Leibniz-Gemeinschaft verabschiedete am 16. November 2021 auf dieser Grundlage die vorliegende Stellungnahme. Der Senat dankt den Mitgliedern der Bewertungsgruppe und des Senatsausschusses Evaluierung für ihre Arbeit.

1. Beurteilung und Empfehlungen

Der Senat schließt sich den Beurteilungen und Empfehlungen der Bewertungsgruppe an.

Das PDI erforscht die Grundlagen epitaktischen Wachstums sowie neuer anorganischer Materialien und Heterostrukturen im Nanobereich mit dem Ziel, innovative Halbleiterbauelemente für neue Zukunftstechnologien zu entwickeln. Das Alleinstellungsmerkmal des PDI ist seine Ausstattung und langjährige Expertise im Bereich der Molekularstrahlepitaxie (MBE), einer Technik, die das kontrollierte Wachstum maßgeschneiderter Struk-

[1] Ausführungsvereinbarung zum GWK-Abkommen über die gemeinsame Förderung der Mitgliedseinrichtungen der Wissenschaftsgemeinschaft Gottfried Wilhelm Leibniz e. V.

turen mit atomarer Präzision ermöglicht. Auf dieser Grundlage verfolgt das Institut Forschungsfragen z. B. auf dem Gebiet der Spintronik, zu akustischen Oberflächenwellen und zu Nanodrähten.

Das PDI ist in vier Abteilungen organisiert, die gemeinsam in sechs Core Research Areas (CReAs) arbeiten. Alle CReAs haben in klar definierten Kompetenzbereichen sehr gute, in einigen Fällen auch ausgezeichnete **Leistungen** erbracht. Seine Forschungsergebnisse veröffentlicht das Institut regelmäßig in den einschlägigen Fachzeitschriften, besitzt aber das Potenzial, noch häufiger in höherrangigen und stärker fachübergreifend rezipierten Zeitschriften zu publizieren. Im Bereich des Transfers der Forschungs- und Entwicklungsarbeiten sind die hervorragenden und stark nachgefragten Materialproben hervorzuheben. Ebenfalls von hoher Bedeutung für die externe Nutzung sind die am PDI entwickelten Quantenkaskadenlaser (QCL). Diese werden u. a. bei astronomischen Anwendungen wie dem Teleskop SOFIA (*Stratospheric Observatory For Infrared Astronomy*) eingesetzt. Darüber hinaus führen die Arbeiten des PDI auch regelmäßig zu Patenten. Das PDI verfügt über eine herausragende Forschungsinfrastruktur. Es wird begrüßt, dass das Institut vorsieht, diese in noch größerem Maße als bisher kleinen und mittleren Unternehmen zugänglich zu machen. Dies sollte es dem PDI ermöglichen, seine Zusammenarbeit mit Industriepartnern auszubauen und somit auch den Transfer in die industrielle Verwertung weiter zu stärken.

Ende 2019 trat der langjährige und sehr erfolgreiche Direktor in den Ruhestand ein. Leider verzögerte sich die Wiederbesetzung bis zum 1. Juli 2021. Während der Vakanz wurden unter der kommissarischen Leitung eines Abteilungsleiters die wissenschaftlichen Arbeiten in den einzelnen CReAs erfolgreich weitergeführt und auch vielversprechende strategische Ideen entwickelt. Die Festlegung längerfristiger Ziele blieb jedoch mit Blick auf den Leitungswechsel weitgehend offen; einige Besetzungen wissenschaftlicher Stellen wurden zurückgestellt. Diese Situation und die 2022 anstehende Neubesetzung einer Abteilungsleitung eröffnen dem neuen Direktor nun großen, zügig zu füllenden Gestaltungsspielraum bei der Ausarbeitung einer **übergreifenden Institutsstrategie** für die nächsten Jahre. Ziel sollte es sein, die verschiedenen Arbeitseinheiten noch stärker als bisher auf ein gemeinsames Thema zu fokussieren.

Die Ausstattung des PDI mit Mitteln der institutionellen Förderung ist zur Erfüllung des derzeitigen Aufgabenspektrums auskömmlich. Die **Drittmitteleinnahmen** des Instituts liegen allerdings nach wie vor auf einem niedrigen Niveau (durchschnittlich p. a. 17 % des Gesamtbudgets zwischen 2017-2019) und müssen erhöht werden. Die wissenschaftliche Expertise und die exzellente Forschungsinfrastruktur bieten dafür beste Voraussetzungen. Positiv festzuhalten ist, dass das PDI die DFG-Abgabe regelmäßig wieder einwirbt.

Das PDI bietet Nachwuchswissenschaftlerinnen und -wissenschaftlern ein hervorragendes Arbeitsumfeld. Die Anzahl der **Promovierenden** war seit der letzten Evaluierung wie empfohlen zunächst angestiegen, ist dann allerdings wieder gesunken und muss nun wieder erhöht werden. Auch die Zahl der **Wissenschaftlerinnen** ist nach wie vor zu niedrig. Das PDI muss die anstehenden Neubesetzungen von wissenschaftlichen Mitarbeiter- und Leitungsstellen nutzen, um den Frauenanteil zu steigern. Dies gilt insbesondere für Leitungspositionen, von denen derzeit keine mit einer Wissenschaftlerin besetzt ist.

Das PDI arbeitet in verschiedenen Projekten eng mit den **Berliner Universitäten** zusammen. Hervorzuheben ist die Einrichtung eines Leibniz-WissenschaftsCampus zur Erforschung von Oxiden, an dem neben der Humboldt-Universität zu Berlin (HU Berlin) und der Technischen Universität Berlin auch das Leibniz-Institut für Kristallzüchtung (IKZ) und das Fritz-Haber-Institut der Max-Planck-Gesellschaft beteiligt sind. Die Zusammenarbeit mit der HU Berlin umfasst zudem auch die gemeinsame Berufung des Direktors des PDI. Es wird begrüßt, dass im Zusammenhang mit der anstehenden Neubesetzung einer Abteilungsleitung derzeit geprüft wird, inwieweit auch auf dieser Ebene künftig gemeinsame Berufungen mit einer Hochschule erfolgen sollen. Der Senat erwartet, dass im Namen des Instituts künftig noch klarer die Mitgliedschaft in der Leibniz-Gemeinschaft zum Ausdruck gebracht wird.

Das PDI erfüllt die Anforderungen, die an eine Einrichtung von überregionaler Bedeutung und gesamtstaatlichem wirtschaftspolitischem Interesse zu stellen sind. Das Institut betreibt auf der Grundlage seiner außergewöhnlichen Forschungsinfrastrukturen international bestens wettbewerbsfähige Forschungs- und Entwicklungsarbeiten, die neuartige informationstechnologische Anwendungen ermöglichen. Das PDI erbringt Leistungen, die in dieser Form nicht an einer Hochschule erbracht werden können. Die Eingliederung in eine Hochschule wird daher nicht empfohlen.

2. Zur Stellungnahme des PDI

Der Senat begrüßt, dass das PDI beabsichtigt, die Empfehlungen und Hinweise aus dem Bewertungsbericht bei seiner weiteren Arbeit zu berücksichtigen.

3. Förderempfehlung

Der Senat der Leibniz-Gemeinschaft empfiehlt Bund und Ländern, das PDI als Einrichtung der Forschung und der wissenschaftlichen Infrastruktur auf der Grundlage der Ausführungsvereinbarung WGL weiter zu fördern.

8 February 2021

Annex A: Status report

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

Contents

1. Key data, structure and tasks

Key data

Year established:	1992
Admission to joint funding by Federal and *Länder* Governments:	1992
Admission to the Leibniz Association:	1992
Last statement by the Leibniz Senate:	2014
Legal form:	One of seven Leibniz institutes of the *Forschungsverbund Berlin e. V.* (a registered non-profit association under private law)
Responsible department at *Land* level:	The Governing Mayor of Berlin, Senate Chancellery – Higher Education and Research
Responsible department at Federal level:	Federal Ministry of Education and Research (BMBF)

Total budget (2019, cf. appendix 3)

€9.6 M institutional funding

€1.7 M revenue from project grants

€72 k revenue from services

Number of staff (2019, cf. appendix 4)

53 research and scientific service

27 service staff

6 administration

Mission and organization

Mission (according to the new institute strategy, *Institutskonzept*, as approved by the Board of Trustees)

"*The Paul-Drude-Institut für Festkörperelektronik (PDI) plays a pathfinding role in pushing the outermost frontiers of materials and nanoscale devices for solid-state electronics and photonics. This exploratory work is firmly grounded on PDI's expertise in molecular beam epitaxy, a materials growth technique with extraordinary control and precision on the atomic scale. In a lively symbiosis between materials science and solid-state physics, PDI investigates the fundamentals of epitaxial growth, novel inorganic materials and nanoscale heterostructures, at the same time exploring the quantum physics of such structures with regard to innovative device concepts.*"

Organization

PDI is organized in four departments, which are defined by the areas of competences of PDI staff and the corresponding research facilities and cover the spectrum from materials synthesis by MBE with associated in-situ and ex-situ structure analysis and the investigation of physical phenomena to the demonstration of prototype devices. In order to address interdisciplinary tasks between materials science and solid-state physics, research within PDI is carried out in currently six “Core Research Areas” (CReAs), where scientists, engineers, and technicians from several departments collaborate for a certain period of time. See appendix 1 for the organizational charts of PDI.

2. Overall concept, activities and results

Overall concept and activities

According to PDI, its research typically places it in an early, exploratory phase, roughly 15 years before results may reach the marketplace, i.e. between fundamental and applied research. In order to ensure a clear orientation toward future devices, PDI selects new projects by their potential for applications. PDI seeks collaboration with industrial partners, typically in third-party funded consortia. Looking beyond specific materials or physical phenomena, PDI’s research has the following **four overarching aims:**

- Tailoring the synthesis of epitaxial materials and hybrid structures having unprecedented crystalline perfection, precisely controlled chemical composition, and/or nanoscale configurations to produce highly controlled electronic, optical, or magnetic properties
- Understanding the fundamental physical properties of these structures and the relationships between their structure and properties
- Devising new concepts for novel device functionalities based on the quantum-mechanical properties of electrons, photons, phonons, spins, and other elementary excitations
- Developing new device concepts for nascent markets and further advancing leading-edge device concepts for existing markets

In order to fulfil its mission, PDI maintains facilities needed to conduct complex scientific research projects, which may encompass the full range from fundamental growth studies, the understanding of basic inorganic materials properties and of fundamental physical effects to the fabrication of devices.

Research at PDI is organized in **six Core Research Areas (CReAs)** described below. The first three CReAs are characterized by a focus predominantly given by scientific methods, and the last three CReAs are defined by a focus on a specific research topic. For a more detailed description of the six CReAs see chapter 7.

i) The *CReA Nanofabrication* is devoted to the fabrication of novel types of thin films and nanostructures with high crystalline perfection. In addition to the traditional focus on III-V compounds, the CReA has widened its scope of epitaxial activities to other semiconductors and materials with further functionalities.

ii) The *CReA Nanoanalytics* aims at clarifying fundamental structure-property relations of low-dimensional systems and nanoscale devices. The work program is based on the development and application of sophisticated experimental and modelling tools for materials analysis with highest sensitivity and resolution down to the single-atom level.

iii) The *CReA Nanoelectronics* explores quantum effects and quantum transport of electrons as well as spins in artificial hetero- and nanostructures such as quantum circuits and ferromagnet-semiconductor hybrid structures, ionic transport in solid electrolytes, as well as materials for topological insulators.

iv) The *CReA III-V Nanowires for Optoelectronics* synthesizes III-V nanowires by both bottom-up and top-down approaches, investigates their fundamental properties, fabricates demonstrator devices, and explores advanced structures enabling novel physical effects. The overall goal is to critically evaluate the suitability of III-V nanowires for optoelectronic applications, to identify the specific application areas in which nanowires are conceptually superior to conventional planar structures, and to demonstrate new device functionalities.

v) The *CReA Control of Elementary Excitations by Acoustic Fields* aims at the control of elementary excitations such as photons, electrons, and spins in semiconductor nanostructures using spatially and time-dependent fields produced by acoustic waves. The research activities within this CReA address basic studies of the interaction between dynamic acoustic fields and solid-state excitations, the development of new materials and structures for acoustic modulation, as well as their exploitation for novel device functionalities.

vi) The *CReA Intersubband Emitters: GaAs-based Quantum-Cascade Lasers* focuses on the development of terahertz quantum-cascade lasers (QCLs) for high-resolution spectroscopy. The activities include the design, the growth, the fabrication, and the determination of the operating parameters of GaAs/(Al,Ga)As QCLs.

Results

Research

Activities at PDI are very much centred on research. Between 2017 and 2019, work at PDI lead to 233 publications in peer-reviewed journals (see appendix 2). PDI highlights the following ten research results:

i) *Metal exchange catalysis during oxide growth:* A catalytic mechanism has been discovered that enables higher growth rates or temperatures during molecular beam epitaxy of β-Ga_2O_3. This mechanism is explained by a thermodynamically driven cation exchange that bypasses the limiting kinetics of intermediate suboxide formation and desorption.

ii) *Selective-area van der Waals epitaxy of two-dimensional heterostructures:* Defect engineering in two-dimensional materials via focused ion beam irradiation allows to fabricate epitaxially aligned h-BN/graphene heterostacks with a high degree of control. This approach has evolved from PDI's findings on defect-mediated van der Waals growth. PDI applied for a patent.

iii) *GaN nanowires on metals:* The self-assembled growth of GaN nanowires has been pioneered for metallic substrates, including TiN films, Ti foil, and graphene. Because of the high electrical and thermal conductivity of metals, this extreme heteroepitaxy of dissimilar materials may prove highly beneficial for applications.

iv) *First experimental demonstration of well-ordered, layered $FeGe_2$ (not existing as bulk material):* By a combination of molecular beam and solid-phase epitaxy, $Fe_3Si/FeGe_2/Fe_3Si$ thin-film stacks have been synthesized as an important step toward the development of vertical spin-selective devices and of materials exhibiting two-dimensional magnetism.

v) *Non-common-atom heterovalent interfaces:* A new strategy for a comprehensive and quantitative structure determination of heterovalent interfaces has been developed. The CdTe-on-InSb case study is used to demonstrate the applicability of transmission electron microscopy methods on all relevant length scales to obtain composition profiles for each atom type.

vi) *Quantum rings engineered by atom manipulation:* Atomic rings were constructed that reveal the generic electronic states of a quantum ring. Their hexagonal shape leads to a perturbed level structure that can be understood in analogy to band gap formation in a one-dimensional crystal, demonstrating the possibility of controlling the electron dynamics in a tunable periodic potential on a semiconductor surface.

vii) *Bent GaAs nanowires:* Controlled bending of GaAs nanowires close to the elastic limit has been demonstrated by the growth of asymmetric lattice-mismatched shells. This bending gives rise to extreme strain gradients influencing charge carrier dynamics and according to PDI elevates the concept of strain engineering to a new level.

viii) *Dynamically tuned lattices of polariton parametric oscillators:* The fine tuning of confined polariton states in an (Al,Ga)As microcavity by an acoustic wave has been shown to enable the realization of complex and scalable non-linear functionalities on a chip such as optical amplifiers, generators of correlated photons, and optical memories.

ix) *Anisotropic spin-acoustic resonance in SiC at room temperature:* Acoustically driven resonant transitions between spin levels with quantum number differences of ±1 and ±2 in atomic-scale centres in SiC have been observed at room temperature and exhibit a non-trivial dependence on the angle between the propagation direction of the surface acoustic wave and the spin quantization orientation.

x) *High-performance GaAs/AlAs THz quantum-cascade lasers for high-resolution spectroscopy:* THz quantum-cascade lasers based on GaAs/AlAs have been demonstrated, which exhibit a much higher wall plug efficiency than lasers using (Al,Ga)As barriers. Lasers with several emission frequencies between 3.3 and 4.7 THz were developed for astronomical observations and for the quantitative determination of the density of atoms/ions in plasma processes.

Research Infrastructure

Regarding the operation of research infrastructures, a few of the facilities that are needed for PDI's research program are made available to a limited extent for external purposes.

In 2019 PDI established with support from the European Regional Development Fund and grants from the Berlin Senate a new Application Laboratory Electron Tomography. It will serve to further develop the electron tomography method and to apply it to materials research and development activities in the field of semiconductor technologies and photonics.

The laboratory and the expertise of the respective scientists will be made available to partners from science and industry.

For more than two decades, PDI has been operating its own beamline PHARAO at the Berlin Synchrotron BESSY II, which is part of the *Helmholtz-Zentrum Berlin*. As a distinctive feature, this beamline is equipped with a heavy-duty goniometer, on which a custom-designed MBE system is mounted. Thus, this experiment allows the in-situ real-time analysis of growth processes by x-ray diffraction. A general condition for accessing experimental time is a successful project proposal.

Transfer

Transfer activities at PDI follow three different routes. First, PDI transfers technological knowledge through the organization of scientific meetings and through collaborations by exchange of samples, ideas, and scientists. This route overlaps directly with PDI's research activities. For example, PDI organized the Compound Semiconductor Week (CSW) 2017 in Berlin and the European Workshop on Molecular Beam Epitaxy (EuroMBE) 2019 in Lenggries.

Second, the institute makes its technological skills available to partners in science and industry by providing customized samples and designs, granting access to experimental techniques, and offering secured intellectual property. The most tangible result with respect to this transfer route are PDI's quantum-cascade lasers (QCLs). In addition to about 30 QCL devices provided to partners in the framework of externally funded projects since 2014, PDI delivered six devices to other research groups for testing potential applications of THz QCLs. Furthermore, PDI sold five QCL devices, two to a company and three to a research institution for use in commercial systems. In terms of intellectual property, between 2017 and 2019 11 patents in 5 patent families were granted, 14 patents in 7 patent families were filed, and 6 patents in 4 patent families were given up (see also appendix 2).

The third route includes traditional outreach formats such as open house events and laboratory tours, offering internships to high school students, participating in the Girl's Day organized in Berlin, but also science-art collaborations, public talks, as well as interdisciplinary debates. The head of the PDI *Department Technology and Transfer* is speaker of the working group Knowledge Transfer of the Leibniz Association.

3. Changes and planning

Development since the previous evaluation

Personnel Changes

The former director of PDI retired at the end of 2019. Since January 2020, the head of the *Department Epitaxy* has been acting director of PDI. The procedure for filling the position of the director in connection with a joint appointment (W3) at the Humboldt-Universität zu Berlin is ongoing. The position was advertised in November 2018.

In addition to the director, there have also been changes among the senior scientists:

- Shortly after the last evaluation, a senior scientist joined the institute and started a research activity on quantum transport investigated at cryogenic temperatures in nanoscale circuits that belongs now to the new *CReA Nanoelectronics*, established in 2020.

- One of the two senior scientists in the *CReA Control of Elementary Excitations by Acoustic Fields* left PDI. His position has been refilled internally.

Furthermore, two senior scientists retired (responsible for analytical scanning electron microscopy and for x-ray diffraction and structural analysis of ferromagnet-semiconductor hybrid structures) and two moved on to other positions in academia (responsible for synthesis of group-III nitride nanowires and for epitaxy of nitride thin films and phase change materials). The re-staffing of these positions will be pursued once the new director has been appointed.

Structural Changes

Among the four Departments that provide the long-term stability in terms of infrastructure and essential expertise, there has not been any change since the last evaluation. On the level of the six CReA the following two main changes were made:

- The *CReA Ferromagnet-Semiconductor Hybrid Structures* was discontinued in 2017, since the respective research activities had decreased below a critical level. Efforts related to the growth of such structures are now embedded in the *CReA Nanofabrication*.
- In 2020, the new *CReA Nanoelectronics* was established. This CReA investigates quantum effects and quantum transport of electrons as well as spins in different nanostructures and materials.

Strategic work planning for the coming years

With respect to the **four overarching aims** of the institute strategy (see chapter 2), PDI has the following plans:

- Regarding the tailoring of the <u>synthesis</u> of epitaxial materials, PDI wants to study how the formation of point defects in Ga_2O_3 depends on growth conditions and how such point defects affect materials properties relevant for power electronics.
- In terms of elucidating fundamental physical <u>properties</u> of semiconductor systems and their correlation with structure, PDI plans to advance electron tomography to the level of obtaining a three-dimensional reconstruction of interfaces with atomic resolution and a corresponding mapping of chemical intermixing.
- With the ambition of devising novel device <u>functionalities</u> based on quantum-mechanical properties, it is PDI's long-term aim to realize quantum circuits made from atomically defined nanostructures representing quantum bits. To this end, the manipulation of individual atoms by scanning tunnelling microscopy (STM) will be combined with lateral control gates and external electrical contacts.
- As a new <u>device</u> concept, PDI works towards a laser for Si photonics based on ordered arrays of group-III arsenide nanowires. PDI has filed for patent protection of a laser concept based on a hybrid cavity composed of nanowires as amplifying material monolithically grown on top of Si waveguide elements providing photonic confinement. To

obtain high peak gain, PDI plans to realize core-shell nanowire heterostructures with a sufficiently thin core diameter to enable lateral quantum confinement.

Furthermore, PDI plans to pursue research by **joint efforts of previously disjunctive activities**:

- One direction is the investigation of advanced quantum circuits. In addition to the above mentioned atom manipulation by STM, it also requires expertise on quantum transport in nanoscale circuits created by electron beam lithography. Furthermore, in a combination of the latter research with PDI's activities on controlling elementary excitations by acoustic waves, the interaction between electrons localized in quantum dots and confined phonons will be studied.
- Within the new focus on ferromagnetism in two-dimensional (2D) materials, PDI plans to explore the synthesis of van der Waals heterostructures comprising $FeGe_2$ or Fe_3GeTe_2 and to investigate structure-property relations with the vision to engineer magnetic functionalities.

Also, PDI highlights further plans belonging to the field of **quantum technology**:

- PDI plans to amend the top-down fabrication of ordered arrays of GaN nanowires with a subsequent thinning of these nanowires by thermal sublimation and then growing (In,Ga)N quantum dots on the nanowire top facets. The vision of this approach is the realization of single photon emitters operating at room temperature in the entire telecommunication wavelength range.
- The (Al,Ga)As microcavities (see chapter 2, highlight viii) may eventually be utilized as the technological basis for a solid-state quantum simulator. To this end, PDI is exploring processing options to reduce the dimensions of the intracavity traps to a size of roughly 0.5 µm.

The plans described above can be implemented with the resources available at PDI. In addition, PDI sees possibilities for **disruptive extensions of its work.** However, according to PDI these would need new fabrication facilities and corresponding personnel, for which PDI would have to secure additional funding. PDI sees the following two directions:

- In view of PDI, the best fabrication option for the realization of the solid-state quantum simulator based on tuneable polariton lattices (see above) would be a cluster comprising a system for molecular beam epitaxy (MBE) of group-III arsenides and a processing chamber with focused ion beam (FIB) and scanning electron microscopy columns. Such a cluster system would enable repeated contamination-free growth-patterning sequences, thus facilitating the three-dimensional fabrication of complex epitaxial heterostructures. Furthermore, in-situ patterning by FIB is attractive also for PDI's activity on 2D materials.

- According to PDI a facility for thermal laser epitaxy (TLE) would overcome technical limitations of the traditionally used MBE and greatly widen the choice of epitaxial materials for the investigation of desirable physical properties. Specifically, such a facility would benefit PDI's plans to explore the growth of hexagonal BN (h-BN) films with a thickness usual for conventional light-emitting devices towards optoelectronics in the deep ultraviolet spectral region.

4. Controlling and quality management

Facilities, equipment and funding

Funding

In 2019, the institutional funding of PDI according to the administrative agreement between the Federal and *Länder* Governments with regard to the joint funding of member institutions of the Leibniz Association (AV-WGL) totalled 9.6 M€.

Between 2017 and 2019, revenue for project grants totalled approx 5.4 M€ (∅ 1.8 M€ p.a.), corresponding to 16 % of the overall budget. Thereof, 1.6 M€ were raised from the EU (∅ 533 k€ p.a.), 1.3 M€ (∅ 433 k€ p.a.) from the Deutsche Forschungsgemeinschaft (DFG), 1.3 M€ (∅ 433 k€ p.a.) from Federal and *Länder* governments, and 1.1 M€ (∅ 366 k€ p.a.) from the Leibniz Association.

From services, PDI generated revenue in the amount of 450 k€ (∅ 150 k€ p.a.). For an overview of PDI's revenue and expenses, see appendix 3.

Equipment

PDI operates a range of molecular-beam-epitaxy equipment. The according growth activities are performed in a 550 square meter cleanroom.

The patterning of wafers before growth experiments, processing between growth steps, post-growth structuring, and further post-processing are performed in the semiconductor technology cleanroom with optical and electron beam lithography, wet-chemical and dry etching, as well as sputtering and electron beam evaporation setups.

The permanent access to a beamline at BESSY II at the *Helmholtz-Zentrum Berlin* (HZB) allows for experimental setups for complex investigations with high-resolution x-ray diffraction.

In addition, the following methods and techniques are available at the institute: continuous-wave and time-resolved photoluminescence spectroscopy, Raman and photoluminescence spectroscopy, Fourier-transform spectroscopy, magneto-transport experiments, scanning electron microscopy including cathodoluminescence spectroscopy, energy- and wavelength-dispersive x-ray spectroscopy, electron backscatter diffraction, transmission electron microscopy, scanning tunnelling microscopy, and electron tomography.

PDI's IT strategy serves three general purposes: managing the office PCs with rapid first-level support, managing services that are accessible from the outside but separate from PDI's inner systems, and managing internal servers and services, data backup, and data protection. This is achieved by integrating the local IT into the corporate IT of the *Forschungsverbund Berlin e. V.* (FVB).

Organisational and operational structure

PDI is one of currently seven institutes of the FVB, with administration being shared between the joint FVB administration and the local administrative unit of PDI. PDI is headed by the Scientific Director and the Managing Director of the FVB.

The departments are defined by the areas of competence of PDI staff and share the responsibility for research resources. Each department is managed by one department head, who together are advising the director in scientific and technological questions. They meet at least once a week with the director.

The CReAs manage the core scientific activities that often involve more than one department. Each CReA is usually managed by one to two senior scientists, one of whom is usually a department head. Through the department heads, the CReA activities are in contact to the scientific managing team of the institute.

Long-term strategies have been defined in the new institute strategy *(Institutskonzept).* Mid-term goals are developed within the CReAs and described annually in the official program budget document, which is subsequently approved by the Director, the Scientific Advisory Board, and the Board of Trustees (see below).

Quality Management

PDI follows the recommendations for good scientific practice as developed by the DFG and adopted by the Leibniz Association. PDI has an ombudsperson. For major concerns, an external ombudsman can be contacted.

Scientific results are to be published in peer-reviewed journals. Before submitting a paper, an internal review process has to be followed. The process is supported electronically by the Publication Manager, a tool that helps trace the stages of the publication from internally submitting the draft, internal review by a scientist not connected to the work to be published, a check for possible intellectual property by the transfer manager, to the iterations of the journals' referee process and, finally, acceptance.

PDI has developed an Open Access Policy. Open access is supported with an institute budget, that, e.g., allows for participation in the DEAL project that was initiated by the alliance of the German science organizations. This project develops novel contract models with major science publishers, which include permanent open access rights for the authors of participating institutions.

The responsibility for the quality management of the scientific infrastructure is assigned to the department heads. They regularly discuss in the weekly meetings with the director and decide on allocation of investment funds. The experiments at the beamline at BESSY II are regularly evaluated externally. The new Application Laboratory for Electron Tomography is evaluated in the frame of the EFRE project which initiated this infrastructure.

The program budget is the central formal document which allows for a discussion and assessment of performance as evidenced by a set of performance indicators between institute and funding bodies. The program budget describes the scientific development within the CReAs and outlines their scientific goals for the coming two years. Part of the annual meetings of the Scientific Advisory Board (see below) is used to assess the performance completion based on the program budget. This assessment and concomitant recommendations are reported to the supervising body. PDI has no performance-based allocation of funds (*Leistungsorientierte Mittelvergabe* – LOM).

Quality management by supervisory board and advisory board

The Scientific Advisory Board (SAB) advises the Director and the Board of Trustees (see below) on fundamental questions concerning the scientific work program. The SAB also carries out an audit between two evaluations as it is common for Leibniz institutes. The SAB is composed of six to twelve scientists, who are closely linked to the research areas of the institute. The appointment period is four years and one consecutive reappointment for four years is possible.

The supervisory board of the PDI is the Board of Trustees (*Kuratorium*) of the FVB, which is responsible for all essential scientific, programme-related and economic issues of all the institutes within the FVB, appoints directors, and confirms joint professorial appointments. Decisions by the Board of Trustees that relate to PDI are prepared by its Institute Committee consisting of the SAB's chairperson and both the representatives of the Berlin Senate Chancellery and the Federal Ministry of Education and Research (BMBF). The institute Director and the Managing Director of the FVB have guest status.

5. Human Resources

As of 31 December 2019, PDI had 86 employees (without assistants, trainees, and scholarship recipients, see annex 4). 53 persons worked in research, comprising the director, 4 department heads, 34 scientists in non-executive positions (18 senior scientists and 16 postdocs), and 14 doctoral candidates. Furthermore, 27 persons worked in service positions and 6 persons had administrative tasks (1 department head also acts as head of administration).

Management

The procedures for appointing leading scientific staff (director and department heads) and joint professors are defined in the guidelines for a joint appointment process (*Leitlinien für gemeinsame Berufungsverfahren der Institute im Forschungsverbund Berlin e. V.*). It is generally recommended to evaluate if the position of a department head should be connected to a joint appointment at one of Berlin's universities. For the position of the director this connection is mandatory. A joint appointment committee of one of Berlin's universities and the FVB then heads the further search process. The regulations take into account the recommendations of the Leibniz Association for the appointment of leading scientific and administrative staff.

Postdoctoral staff

An average of fifteen postdocs are working at the PDI. PDI strives to provide support for and transparency about the next career steps in and out of science. PDI supports postdoctoral researchers by integration into PDI's research, by supervision and mentoring. Postdocs are encouraged to supervise Ph. D. students, and they are supported with their conference contributions and international exchanges. If the postdoctoral researcher aims at a professorship, PDI supports the possibility to pursue a Habilitation at one of Berlin's universities.

While the institute aims at keeping the best scientific staff as senior scientists by offering permanent positions, there is no tenure-track program. Since 2017, 1 postdoc moved on to a permanent position (senior scientist) at PDI. Furthermore, 2 senior scientists, 6 postdocs, and 1 PhD student moved on to external leading positions in science (8) or industry (1).

Doctoral Candidates

As of 31 December 2019, there were 14 doctoral candidates working at PDI. Between 2017 and 2019, 17 doctoral candidates successfully completed their work. Positions are initially awarded for two years with the explicit intent to extend it for a third year and the possibility for additional short-term extensions up to another nine months. It is expected that the main experimental scientific work is finished after three years and that at this stage an outline of the thesis is available. The median duration of doctorates is 4 years until handing in the thesis.

Each doctoral student is assigned to a supervisor. Furthermore, the director is often formally and actively supervising the doctoral theses. The doctoral candidates discuss their results in internal seminars and usually present their early scientific work in talks or posters at the spring conference of the German Physical Society. They also organize their own seminar series, in which they present their research to each other or study topics of joint interest. They have the possibility to attend summer schools or, at a later stage, international conferences to present their results. Through the graduate school of Humboldt-Universität zu Berlin, doctoral students have access to parts of the structured doctoral program of the university.

PDI's support of doctoral candidates takes into account the Career Guidelines of the Leibniz Association. Additional guidance will be established in PDI's own guidelines for doctoral students. After completing their thesis, doctoral candidates are encouraged to sign in to a loosely managed alumni network on the social platform linkedin.

Non-scientific staff

All non-scientific staff are encouraged to participate in advanced training. The members of the machine shop visit manufacturing systems fairs and receive training when new equipment is acquired. The molecular beam epitaxy (MBE) technicians participate in the German MBE Workshop.

Administrative staff receives invitations to all vocational training measures of FVB, and specific training is offered through discussion with the department head. PDI's offers administrative traineeships in collaboration with the central administration of FVB. The core of the vocational training lies in the central administration with stints of the trainees at PDI. This collaboration offers one traineeship per year.

Equal opportunities and work-life balance

Equal opportunities

As of 31 December 2019, out of 53 employees in "Research and scientific services" (see appendix 4) 7 were female (13 %). Out of the 5 leading scientists (director and four department heads) none was female. Among the 34 scientists in non-executive positions, 2 were female (6 %). Among the 14 doctoral candidates, 5 were female (36 %).

The gender equality officer is involved in promoting PDI as a woman-friendly employer by organizing Girls Days and networking events for female doctoral students. She is involved in every hiring process, discusses possible systemic hurdles for women pursuing scientific careers, coordinates with her colleagues of the other FVB institutes, and is included in the group of gender equality officers at the Leibniz Association.

Work life balance

PDI supports work-life balance through individual solutions from special arrangements of working hours, flexible response to especially demanding situations, and encouragement of maternal/paternal leave. In 2018, PDI has been re-certified by the audit "berufundfamilie" (conferred through the berufundfamilie Service GmbH after full evaluations) for its engagement in pursuing a family-friendly human resources policy. PDI is evaluating its experience with mobile working and home office solutions that were set up to react to the covid-19 pandemic.

6. Cooperation and environment

Cooperation with universities

The institute is connected with the *Humboldt-Universität zu Berlin* (HU Berlin) on the basis of a cooperation agreement. The contract regulates the joint appointment of the institute's director as a full professor with reduced teaching obligations (S-Professorship). This joint appointment enables collaborative research, training of students (academic supervision of Bachelor, Master, and doctoral theses), and the integration of the institute in comprehensive research activities such as Collaborative Research Centres (CRCs) or Research Training Groups and other networks of the university.

PDI is also associated with the *Technische Universität Berlin* (TU Berlin) through an extraordinary professorship (*außerplanmäßige Professur*) of the head of the *Department Semiconductor Spectroscopy* since 2001. He teaches at the TU Berlin and conducts the academic supervision of Master and doctoral theses. In 2016, a senior scientist in the same department became private lecturer (*Privatdozent*) at the *Freie Universität Berlin* (FU Berlin), where he also teaches courses and conducts academic supervision.

Since the last evaluation, scientists of PDI participated in two DFG-funded Collaborative Research Centres at HU Berlin (until 2015) and FU Berlin (until 2017). Furthermore, PDI participated in one DFG-funded Priority Program (until 2015). In addition, there are individual projects funded by the DFG at PDI involving at least one informal partner, often at a German university.

PDI is a coordinator of the Leibniz ScienceCampus "Growth and fundamentals of oxides for electronic applications" (GraFOx) funded through the Leibniz Association. The ScienceCampus model promotes cooperation between Leibniz institutes and universities. Partners in GraFOx are the *Leibniz-Institut für Kristallzüchtung* (IKZ) in Berlin, HU Berlin, TU Berlin, and the *Fritz-Haber-Institut* of the Max Planck Society. The primary goals of GraFOx are to perform joint research on oxide electronics and to educate and promote young scientists in solid-state physics. The second funding period of GraFOx started in 2020.

Cooperation with non-university partners

PDI is engaged with other Leibniz institutes in two collaborative projects of the Leibniz competition procedure. In the project *TERAPLAS - Terahertz detection of atoms in plasma processes,* PDI cooperates with the Leibniz Institute for Plasma Science and Technology (INP) in Greifswald and in the project *BaSTeT- Barium stannate based heterostructures for electronic applications* with the IKZ in Berlin.

The institute collaborates with the Institute of Optical Sensor Systems of the German Aerospace Centre (*Deutsches Zentrum für Luft- und Raumfahrt*) in Berlin. Furthermore, since the last evaluation, PDI was and is involved in three cooperative projects with university and non-university partners funded by the BMBF, two of them are still ongoing.

International cooperation

In connection with the 2019 established Application Laboratory Electron Tomography, there are collaborations with the *Université de Montpellier* on dislocation tomography, the *Universidad Politécnica de Madrid* (Spain) on nanowire tomography, and the *Eidgenössische Technische Hochschule* (*ETH) Zürich* (Switzerland) on interface tomography. Furthermore, there is an agreement with the *Fraunhofer-Institut für Angewandte Festköperphysik* in Freiburg as the basis for future cooperation.

PDI participated in five cooperative projects funded by the European Union (PASTRY, DEEPEN, SPRInG, SAWtrain, BeforeHand), one of them is still ongoing. Furthermore, there are bilateral projects with the *Institut Néel* in Grenoble (France), the *Laboratoire National des Champs Magnétiques Intenses*, Toulouse (France), the Hebrew University of Jerusalem (Israel), and the Institute of Solid-State Physics, Russian Academy of Sciences, Moscow (Russia). The latter takes place within a cooperation with the *Walter Schottky Institut* of the *Technische Universität München*.

Other collaborations

The PDI has also exchanged scientific staff bilaterally with universities in Montpellier and Grenoble (France) within the *Project Based Personnel Exchange Program* funded by the *Deutscher Akademischer Austausch Dienst* (DAAD). In 2019, PDI also hosted one recipient of a Leibniz-DAAD Research Fellowship from Suzhou Institute of Nano-Tech and Nano-Bionics, Chinese Academy of Sciences, Suzhou (China).

Between 2014 and 2019, PDI hosted seven recipients of a Humboldt Research Fellowship. In addition, a total of 162 scientists visited PDI with "Guest Scholar Agreement" for at least one week or longer, 55 of them for more than 3 months.

Institution's status in the specialist environment

According to PDI, the institute is one of the very few institutions which combine efforts in epitaxial growth with structural and interface investigations, detailed optical spectroscopy, and the processing of demonstrator devices. On the national level, PDI names as institutes that take a similar position the *Walter Schottky Institut* (WSI) and the WSI Center for Nanotechnology and Nanomaterials of the *Technische Universität München* as well as the *Peter-Grünberg-Institut* (PGI) of the *Forschungszentrum Jülich*.

On an international level, PDI names the *CNRS-Centre de Recherche sur l'Heteroepitaxie et ses Applications* (CRHEA) in Valbonne (France) as well as the Department of Materials and the Department of Electrical Engineering of the University of California, Santa Barbara (USA).

7. Core Research Areas of PDI

CReA Nanofabrication

[As of 31 December 2019: 9.7 FTE Research and scientific services, 2.6 FTE Doctoral candidates]

The CReA is devoted to the fabrication of novel types of crystalline thin films and nanostructures. For the desirable high level of control over fabrication, the CReA studies the underlying fundamental growth mechanisms. Research is mainly based on molecular beam epitaxy (MBE). Materials for growth are chosen on the basis of their application perspectives. In addition to conventional arsenide and nitride III-V compound semiconductors, the CReA presently works on ferromagnetic Heusler alloys such as Co_2FeSi in hybrid structures, wide-bandgap semiconducting oxides such as Ga_2O_3, phase change materials in the alloy system Ge-Sb-Te, and two-dimensional (2D) materials such as hexagonal BN (h-BN). Another typical example of work is the fabrication of heterostructures in highest complexity or combining dissimilar materials. Current examples for the physical phenomena and application perspectives that are pursued include non-volatile memories, gas sensing, power electronics, phenomena and applications based on electron spin, as well as 2D ferromagnetism.

Between 2017 and 2019, the CReA published 82 articles in peer-reviewed journals. The revenue from project grants totalled approx. 1.35 M€ (∅ 450 k€ p.a.), with 940 k€ spent from the Leibniz Association, and 350 k€ from the EU. In addition, the CReA applied for two patents. In the same period, five doctoral degrees were completed.

CReA Nanoanalytics

[As of 31 December 2019: 11 FTE Research and scientific services, 5.3 FTE Doctoral candidates]

The central aim of the CReA is to clarify the fundamental structure-property relation in semiconductor materials. The work program is based on the development and application of experimental and modelling tools for materials analysis with highest sensitivity and resolution down to the single-atom level. Research addresses the following key aspects: (I) Interfaces in epitaxial heterostructures, (II) order-disorder phenomena and phase transitions, (III) microstructure of metastable and nano-scale systems, (IV) manipulation and spectroscopy of materials at the single-atom scale. At the PHARAO beamline at the synchrotron BESSY II, synchrotron x-ray diffraction (XRD) is performed for the in-situ investigation of epitaxial layers during growth. Advanced transmission electron microscopy (TEM) and scanning (S)TEM techniques including diffraction, imaging and spectroscopy as well as scanning tunnelling microscopy (STM) and spectroscopy are applied to quantitatively analyse the structural, chemical, and electronic properties of the material systems with highest spatial resolution. Experimental results are compared with computer simulations and supported by theoretical modelling. Aside from the analytical aspect, the CReA uses operational tools to deliberately modify material structure by the focused ion beam technique on the length scale between micron to nanometer and by STM on the scale of single atoms.

Between 2017 and 2019, the CReA published 73 articles in peer-reviewed journals. The revenue from project grants totalled approx. 2.4 M€ (∅ 800 k€ p.a.), with 1.13 M€ spent from the EU, 650 k€ from the DFG, and 600 k€ from federal and *Länder* governments. In addition, the CReA applied for one patent. In the same period, four doctoral degrees were completed.

CReA Nanoelectronics

[As of 31 December 2019: no personnel was assigned to the CReA since it was established in 2020]

The CReA explores quantum effects and quantum transport of electrons as well as spins in artificial hetero- and nanostructures, ionic transport in solid electrolytes, and materials for topological insulators. Nanoscale quantum circuits fabricated by electron beam lithography are investigated by transport experiments at very low temperatures and also in high magnetic fields. Quantum transport is also investigated under the influence of superconductivity. Spin transport phenomena are studied in ferromagnet/semiconductor hybrid structures. Topological insulators also provide an interesting system for the investigation of spin transport, since they contain metallic helical surface states, for which spin and momentum are coupled to each other.

CReA III-V Nanowires for Optoelectronics

[As of 31 December 2019: 5.5 FTE Research and scientific services, 0.7 FTE Doctoral candidates]

The goal of the CReA is to inspire and demonstrate new functionalities for optoelectronic applications by employing III-V nanowires. To this end, the CReA investigates fundamental nanowire properties that crucially influence such applications to assess nanowire suitability. The CReA grows both group-III-nitride and group III-arsenide nanowires by molecular beam epitaxy (MBE) but pursues also top-down approaches. Synthesis is an important research direction, because of the need to control nanowire composition, doping, dimensions, and arrangement as a means to tailor nanowire properties. With respect to the latter aspect, special attention is paid to phenomena that are a direct consequence of the peculiar wire-like shape and nanometric size and are independent of the material the nanowires consist of. Specifically, nanowire microstructure properties are analysed as well as optical and electronic properties. Furthermore, the CReA employs technology to guide growth, enable electrical measurements, and process demonstrator devices. Particular interest lies on advanced structures that exploit nanowire specifics to enable functionalities that are inherently impossible for planar structures. The application perspectives range from single photon emission for quantum communication, to utilizing sun light for the conversion of CO_2 into valuable chemicals, to optoelectronic devices for the deep ultraviolet spectral range, and to a monolithically integrated laser for Si photonics.

Between 2017 and 2019, the CReA published 50 articles in peer-reviewed journals. The revenue from project grants totalled approx. 640 k€ (∅ 220 k€ p.a.), with 500 k€ spent from federal and *Länder* governments. In addition, 6 patents were granted, and the CReA applied for seven more. In the same period, three doctoral degrees were completed.

CReA Control of Elementary Excitations by Acoustic Fields

[As of 31 December 2019: 5.5 FTE Research and scientific services, 0.7 FTE Doctoral candidates]

The CReA aims at the control of elementary excitations in semiconductor nanostructures using the space- and time-dependent fields produced by acoustic waves. The studies are motivated by the fact that acoustic fields interact with a wide range of optical, electronic, and magnetic excitations in semiconductors and thus provide a convenient tool for the tuneable spatial and temporal modulation of these properties without introducing lateral interfaces, which are normally deleterious for the electronic properties. In most cases, these dynamic fields are created by high-frequency (0.5-20 GHz) surface or bulk acoustic waves (SAWs or BAWs) excited by piezoelectric transducers on the surface of the semiconductor structures. Recent technological developments have reduced the spatial and temporal periods of piezoelectrically excited fields to the sub-µm and sub-ns ranges, respectively. These values are approaching the characteristic response times of semiconductor excitations, thus opening the way for their coherent coupling to vibrations. Finally, the moving character of acoustic waves can be used to transport excitations with the well-defined acoustic velocity. The research activities within this CReA address basic studies of the interaction between dynamic acoustic fields and solid-state excitations, the development of new materials and structures for acoustic modulation as well as their exploitation for novel device functionalities.

Between 2017 and 2019, the CReA published 25 articles in peer-reviewed journals. The revenue from project grants totalled approx. 630 k€ (∅ 210 k€ p.a.), with 450 k€ from the DFG, and 110 k€ from federal and *Länder* governments. In addition, five patents were granted and the CReA applied for one more. In the same period, one doctoral degree was completed.

<u>CReA Intersubband Emitters: GaAs-based Quantum-Cascade Lasers</u>

[As of 31 December 2019: 5.2 FTE Research and scientific services]

The CReA focuses on the development of terahertz (THz) quantum-cascade lasers (QCLs) for high-resolution spectroscopy. The activities include the design, the growth, the fabrication, and the determination of the operating parameters for these lasers. For the design, the CReA developed a customized numerical model for carrier transport, which is being continuously extended and improved. The precise growth of THz QCLs is accomplished using molecular beam epitaxy with a spectroscopic in-situ growth control. In order to achieve sufficiently high output powers under continuous-wave operation and circular beam profiles, the CReA fabricates Fabry-Pérot lasers based on single-plasmon waveguides. In the past years, the CReA focused on GaAs/AlAs-based THz QCLs, which are currently covering frequencies between 2.2 and 5.7 THz, for real-world applications. An example is the development of THz QCLs for high-resolution absorption spectroscopy in order to determine the density of particular atoms and ions in plasma processes. Key challenges are the further increase of the wall plug efficiency to reduce the necessary cooling power and the increase of the operating temperature to achieve passive cooling.

Between 2017 and 2019, the CReA published 12 articles in peer-reviewed journals. The revenue from project grants totalled approx. 270 k€ (∅ 90 k€ p.a.), with 140 k€ from the DFG, and 130 k€ from the Leibniz Association. In addition, the CReA applied for three patents. In the same period, one doctoral degree was completed.

8. Handling of recommendations from the previous evaluation

PDI responded as follows to the 11 recommendations of the last external evaluation (highlighted in *italics*, see also statement of the Senate of the Leibniz Association issued on 17 July 2014):

1) Based on PDI's excellent material samples, many innovative ideas are generated for further research topics in the various Core Research Areas. However, the strategic guidelines should be more stringently defined as a reference for determining the development of research topics at PDI. The ***institute's strategy*** *2009 (Institutskonzept 2009) leaves too many open questions. The approach of using the institute's strengths in methodology as the basis for the long-term strategy is convincing. However, PDI must exploit its excellent methodological expertise and material samples to develop and select scientifically productive physical and methodological questions more systematically than it has so far.*

In cooperation with the Scientific Advisory Board, the institute strategy (*Institutskonzept)* was revised and updated in essential points on mission, scientific concept and strategy. Subsequently, the new version has been approved by the Board of Trustees of the Forschungsverbund Berlin e.V. (FVB) in 2018. Especially the strategy part was described in more detail and brought in line with the current scientific profile of the institute (for more details, see Chapter 2 and 3).

2) PDI should have an eye to ***industrially relevant applications*** *when making decisions on selecting scientifically productive questions. In order to determine strategic goals it would,* *therefore, be recommendable to consult with partners in industry. An attempt should be made to involve them in research projects to a greater extent than has been the case so far, both as active and, for example, as financially active participants in (co-)financing doctoral positions. At the same time, PDI should not shy away from stating clearly that its research can often only aim to develop new devices in the long term. Given the institute's emphasis on fundamental research and its comparatively small size, this is quite plausible.*

According to PDI, the institute has formed several strategic collaborations with major industrial partners, including Osram Opto Semiconductors, Micron Semiconductors Italia, and CreaTec Fischer & Co GmbH, a well-known German manufacturer of highly customized and application-oriented systems and components for ultra-high vacuum technology, molecular beam epitaxy, and low-temperature scanning tunneling microscopy/atomic force microscopy. These industrial partnerships play an important role to keep the focus of PDI's strategic goals on industrially relevant technologies. This approach is further supported by regular discussions with the industry representatives in PDI's Scientific Advisory Board.

*3) PDI should continue to increase the proportion of **third-party funding** in the budget.*

The proportion of third-party funds in the total budget of the institute has remained almost constant in recent years, with only minor fluctuations, although the total number of projects has slightly increased. PDI selects projects primarily on the basis that they fit into the current Core Research Areas or reflect potential research interests. According to PDI, the initiation of collaborations with renowned partners worldwide plays in this context a major role, in line with the respective updated institute strategy.

Alternatively, in order to possibly increase the share of third-party funding, the PDI is intensifying its efforts to offer its research infrastructure and service to small and medium-sized companies in the greater Berlin-Brandenburg area, whereby internal research work must not be affected by this—an approach that must be coordinated with the new director. PDI expects that these industry contacts should in turn open up new opportunities for the institute to acquire third-party funding.

*4) PDI must develop an **IT strategy**.*

The IT strategy primarily refers to the following three areas: Back-up systems, access control for PDI's intranet, and cybersecurity. Here, according to PDI, many substantial improvements have been made:

- PDI acquired a 'strongbox' for archiving scientific data which allowed to take this major portion of data volume out of the shared backup system of FVB, making it faster to recover and cheaper to operate. For long-term backup of all data PDI uses a combination of the backup system of FVB in Adlershof and a comprehensive tape-based backup system in a cooperative arrangement with the adjacent Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS).
- PDI runs its own intranet which is physically hosted at the institute. It includes a cloud-based data-sharing service, which is separated from the external internet and has restricted access for Institute's guests.

- The main responsibility for cybersecurity, as represented in the Institute's Sicherheitskonzept, has been taken over by the Forschungsverbund IT Services (FVB-IT) and was upgraded in recent years. The recently installed modern firewall at FVB protects all institutes from cyberattacks and serves as perimeter firewall for PDI. Incoming emails are scanned for viruses and malware by Deutsches Forschungsnetz (DFN). Through the membership with DFN, PDI (like all institutes of FVB) can issue certificates which are used to sign and encrypt emails and documents and to provide secure VPN connections where needed.

5) The institute should intensify its ***cooperation*** *with Berlin universities as well as with other non-university research institutions at home and abroad. Its material samples make it an extremely attractive partner. PDI is encouraged to use this notable expertise to approach other institutions more proactively than it has done in the past.*

PDI is directly linked to the *Humboldt-Universität zu Berlin* (HU Berlin) through a joint appointment of the director as a full professor with reduced teaching load (S-Professor). PDI is also associated with the Technische Universität Berlin (TU Berlin) through an extraordinary professorship (außerplanmäßige Professur) since 2001. In 2016, a PDI scientist became private lecturer (Privatdozent) at the *Freie Universität Berlin* (FU Berlin).

According to PDI, the number of externally funded large research networks in which PDI participates and collaborates with universities and non-university research institutes in Berlin, Germany, and Europe has been substantially increased:

- Leibniz ScienceCampus funded through the Leibniz Association: GraFOx (2016–2024)
- Cooperative projects funded by Bundesministerium für Bildung und Forschung: LETOIG (2015–2019), MILAS (2018–2021), InterPOL (2018–2021)
- Cooperative projects funded by the European Union: DEEPEN (2014–2016), SPRInG (2015–2018), SAWtrain (2015–2019), BeforeHand (2019–2021)

Within a number of individual projects funded by the DFG, PDI also collaborates with universities and non-university research institutes in Germany and worldwide.

6) The institute should specifically analyse which projects would be promising for involving companies – for example by financing doctoral positions. At present, this kind of ***collaboration with industry*** *is not being utilised.*

According to PDI, the institute actively approached major players like Robert Bosch GmbH and Osram Opto Semiconductors GmbH and learned that in view of the long time to market associated with the very fundamental character of PDI's research and the relatively low technology readiness level, collaborations are attractive for them only in the framework of externally funded research networks. PDI has pursued this route in EU projects. It has become obvious to PDI, however, that this might change considerably if the targeted partners are small and medium-sized regional enterprises (SMEs) and the cooperation involves access to PDI's research infrastructure and services. A first step is the successful start of the Application Laboratory Electron Tomography. Furthermore, an extension of operating hours of the semiconductor technology cleanroom with its postprocessing capacities may be realizable – in cooperation with SMEs to the benefit of both sides.

7) Even if the relatively low overall figures for women in physics in Germany are taken into account, ***very few women work at PDI****, irrespective of the level of academic qualification or hierarchy. The situation is unsatisfactory. The target quotas set by PDI when introducing the cascade model are not ambitious enough and must be increased.*

According to PDI, the institute is aware of this problem and actively promotes gender equality on the basis of recommendations by the Deutsche Forschungsgemeinschaft and the Leibniz-Gemeinschaft and is implementing the essential features of the 'Implementation Agreement on equal opportunitites' for the Leibniz-Gemeinschaft (Ausführungsvereinbarung Gleichstellung). The institute has an equal opportunity commissioner and a deputy.

According to PDI, its family-friendly policy is very well received – having a number of male and female staff making use of maternal/paternal leave possibilities and the flexibility of 'team-consensus flexible working hours' – which allows for an adaptation of the personal working hours that is aligned with the necessities of work in the research team.

PDI supports flexible solutions that facilitate a life-work balance. Individual agreements on working hours are possible. Important institute meetings and seminars are terminated before 4 pm to enable parents to pick up children from child care or to assist other family members. PDI is certified and re-certified by BerufUndFamilie GmbH.

In the area of technical personnel, the proportion of female staff has already risen to over 50 %; the quota of female doctoral students is a remarkable 40 %.

8) It should be possible to attract ***more doctoral candidates*** *in working at PDI. As only a few scientists at PDI are entitled to supervise doctorates, cooperation should be sought with university teachers.*

According to PDI, the number of doctoral students has been increased from 20 in 2015 to 30 in 2017 (cumulative values). In 2019, the number of students dropped again somewhat because of the impending change of director. The majority of students obtain their doctorates at the HU Berlin, but there are also a few doctoral theses that are carried out in connection with the TU and FU Berlin.

9) PDI's doctoral candidates should be part of a ***structured doctoral programme****. PDI does not necessarily have to create such a programme on its own but could do so in cooperation with a university and possibly other institutions.*

All doctoral students have access to the Graduate School of the HU Berlin that offers a wide variety of lectures and training programs. In addition, a large number of students has been involved in the programs offered within research networks such as SAWTrain, SPRInG, and GraFOx. Currently, PDI is involved in the preparation of an application to the DFG for a Research and Training Group (*Graduiertenkolleg*) organized by HU Berlin.

10) It is recommended to establish ***discussion and decision-making structures*** *to extend the existing informal mechanisms. In this context the following issues should be defined: how long-term strategies are declared to be binding, who is responsible for implementation and at which level (entire institute, Core Research Area), and at which intervals decisions and results should be evaluated.*

Long-term strategies have been defined in the new institute's strategy (*Institutskonzep*t), in whose drafting all senior scientists were involved. Scientific goals are continuously developed within the CReAs and described annually in the official program budget document, which is subsequently approved by the director, the Scientific Advisory Board, and the Board of Trustees. An intensive exchange of ideas on future research topics and projects are initiated and discussed upon primarily at the regular CReA meetings and decided by CReA managers. Following the institute seminars and colloquia, discussions are continued across CReAs, which can then lead to new cooperative projects. Proposals for third-party projects are planned by senior scientists, and they organize and implement the projects within the CReA as principal investigators. The decision on project applications is discussed between the director and the department heads.

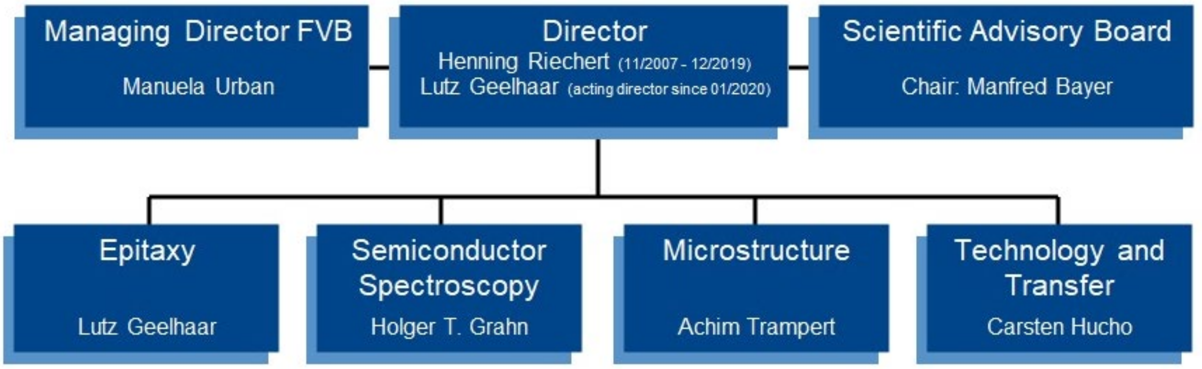
11) Given the size of the institute the process of determining long-term strategies is made potentially more difficult at present by the almost overly-complex ***matrix structure****. The establishment of Core Research Areas at PDI is convincing and has proved its worth. It should be examined whether it is still necessary to perpetuate the department structure with responsibility for staff and budgeting that exist beside the CReAs.*

According to PDI, the institute is organized in a matrix structure consisting of departments and CReAs that ensures both, the indispensable long-term basis in research infrastructure and a highly flexible environment that allows a quick adjustment of the research focus. It has been approved by the Scientific Advisory Board as extremely suitable. It simply reflects the basic idea that research projects are not defined within the boundaries of (personnel) departments but rather cut across them.

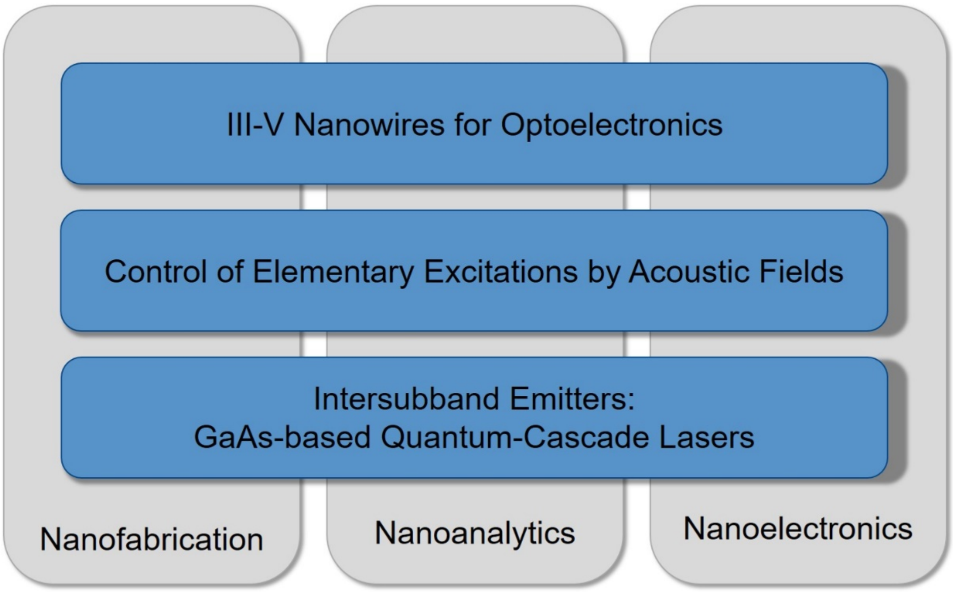
Appendix 1

Organisational Chart

i) Organizational Structure (four Departments)



ii) Research Structure (six Core Research Areas, three defined by methods, three by topics)



iii) Matrix Structure (four Departments working together in six Core Research Areas)

CReAs → / Depart-ments ↓	Nanofabrication	Nanoanalytics	Nanoelectronics	III-V Nanowires for Opto-electronics	Control of Elementary Excitations by Acoustic Fields	Intersubband Emitters: GaAs-based Quantum-Cascade Lasers
Epitaxy						
Microstructure						
Semiconductor Spectroscopy						
Technology and Transfer						

Appendix 2

Publications

Type of publication	2017	2018	2019
Monographs			
Individual contributions to edited volumes	2	2	3
Articles in peer-reviewed journals	91	66	76
Articles in other journals	1		
Working and discussion papers		4	
Editorship of edited volumes			

Industrial property rights

	2017	2018	2019
Patents (granted / applied)	-/6	8/5	3/3
Other industrial property rights (granted / applied)			
Exploitation rights / licenses (number of patents covered)			

Appendix 3 Revenue and Expenditure

	Revenue	2017 k€	2017 %	2017 %	2018 k€	2018 %	2018 %	2019 k€	2019 %	2019 %
Total revenue (sum of I., II. and III.; excluding DFG fees)		**11, 877.3**			**11, 759.6**			**11, 572.2**		
I.	**Revenue (sum of I.1., I.2. and I.3)**	**11, 483.6**	100 %		**11, 404.5**	100 %		**11, 347.1**	100 %	
1.	INSTITUTIONAL FUNDING (EXCLUDING CONSTRUCTION PROJECTS AND ACQUISITION OF PROPERTY)	9, 348.7	81 %		9, 482.2	83 %		9, 577.7	84 %	
1.1	Institutional funding (excluding construction projects and acquisition of property) by Federal and *States* governments according to AV-WGL	9, 348.7			9, 482.2			9, 577.7		
1.2	Institutional funding (excluding construction projects and acquisition of property) not received in accordance with AV-WGL									
2.	REVENUE FROM PROJECT GRANTS	1,803.8	16 %	100 %	1,871.9	16 %	100 %	1,697.0	15 %	100 %
2.1	DFG	317		15 %	309,6		16 %	706,8		40 %
2.2	Leibniz-Gemeinschaft (competitive procedure)	177,2		8 %	542,1		28 %	402,4		23 %
2.3	Federal, *States* governments	491,4		23 %	396,1		21 %	388,7		22 %
2.4	EU	796,9		38 %	615,4		32 %	177,8		10 %
2.5	Industry	10		1%						
2.6	Foundations	11,3		1%	8,7			21,3		1%
3.	REVENUE FROM SERVICES	331,1	3%		50,4			72,4	1%	
3.1	Revenue from commissioned work	11,1			7,7			1,2		
3.2	Revenue from publications									
3.3	Revenue from exploitation of intellectual property for which the institution holds industrial property rights (patents, utility models etc.)									
3.4	Revenue from exploitation of intellectual property without industrial property rights									
3.5	Revenue from other services: dissemination events	320			42,7			71,2		
II.	**Miscellaneous revenue** (e.g. membership fees, donations, rental income, funds drawn from reserves)	**393,7**			**355,1**			**225,1**		
III.	**Revenue for construction projects** (institutional funding by Federal and *States* governments, EU structural funds, etc.)									

	Expenditures	2017 k€	2018 k€	2019 k€
Expenditures (excluding DFG fees)		**9, 753.5**	**9,845**	**9, 804.1**
1.	Personnel	5, 753.6	5, 640.3	5, 599.8
2.	Material expenses	2, 467.2	2, 825.5	2, 344.1
2.1	*Proportion of these expenditures used for registering industrial property rights (patents, utility models etc.)*	25	56,3	52,1
3.	Equipment investments	820,6	796,2	807,9
4.	Construction projects, acquisition of property			
5.	Other operating expenses	712,1	583	1, 052.3
DFG fees (if paid for the institution – 2.5% of revenue from institutional funding)		231,3	235,8	238,3

Appendix 4

Staff

(Basic financing and third-party funding / proportion of women (as of: 31 December 2019))

	Full time equivalents		Employees		Female employees		foreigners
	Total	on third-party funding	Total	on temporary contracts	Total	on temporary contracts	Total
	Number	Percent	Number	Percent	Number	Percent	Number
Research and scientific services	**46.54**	**31**	**53**	**59**	**7**	**86**	**20**
1st level (scientific directors)	1	0	1	0			
2nd level (department heads)	3.5	0	4	0			
3rd level (group leaders or equi.)							
Junior research group leaders (if applicable)							
Further academic staff in executive positions							
Scientists in non-executive positions (A13, A14, E13, E14 or equivalent)	32.80	30	34	50	2	50	15
Doctoral candidates (A13, E13, E13/2 or equi.)	9.24	50	14	100	5	100	5
Service positions	**25.79**	**3**	**27**				
Laboratory (E13 senior service)	0.82	0	1				
Laboratory (E9 to E12, upper-mid-level service)	13.97	6	15				
Laboratory (E5 to E8, mid-level service)	2	0	2				
Workshops (E9 to E12, upper-mid-level service)	1	0	1				
Workshops (E5 to E8, mid-level service)	3	0	3				
Library (E9 to E12, upper-mid-level service)	1	0	1				
Information technology - IT (E9 to E12, upper-mid-level service)	1	0	1				
Information technology - IT (E5 to E8, mid-level service)	1	0	1				
Building service (E5 to E8, mid-level service)	2	0	2				
Administration	**6.27**	**0**	**7**				
Head of the administration	0.5	0	1[1]				
Staff positions (from E13, senior service)	2	0	2				
Internal administration (financial administration, personnel etc.) (E9 to E12, upper-mid-level service)	3.77	0	4				
Student assistants	0.59	64	2				
Trainees	**1**	0	1				
Scholarship recipients at the institution	**1**	0	1				1
Doctoral candidates							
Post-doctoral researchers	1	0	1				1

[1] Same person as one of the department heads listed under "Research and scientific services".

14 July 2021

Annex B: Evaluation Report

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

Contents

1. Summary and main recommendations

The Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e. V. (PDI) explores epitaxial materials with new functionalities, with the aim of developing innovative semiconductor devices for future information technologies. The PDI's particular unique feature is its long-term expertise in molecular beam epitaxy (MBE), a technique that allows controlled growth of tailored structures with atomic precision. The PDI's research is organised in four departments, which together address six Core Research Areas (CReAs). All CReAs work successfully in clearly defined areas of competence and produce results that are very important also for work taking place outside the PDI.

The research work carried out in the CReAs is very good, and at times excellent, and is based on outstanding research infrastructure. Its instruments and equipment in the area of molecular beam epitaxy in particular set the institute apart, even by international standards. Based on its research work, the PDI successfully transfers results into technological applications. In particular, the excellent material samples produced at the PDI are in high demand even outside the institute. The same applies to devices developed at the PDI, in particular the terahertz quantum-cascade lasers (QCLs), which are used e.g. for astronomical investigations, such as the detection of oxygen in the thermosphere of Mars. In addition, the PDI's work regularly leads to patent applications.

In 2018, the PDI developed its strategic guidelines further, as recommended during the last evaluation. However, strategic development stalled in 2019 when the long-serving and very successful director retired and the institute was unable to fill his post. The PDI is currently still under the provisional leadership of a department head. He is doing a very good job. The individual CReAs have been able to continue successfully with their research work and the initial ideas regarding an overarching direction for the PDI, with a focus on quantum technology, certainly make sense. However, these and other strategic issues with regard to the PDI as a whole cannot be pursued without the new PDI director in post.

Against the backdrop of the directorship vacancy, it is understandable that the posts of four senior scientists who have left in the meantime have not yet been filled. However, since the PDI is a comparatively small institute (47 full-time equivalents in research and scientific services, see chapter 5), this presents another serious obstacle to its further development. Another important personnel decision is coming up in 2022, when one of the long-serving department heads will retire. Overall, the PDI is facing a period of far-reaching changes.

Special consideration should be given to the following main recommendations in the evaluation report (highlighted in **bold face** in the text):

Overall concept, activities and results (chapter 2)

1. The PDI's very good research results are regularly **published** in the relevant peer-reviewed journals and are highly visible in the respective scientific communities. The PDI does have the potential, however, to publish even more frequently in higher-ranking journals seen by an even broader readership.
2. It is good to see that the PDI plans to make its **outstanding infrastructure** even more widely accessible to medium-sized regional enterprises (SMEs). This should enable the

PDI to expand its collaboration with industry partners and so to further strengthen the translation of its research and development work into industrial application.

<u>Changes and planning</u> (chapter 3)

3. The planned **recruitment of a new scientific director** in a joint appointment procedure (W3 professor) with Humboldt-Universität zu Berlin will be of key importance for the further development of the PDI. The committees involved in the appointment must now complete the process quickly, as planned, and appoint a researcher with an excellent scientific track record to lead the PDI.

   Under the new director, the institute should develop an **overall strategy** as a framework to give the work of the six CReAs an even sharper focus on an overarching theme. In doing so, the PDI must keep an eye on the application potential of its research results. At the same time, particularly in new research fields, there will continue to be a need for a strong focus on basic research to start with. This is the only way to achieve real advances in innovation.

   The **senior scientist vacancies** must be filled as quickly as possible, in line with the overall strategy. Another important personnel decision is approaching in mid-2022, when one of the long-serving department heads is due to retire.

<u>Controlling and quality management</u> (chapter 4)

4. As part of its overall strategy, the PDI should clarify to what extent it should be trying to obtain funding for basic and applied research projects. The requirement to increase **third-party funds** continues to apply. The scientific expertise, outstanding material samples and excellent research infrastructure provide the ideal conditions to achieve this. In addition to submitting further funding applications to the DFG, the PDI also has the potential to apply successfully for ERC grants. And at EU level, the FET Open (Future and Emerging Technologies) programme is a potential source of funding. In view of the increased focus on quantum technology, there are also many possibilities to apply for funds through calls for proposals issued by the German Federal Ministry of Education and Research (BMBF).

<u>Human resources (chapter 5)</u>

5. Thanks to its excellent instruments and equipment and stimulating scientific environment, the PDI offers outstanding conditions for training **doctoral candidates**. Against this background, a recommendation was made during the last evaluation to increase the number of doctoral candidates. As of 31 December 2012, there were 19 (incl. 3 scholarships). The number rose to 25 in 2017 and fell again following the retirement of the director to 14 on 31 December 2019. The PDI now needs to increase the number of doctoral candidates again.

6. Out of 53 employees in research and scientific services, 7 were female (13 %). 5 of the 14 doctoral students were female (36 %). Among the 34 scientists in non-executive positions, 2 were female (6 %). None of the leading scientists is female. The number of **female scientists** at the PDI is still too low. The PDI must take advantage of job vacancies,

especially the existing vacancies in leadership positions, to make significant improvements in this regard.

Cooperation and environment (chapter 6)

7. In order to further strengthen its university connections, the PDI should check, when it comes to filling department head positions in the future, whether **joint appointments** with a university are possible at this level too. This would also help increase the number of doctoral candidates at the PDI.

2. Overall concept, activities and results

Overall concept

The Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e. V. (PDI) explores epitaxial materials with new functionalities, with the aim of developing innovative semiconductor devices for future information technologies. The PDI's particular unique feature is its long-term expertise in molecular beam epitaxy (MBE), a technique that allows controlled growth of tailored structures with atomic precision.

The PDI's research is organised in four departments, which together address six Core Research Areas (CReAs). The first three CReAs are characterised by a focus driven primarily by scientific methods, and the last three CReAs are defined by a focus on a specific research topic. All the CReAs achieve very good results in clearly defined niche areas of competence that are also highly significant for work conducted outside the PDI. This work not only leads to scientific publications, but also to patents, material samples and scientific devices (see below).

Activities and results

Research

The PDI's research performance is very good, and at times excellent. Highlights worth mentioning include wide-band gap semiconducting oxides such as Ga_2O_3, a new compound which has been predicted to outperform GaN and SiC as a materials basis for high-power electronics. Other very successful research has shown that surface acoustic waves (SAWs) can modulate the optical properties of light emission centres in hexagonal boron nitride (h-BN). These results are promising in terms of future quantum technology applications. Another example is the institute's many years of research in the field of quantum cascade lasers (QCLs), which is reflected in scientific publications and in the development of innovative devices that are in high demand (see below under 'Transfer').

The PDI's very good research results are regularly published in the relevant peer-reviewed journals and are highly visible in the respective scientific communities. The PDI does have the potential, however, to publish even more frequently in higher-ranking journals seen by an even broader readership.

Infrastructure

The PDI has outstanding research infrastructure. Its instruments and equipment in the area of molecular beam epitaxy in particular, which include a semiconductor technology cleanroom, set the institute apart, even by international standards.

In addition, the PDI operates the PHARAO beamline of the BESSY II synchrotron at Helmholtz-Zentrum Berlin. This gives the PDI excellent possibilities to analyse material samples and growth processes. It is good to see that the PDI has provided access for external researchers to use the beamline, following a recommendation in the last evaluation.

Furthermore, in 2019, with support from the European Regional Development Fund and grants from the Berlin Senate, the PDI established a new Application Laboratory for Electron Tomography. This gives the PDI the possibility to further develop the electron tomography method in the field of semiconductor technologies and photonics.

It is good to see that the PDI plans to make its outstanding infrastructure even more widely accessible to medium-sized regional enterprises. This should enable the PDI to expand its collaboration with industry partners and so to further strengthen the translation of its research and development work into industrial application (see below).

Transfer

Based on its research work, the PDI successfully carries out various forms of knowledge and technology transfer. In particular, the excellent material samples produced at the PDI provide the basis for various further research projects, both inside and outside the PDI.

Worth highlighting also is the development of terahertz quantum cascade lasers (QCLs), which are used e.g. for astronomical research, such as detecting oxygen in the thermosphere of Mars and measuring the velocity distribution of gas clouds in star-forming regions. Since 2014, the PDI's QCLs have been operated in the German REceivers for Astronomy at Terahertz Frequencies (GREAT/upGREAT) during approximately 50 missions on board the Stratospheric Observatory For Infrared Astronomy (SOFIA). The PDI has provided 30 QCLs to partners within the framework of externally funded projects, and 6 to other research groups for testing applications. Furthermore, 5 QCLs have been sold to companies or research institutes.

In addition, the PDI's work regularly leads to patent applications. The institute pursues a coherent patent strategy. Between 2017 and 2019, 11 patents in 5 patent families were granted, 14 patents in 7 patent families were filed, and 6 patents in 4 patent families were given up.

3. Changes and planning

Development since the previous evaluation

Since the last evaluation, the PDI's research work in the individuals CReAs has continued successfully. The CReA for Ferromagnet-Semiconductor Hybrid Structures was closed in

2017 and in 2020 a new CReA for Nanoelectronics was established. The realignment achieved by this move makes sense.

In 2018, the PDI also developed its strategic guidelines further, as recommended during the last evaluation. However, strategic development stalled in 2019 when the long-serving and very successful director retired and the institute was unable to fill his post. The PDI is currently still under the provisional leadership of a department head. He is doing a very good job and the initial ideas regarding an overarching direction for the PDI with a focus on quantum technology certainly make sense. However, these and other strategic issues with regard to the PDI as a whole cannot be pursued without the new PDI director in post.

Against the backdrop of the directorship vacancy, it is understandable that the posts of four senior scientists who have left in the meantime have not yet been filled. However, since the PDI is a comparatively small institute (47 full-time equivalents in research and scientific services, see chapter 5), this is another serious obstacle to its further development. Another important personnel decision is approaching in 2022, when one of the four long-serving department heads is due to retire. Overall, the PDI is facing a period of far-reaching changes.

Strategic work planning for the coming years

The planned recruitment of a new scientific director in a joint appointment procedure (W3 professor) with Humboldt-Universität zu Berlin will be of key importance for the further development of the PDI. The committees involved in the appointment must now complete the process quickly, as planned, and appoint a researcher with an excellent scientific track record to lead the PDI.

Under the new director, the institute should develop an overall strategy as a framework to give the work of the six CReAs an even sharper focus on an overarching theme. In doing so, the PDI must keep an eye on the application potential of its research results. At the same time, particularly in new research fields, there will continue to be a need for a strong focus on basic research to start with. This is the only way to achieve real advances in innovation.

The senior scientist vacancies must be filled as quickly as possible, in line with the overall strategy. Another important personnel decision is approaching in 2022, when one of the long-serving department heads is due to retire.

4. Controlling and quality management

Funding

The provision of <u>institutional funding</u> according to the administrative agreement between the Federal and *Länder* governments is sufficient to cover the PDI's current portfolio of activities. It has risen since the last evaluation from €7.9m (2012) to €9.6m (2019).

The PDI's level of <u>third-party funding</u> is still low. Although it increased from an average of €1.6m p.a. in 2010–2012 to an average of €1.9m p.a. in 2017–2019, third-party funding as a proportion of the total budget was only 17 % p.a. on average in 2017–2019, compared with 18 % p.a. in 2010–2012, because institutional funding increased more rapidly. Although more funds are now obtained from the EU and through the Leibniz Association's competition process, funds obtained from the DFG and from the Federal and *Länder* governments have fallen. A positive point to note is that, as before, DFG income has exceeded the DFG fee each year.

As part of its overall strategy, the PDI should clarify to what extent it should be trying to obtain funding for basic and applied research projects. The requirement to increase third-party funds continues to apply. The scientific expertise, outstanding material samples and excellent research infrastructure provide the ideal conditions to achieve this. In addition to submitting further funding applications to the DFG, the PDI also has the potential to apply successfully for ERC grants. And at EU level, the FET Open (Future and Emerging Technologies) programme is a potential source of funding. In view of the increased focus on quantum technology, there are also many possibilities to apply for funds through calls for proposals issued by the German Federal Ministry of Education and Research (BMBF).

Equipment and IT strategy

The PDI has outstanding equipment. Its instruments and equipment in the area of molecular beam epitaxy in particular set the institute apart, even by international standards. In order to ensure the equipment continues to be state of the art, there is a need for forward-looking financial planning. The PDI is well aware of this and has already presented initial ideas for two future investments. The plan for a facility for thermal laser epitaxy (TLE) appears more promising than the plan for a chamber with focused ion beam (FIB). It is to be welcomed that the PDI will not be pursuing these or other plans until the new director is in post.

As recommended during the last evaluation, the PDI has worked with the Forschungsverbund Berlin (FVB) to develop a coherent IT strategy, which now complies with current technical standards.

Organisational and operational structure

The organisational and operational structure of the institute has proved effective in recent years. The PDI's research is organised in four departments. Each department is managed by a department head, and together the four heads of department advise the director on scientific and technological matters. Together, the departments address six Core Research Areas (CReAs). The first three CReAs are characterised by a focus driven primarily by scientific methods, and the last three CReAs are defined by a focus on a specific research topic.

Quality management

The institute's quality management is well aligned with the established standards. The PDI follows the recommendations for good scientific practice as developed by the German Research Foundation (DFG) and adopted by the Leibniz Association. The PDI has introduced internal control mechanisms, e.g. establishing an internal review process that has to be followed before submitting a paper. These are welcome developments. It is also worth mentioning that the institute has developed an open access policy to remove barriers to access for the PDI's publications.

Quality management by the advisory board and supervisory board

The PDI's Scientific Advisory Board fulfils its mission conscientiously and fairly. In 2017, it conducted the audit that Leibniz institutions are expected to hold between two evaluations.

Together with six other Leibniz Institutes, the PDI is part of the Forschungsverbund Berlin (FVB), whose Board of Trustees fulfils its function as a supervisory body in an acceptable manner.

5. Human Resources

As of 31 December 2019, the PDI employed 53 people in research and scientific services (47 full-time equivalents [FTE]). This number has decreased from 62 at the time of the last evaluation (53 FTE). This downward trend is partly due to the fact that the number of positions in the service category increased over the same period from 24 to 27 (see Status Report, appendix 4). At the same time, some positions are currently vacant and will only be filled under the new scientific director.

Management

The PDI's four very experienced department heads are doing a good job. Since the former director left, one of the department heads has been acting as provisional director of the PDI. He is doing very well, which means research work in the individual CReAs has been able to continue successfully. However, it is not currently possible to address strategic issues that concern the PDI as a whole.

The procedures for appointing the director as a university professor are defined in the guideline on joint appointment procedures of the institutes in the Forschungsverbund Berlin (FVB). A joint appointment committee involving one of Berlin's universities and the FVB heads the search process. For the director, the connection to a university is mandatory. For department heads, a joint appointment is possible but not mandatory. At the current time, none of the department heads has been jointly appointed with a university (see recommendation in chapter 6).

Doctoral candidates and postdoctoral staff

Thanks to its excellent instruments and equipment and stimulating scientific environment, the PDI offers outstanding conditions for training doctoral candidates. Against this background, a recommendation was made during the last evaluation to increase the number of doctoral candidates. As of 31 December 2012, there were 19 (incl. 3 scholarships). The number rose to 25 in 2017 and fell again following the retirement of the director to 14 on 31 December 2019. The PDI now needs to increase the number of doctoral candidates again.

The pleasing temporary rise in the number of doctoral candidates also led to an increase in the number of completed PhD theses, which rose from 9 in 2010–2012 to 17 in 2017–2019. The median time to submission was approximately 4 years.

In line with a recommendation from the last evaluation, the doctoral researchers are now more closely integrated in structured doctoral programmes, such as the Graduate School at Humboldt-Universität zu Berlin, or in projects with third-party funding. The measures are supplemented with seminars within the institute that discuss the researchers' own results or new research topics.

With its diverse research infrastructure facilities, the PDI also offers excellent opportunities for postdocs. An average of 15 postdocs work at the PDI. While the institute aims to keep the best scientific staff as senior scientists by offering permanent positions, there is no tenure-track programme. Since 2017, 1 postdoc has taken up a permanent position (senior scientist) at the PDI. Furthermore, 2 senior scientists, 6 postdocs, and 1 doctoral student moved on to external leading positions in science (8) or industry (1).

Equal opportunities and work-life balance

Out of 53 employees in research and scientific services, 7 were female (13 %). 5 of the 14 doctoral students were female (36 %). Among the 34 scientists in non-executive positions, 2 were female (6 %). None of the leading scientists is female. The number of female scientists at the PDI is still too low. The PDI must take advantage of job vacancies, especially the existing vacancies in leadership positions, to make significant improvements in this regard.

The measures to support a better work-life balance are appropriate. In 2018, the PDI was re-certified by the 'berufundfamilie' audit. Because of the Covid-19 pandemic, the PDI offered extended options for mobile working and working from home. It is good to see that the institute is assessing to what extent these measures can remain in place once the pandemic is over.

6. Cooperation and environment

Cooperation with universities

The PDI is closely connected with Humboldt-Universität zu Berlin (HU Berlin) on the basis of a cooperation agreement. The contract regulates the joint appointment of the institute's director as a W3 professor. The appointment procedure for the position of the new scientific director is currently in progress.

The PDI also benefits from its association with Technische Universität Berlin (TU Berlin) through an extraordinary professorship (*außerplanmäßige Professur*) – a role assigned to the head of the Department of Semiconductor Spectroscopy since 2001. Furthermore, in 2016, a senior scientist became a private lecturer (*Privatdozent*) at Freie Universität Berlin (FU Berlin), where he teaches courses and conducts academic supervision. **In order to further strengthen its university connections, the PDI should check, when it comes to filling department head positions in the future, whether joint appointments with a**

university are possible at this level too. This would also help increase the number of doctoral candidates at the PDI.

A very welcome development is the establishment of the Leibniz ScienceCampus GraFOx (Growth and Fundamentals of Oxides for electronic application), which also involves the Leibniz Institute for Crystal Growth (IKZ) and the Fritz Haber Institute of the Max Planck Society, as well as HU Berlin and TU Berlin.

Other collaborations

The PDI cooperates very closely with Helmholtz-Zentrum Berlin (HZB). The research on the PHARAO beamline of the BESSY II synchrotron at the HZB is of particular importance here. Another fruitful long-term collaboration is with the German Aerospace Centre (DLR) in Berlin in the field of quantum cascade lasers.

Among the collaborations with industrial enterprises, one worth highlighting is the partnership with OSRAM in the field of nitride-based optoelectronic devices. The PDI also collaborates closely with a company called CreaTec in the area of scanning tunnelling microscopy. In addition, the institute is involved in various networks that promote the transfer of developments to industrial application, such as Optec-Berlin-Brandenburg (OpTecBB), a regional competence network for optical technologies and microsystems technology. The PDI should continue to strengthen its collaboration with industrial enterprises, as planned. In this context, it is good to see that the PDI is planning to make its outstanding infrastructure even more widely accessible to medium-sized regional enterprises (see chapter 2).

In addition, the PDI works with other national and international partners on projects that are often financed with third-party funding. The PDI’s standing in the global scientific community is also evident in the fact that between 2014 and 2019, a total of 162 scientists visited the institute under guest scholar agreements for a period of one week or longer, 55 of them for more than 3 months.

7. Core Research Areas of PDI

Core Research Area I: Nanofabrication

[12.31 FTE, of whom 9.67 FTE research and scientific services staff, and 2.64 FTE doctoral candidates]

Coordinated by the acting director of the PDI, CReA I very successfully investigates fundamental growth mechanisms and fabricates novel types of crystalline thin films and nanostructures. Together with the second large CReA (Nanoanalytics, see below), it has played a significant role in ensuring that the PDI is regarded as one of the leading institutes internationally in the field of molecular beam epitaxy (MBE) of III-As and III-N compound semiconductors. Since the last evaluation, the group has successfully started the epitaxy of various semiconducting oxides as an entirely new material class and also widened the range of 2D materials grown by MBE.

The very good research results are published in appropriate journals. However, the CReA has the potential for even more publications in high-ranking journals seen by an even broader scientific community. It is good to see that third-party funding has increased since the last evaluation. The Leibniz ScienceCampus GraFox funded by the Leibniz Association (see chapter 6) that conducts research into oxide electronics deserves a special mention here. Both the research results and the unique samples produced by the CReA offer outstanding opportunities to obtain additional third-party funding through the very competitive procedures run by the DFG, the EU and even the ERC.

The CReA's future plans are very reasonable. In particular, the plans to grow thick h-BN layers for UV light sources or perovskite oxides have a high potential for excellent results. They also offer possibilities to expand cooperative partnerships in academia and industry and further increase the international visibility of the CReA.

Core Research Area II: Nanoanalytics

[16.22 FTE, of whom 10.94 FTE research and scientific services staff, and 5.28 FTE doctoral candidates]

CReA II successfully analyses fundamental structure-property relationships of low-dimensional systems and nanoscale devices. The research results contribute to the fundamental understanding of physical growth processes and are also very important for the other CReAs. The research on the PHARAO beamline of the BESSY II synchrotron deserves a special mention. Here, X-ray diffraction (XRD) is used for the in-situ investigation of epitaxial layers during growth. It is good to see that an upgrade has been carried out to allow even higher resolutions and that the facility is now also available to external users. Another very positive development is the establishment of the new Application Laboratory for Electron Tomography, which opens up options for other innovative research work, such as the analysis of 3D interfaces using scanning transmission electron microscopy (STEM). The basic research relating to scanning tunnelling microscopy (STM) manipulation at the level of single atoms is very exciting. However, there are few links between this research and the CReA's other activities.

The CReA's very good research results are published in appropriate journals. As was the case at the last evaluation, this CReA obtains the highest amount of third-party funding within the PDI, especially from the DFG and at EU level. With its impressive research work, it should even be able to increase its third-party funding still further, for instance through funding from the ERC or within the EU's FET Open programme (Future and Emerging Technologies). It is good to see that the number of completed PhD theses has increased since the last evaluation.

The plans for the future make sense. They include research in the field of point defects and modelling by FEM (finite element method) and 3D reconstruction of the topology of buried interfaces with atomic resolution, e.g. using GaAs-based quantum cascade lasers. It is important that the group keeps an eye on the balance of theory and experiment, as planned.

Core Research Area III: Nanoelectronics

[established 2020, no key data]

The CReA for Nanoelectronics was first set up in 2020, following the closure of the very successful CReA for Ferromagnet-Semiconductor Hybrid Structures in 2017. The realignment achieved by this move makes sense. The topics selected for this new CReA are very promising and have a clear potential for excellent results. The group aims to explore quantum effects and quantum transport of electrons, as well as spins in artificial hetero- and nanostructures, ionic transport in solid electrolytes, and materials for topological insulators.

For the further development of the CReA, the number of different projects, which is still high, should be reduced to improve the coherence of the research work. The future profile of the CReA should be developed in line with the overall strategy of the new PDI director. The CReA should also check to what extent theoretical questions can be included in its work. In addition, collaboration with the other CReAs and with groups outside the PDI should be strengthened.

Core Research Area IV: III-V Nanowires for Optoelectronics

[6.12 FTE, of whom 5.46 FTE research and scientific services staff, and 0.66 FTE doctoral candidates]

CReA IV conducts research into III-V nanowires and uses the results to develop optoelectronic applications with new properties and functions. Since the last evaluation, the work on GaN and GaAs nanowires and further heterostructures grown by MBE has led to very good fundamental results, e.g. the controlled strain bending of nanowires. The CReA is one of the leading groups internationally in this field. Its work in the field of photocathodes for CO_2 reduction is also interesting, but rather peripheral.

The CReA's very good research results are published appropriately, but the CReA has the potential to publish even more frequently in highly visible journals. It is good to see that the research results are reflected in a large number of patents as well. Third-party funding has risen slightly since the last evaluation, but there is still potential for further increases. The number of doctoral candidates should also be increased again.

The plans for the future make sense. Among other things, they envisage the manufacture of faster optoelectronic devices by strain relief and metallic and graphene substrates for power electronics. These projects have a high application potential, especially in the field of quantum technology and are therefore also extremely interesting for industry partners. The CReA should check to what extent the growth of GaN nanowires on metals as an important alternative to graphene can be extended to other materials.

Core Research Area V: Control of Elementary Excitations by Acoustic Fields

[6.19 FTE, of whom 5.53 FTE research and scientific services staff, and 0.66 FTE doctoral candidates]

CReA V regularly produces excellent research results pertaining to the control of elementary excitations by acoustic fields. It is one of the leading research groups in this field internationally and, as a result, is in demand as a cooperation partner even at international level. Research that deserves a particular mention includes the work on super-high frequency acoustic generation as well as the resulting interactions with materials and microstructures. The CReA is pursuing a very coherent work programme with a good balance between basic and applied research. The results are used in the fields of photonics, optomechanics and magnetoacoustics.

The outstanding research results are very well publicised and are highly visible in the scientific community. It is also very good to see that the research work regularly leads to patent applications. Research is excellently complemented by third-party funded projects. Based on its impressive research achievements, the CReA has the potential to acquire more third-party funding from the DFG and at EU level. This would also mean that it could employ more doctoral researchers.

The group's future plans make sense. On the one hand, they are based on very relevant technological aspects, e.g. acoustic modes in planar acoustic waveguides. And on the other, they include basic research on the use of bound excitons or the acoustic control of colour centres.

Core Research Area VI: Intersubband Emitters: GaAs-based Quantum-Cascade Lasers

[5.20 FTE, of whom 5.20 FTE research and scientific services staff]

CReA VI has a long and outstanding international track record in the research and development of terahertz quantum-cascade lasers (QCLs). This excellent work includes the design, growth and fabrication of GaAs/(Al,Ga)As QCLs as well as determination of the operating parameters. Some of the results have been achieved through a long-standing, very fruitful collaboration with the German Aerospace Centre (DLR). The lasers they have developed are used e.g. in the German REceiver for Astronomy at Terahertz Frequencies (GREAT) in the Stratospheric Observatory for Infrared Astronomy (SOFIA).

The research results are regularly published in very good journals. Important results from this CReA also include the provision of over 30 QCLs for partners in science and industry and the sale of a further five QCLs. The applied research offers very good opportunities for increasing third-party funding, especially from industry partners. The number of doctoral candidates should be increased.

The further development plans make sense. In particular, increasing the working temperature of the QCLs is a technologically important target. The aim should be to unlock new fields of application for QCLs through further developments. Other intersubband devices should also be researched. In addition, the CReA should assess to what extent further strategic collaborations, like the new partnership with the Laboratoire National des Champs Magnétiques Intenses (LNCMI) in France, could be beneficial when it comes to implementing the plans.

8. Handling of recommendations of the last external evaluation

The PDI has addressed the recommendations from the last evaluation in a satisfactory manner, but since the director retired in 2019, the PDI is still in a transition phase. In parts, the recommendations made by the Leibniz Association Senate in 2014 (see Status Report, pp. A-18ff) still apply.

Appendix

List of Participants

1. Review Board

Chair (Member of the Leibniz Senate Evaluation Committee)

Roland **Sauerbrey**	Helmholtz-Zentrum Dresden-Rossendorf

Deputy Chair (Member of the Leibniz Senate Evaluation Committee)

Hans-Peter **Seidel**	Max Planck Institute for Informatics, Saarbrücken

Reviewers

Katharina **Al-Shamery**	Institute of Physical Chemistry, University of Oldenburg
Ulrike **Diebold**	Institute of Applied Physics, TU Wien, Austria
Catherine **Gourdon**	Institut des NanoSciences de Paris (INSP), France
Moïra **Hocevar**	Institut Néel CNRS, Grenoble, France
Edmund **Linfield**	School of Electronic and Electrical Engineering, University of Leeds, UK
Daniel **Neumaier**	School of Electrical, Information and Media Engineering, University of Wuppertal
Michael **Oestreich**	Institute of Solid State Physics, University of Hannover
Josef **Zweck**	Institute of Experimental and Applied Physics, University of Regensburg

Representative of the federal government

Volker **Wiesenthal**	Federal Ministry of Education and Research, Bonn

Representative of the Länder *governments (Member of the Leibniz Senate Evaluation Committee)*

absent with apologies

6 August 2021

Annex C: Statement of the Institution on the Evaluation Report

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

PDI thanks the members of the Review Board for their comprehensive assessment and their flexibility to carry out the evaluation process despite the extraordinary conditions imposed by the pandemic. We appreciate the highly valuable, constructive feedback.

We are very pleased with the truly positive evaluation result, which encourages our scientists and support staff to continue striving for excellence in our scientific work. Particularly motivating for us is that our research infrastructure has been assessed as “outstanding”, which will help us to attract exceptional doctoral candidates, postdoctoral scholars, and visiting scientists also in the future.

We are very grateful that the Review Board has recognized PDI’s transition phase at the time of the evaluation - the position of the institute director had been vacant for an extended period of time. We are therefore delighted to announce that Prof. Roman Engel-Herbert has started as the new PDI director July 1st, 2021. We are already engaged in inspiring exchange to refine the scientific strategy for the institute including new research activities beyond the current portfolio. Many elements of an evolving overall strategy have been presented at the evaluation and gained the support of the Review Board.

We welcome and value the additional recommendations provided in this evaluation report as a constructive and stimulating input that we will take into account in our ongoing discussions to shape a scientifically prosperous future for PDI.