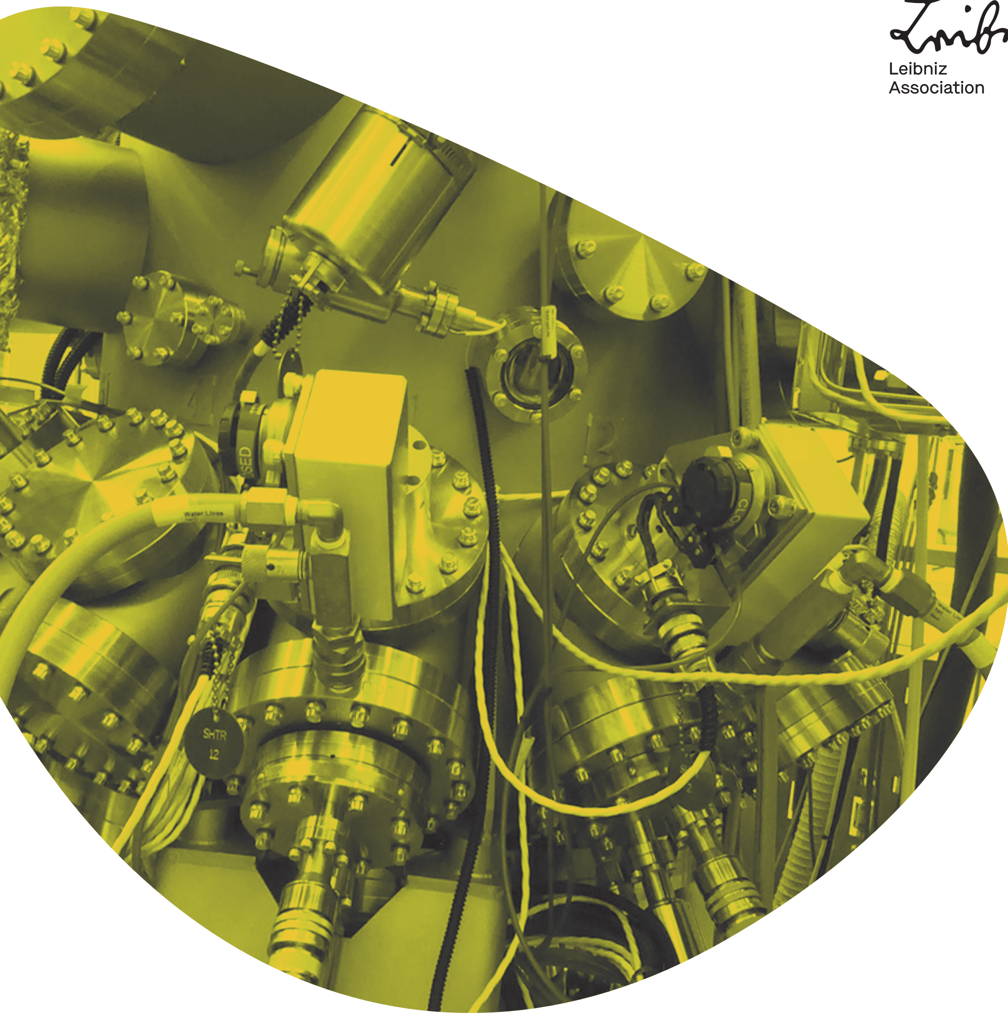

Light, Matter, Information

Section "Mathematics, Natural Sciences, Engineering"

01 Introduction

04 Research focus areas of the section “Mathematics, Natural Sciences, Engineering”

- Communication technologies and microelectronics
- Quantum technologies and space applications
- Materials research, materials and process engineering, nanotechnology
- Optics and photonics
- Biotechnology and living matter
- Biomedical research and health technologies
- Astrophysics and Earth’s atmosphere
- Mathematics and modelling
- Artificial intelligence
- Digital transformation, research data management and infrastructures

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Introduction

New technologies and materials are essential drivers of economic progress in a modern industrial society. They safeguard our standard of living and lay the foundations for meeting future challenges – such as the energy transition, digitalisation, modern global communication networks, climate change, or an ageing society.

The Section "Mathematics, Natural Sciences, Engineering" of the Leibniz Association is ideally positioned to address challenges such as these in an interdisciplinary manner and to offer flexible solutions. It not only conducts excellent research, but also provides the necessary information infrastructures, technology platforms, and venues for scientific exchange. This includes developments at the interface of physics, life sciences, materials science, and engineering that open up new options in the future fields of energy, health, and sustainable production, and forge new value chains. Its institutes complement fundamental research at the highest level with application-oriented topics through to tested products. Efficient concepts for knowledge and technology transfer facilitate the translation of research results – for example in the medical field, in energy, climate and environmental technology, or in the mobility and microelectronics sectors.

This brochure presents the connecting thematic clusters of research within the section:

- **Communication technologies and microelectronics**
- **Quantum technologies and space applications**
- **Materials research, materials and process engineering, nanotechnology**
- **Optics and photonics**
- **Biotechnology and living matter**
- **Biomedical research and health technologies**
- **Astrophysics and Earth's atmosphere**
- **Mathematics and modelling**
- **Artificial Intelligence**
- **Digital transformation, research data management and infrastructures**

Across sections, the institutes collaborate significantly within the Leibniz Research Alliances "Health Technologies", "Advanced Materials Safety", and "INFECTIONS" with other Leibniz institutes.

Further synergies arise within the Leibniz Research Networks "Mathematical Modelling and Simulation" (MMS), "Stem Cells and organoids", "Bioactive Compounds", "Preservation", "Earth and Societies", "Leibniz-Data", "Evidence-Based Science Communication", "Central and Eastern Europe", and "China".

The Leibniz institutes also collaborate closely with universities, for example in thematic Joint Labs and Leibniz ScienceCampi, and are furthermore embedded in numerous national and international cooperations with scientific institutions, research organisations, universities, and industry partners. They actively contribute to the Leibniz Labs "Pandemic Preparedness" and "Systemic Sustainability".

Technological sovereignty

Technological sovereignty, as a central topic in innovation policy for the coming decade, will sustainably transform and shape the European research and development landscape. Mastery of key technologies is the foundation for Europe's economic and political independence and societal resilience, grounded in our democratic values. Technological sovereignty rests on a delicate balance between dependency and autarky, and requires command of as many systemically interconnected competencies as possible along the value chain within the European Research Area.

Leibniz institutes of the section have joined forces on the topic of "Technological Sovereignty" in order to develop holistic contributions by the Leibniz Association to European solutions in this field. Key technological topics such as artificial intelligence, quantum technology, future communications, raw material dependencies, health technologies, smart factory, digitalisation, etc. are being developed in the form of Leibniz clusters of networked Leibniz institutes together with external partners from science, industry, and policy. They also take into account current framework programmes[1] of the Federal Government and address current challenges in the field of research and innovation.

The Leibniz Association positions itself as complementary to universities and other non-university research organisations. The central Leibniz approach consists of linking scientific and technological expertise in a systemic approach **from basic research through applied research to the tested product**.

One example of this is the collaboration between two Leibniz institutes (FBH and IHP) with institutes of the Fraunhofer-Gesellschaft in the Research Fab Microelectronics Germany (Forschungsfabrik Mikroelektronik Deutschland) and within the framework of the European Chips Act on the pilot line for "Advanced Packaging and Heterogeneous Integration for Electronic Components and Systems" (APECS).

A further component for securing technological sovereignty is the education and training of skilled professionals. The Leibniz institutes of the section are engaged in this regard both within their individual institutes and in national and international consortia.

1 See also the Framework Programme "Research and Innovation for Technological Sovereignty" of the Federal Ministry of Research, Technology and Space.

Research focus areas of the section “Mathematics, Natural Sciences, Engineering”

The strategic orientation of the section is articulated in nine research focus areas, which describe the competencies and infrastructures of the Leibniz institutes. With its **Hightech-Agenda**[2], the Federal Government has identified several key technologies that are at the centre of the section‘s research: **microelectronics**, **quantum technologies**, **artificial intelligence**, **biotechnology**, **fusion**, and **climate-neutral technologies**. The Leibniz institutes of the section, with their systemic approach from basic research to application, conduct research on technologies along complex value chains for Germany‘s technological sovereignty and the competitiveness of its scientific and economic landscape.

Communication technologies and microelectronics

In the coming years, the rapid development of **communication technologies** and the **digitalisation** of society will continue. In addition to new forms of communication between people, the wireless and autonomous exchange of information between objects, vehicles, and machines will far outpace this sector and become part of everyday life as the Internet of Things and Industry 4.0. This development brings new challenges for microelectronics and **communication technologies**: very high data rates, short response times, lower energy consumption, and new requirements regarding resilience and data security.

Classical approaches such as continued – but increasingly demanding – CMOS scaling (More Moore) continue to shape the further development of microelectronics. In the future, **quantum technologies**, neuromorphic, and sensory systems will significantly determine the performance and functionality of technical systems, complementary to CMOS technology. In these future-relevant thematic fields, the Leibniz institutes of the Section work across a spectrum from basic research through to the provision and testing of prototype solutions, thereby contributing significantly to the future technological sovereignty of Germany and Europe.

The Leibniz institutes of the section develop crystals, heterostructures, and microelectronic **semiconductor devices** and technologies based on

2 Direct references of the section‘s research topics to the Hightech Agenda are highlighted by yellow underlines.

silicon, compound semiconductors, and entirely new materials. In doing so, they have already achieved cut-off frequencies of up to approximately 700 gigahertz, opening up new possibilities for high-speed data transmission, radar, and sensing. Current research projects aim at even higher frequencies in the terahertz range and the integration of technologies and technology modules.

The technologies are used in institute-owned **pilot lines** for the fabrication of crystals, wafers, photonic components, circuits, laser diodes, and systems as prototypes for research projects. Small-batch production is carried out for industrial partners. Plasma-assisted processes for structuring, cleaning, and coating play a central role in the further development of micro- and nanoelectronic components.

Examples of new **communication systems** include Gigabit WLAN for data rates exceeding 100 gigabits per second at frequencies up to approximately 300 gigahertz, as well as wireless sensor networks and components for fibre-optic communication. In recent years, the integration of indium phosphide with silicon technologies has been demonstrated – an example of hybrid integration. Such solutions are applied primarily in wireless and broadband communication.

Entirely new possibilities arise from the closer integration of expertise in **microelectronics** with the research of more materials-oriented Leibniz institutes. These explore new oxide, metallic, organic, and hybrid functional and nanomaterials and structures that hold great potential for future micro- and nanotechnologies, in efficient power electronics, or for photonic-electronic integrated circuits. Aspects of integrated smart systems, nanoelectronics, and quantum computing are also being addressed.

Quantum technologies and space applications

Quantum technologies exploit the sometimes striking “peculiarities” of quantum physical phenomena compared to classical physics, in order to realise novel technical solutions in various fields such as **computing**, **communication**, and **sensing**. They are capable of both improving the performance of existing, conventional solutions and providing answers to problems for which no established approaches yet exist. The Leibniz institutes of the section work at different positions along the value chain of photonic and electronic technologies. The key technologies for such applications range from ‚quantum-grade‘ materials development, diode lasers, and hypersensitive detector systems to systems such as compact optical or even nuclear clocks of the next generation.

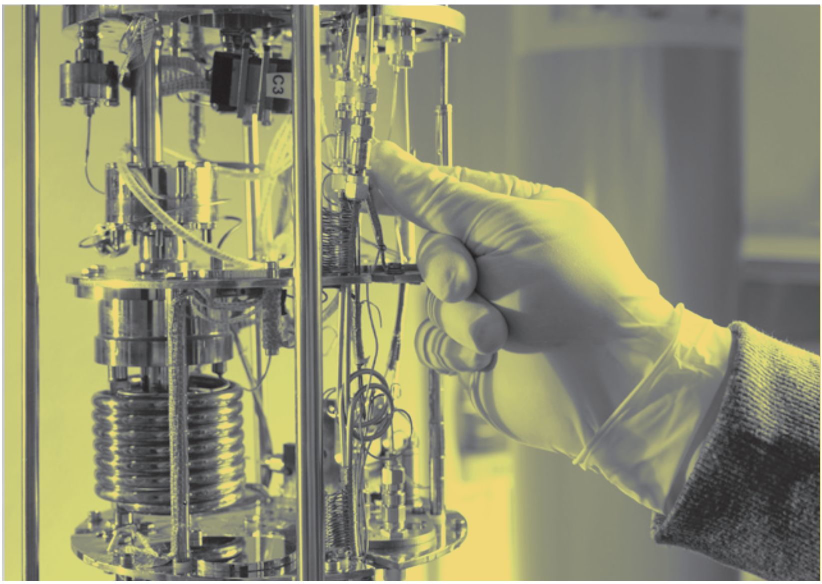
Quantum computers will solve pressing problems that cannot be addressed with classical computers: in the field of cryptography, for example, they are expected to be able to decrypt messages that are currently considered secure – with today‘s and near-future classical computers. They also enable eavesdropping-proof protocols. Developments for quantum information technology include, for example, isotopically pure semiconductor systems that exploit entangled electrons, or ultra-precise single-photon sources. These new emitters are to be realised on the basis of artificially controlled atomic defects – the so-called colour centres – in various semiconductor systems, such as diamond or silicon carbide. In addition, compact and robust high-power lasers with narrow and ultra-narrow linewidths, as well as their light control units, are indispensable for quantum computers based on neutral atoms and ions, as they enable future quantum network applications.

Further applications target sensing, since **quantum sensors** can achieve extreme measurement accuracies and previously unattainable sensitivities: from magnetic field detection for biophysical applications, through improved imaging in the mid-infrared range, to precise timekeeping for navigation – the innovations and realisations of quantum technologies will bring breathtaking new technological improvements. Their realisation is an active subject of research and translation at the Leibniz institutes of the section. The development of tailored quantum materials together with designer laser pulses is an important branch of research in which entirely new applications can be unlocked through extraordinary sensitivity.

Precision measurements test quantum theories and prepare the instrumentation of the next generation. For example, spectroscopy of simple systems advances quantum electrodynamics, quantum chemistry, and many-body theories.

Quantum technologies are also indispensable for demanding **space applications**. They are used in a variety of ways, including to detect mass movements on Earth and to measure the effects of climate change. Magnetometers, in turn, support planetary exploration, while optical atomic clocks lay the foundation for the next generation of global **navigation satellite systems**.

Leibniz institutes of the section possess comprehensive know-how and an excellent infrastructure to realise robust and high-performance materials, components, modules, and systems that meet the demanding conditions of space and quantum technologies.



Materials research, materials and process engineering, nanotechnology

Materials with new properties and functions are indispensable for the development of novel technologies. Topics of sustainability and the **circular economy**, as well as the **reduction of raw material dependencies**, are of particular importance. New materials enable system solutions in the chemical and pharmaceutical industries, in medical, communication, transport, and energy technology. They are also innovation drivers for mechanical and automotive engineering, as well as for rail transport and aerospace. In this context, coordinated process chains and comprehensive materials testing and analysis play a major role in engineering research, the findings of which find direct application in industrial practice.

The materials science Leibniz institutes of the section address the materials-oriented requirements of the future and investigate and further develop materials, explore processes, design and manufacturing methods, and thus focus on the entire spectrum from the smallest powder particles to large components. They research and develop **materials from different material classes**: functional materials with broad application potential in communication technology and biomedicine, as well as high-performance composite materials, nanostructured materials, polymers, and catalysts, which are particularly indispensable in lightweight construction, energy technology, and the chemical industry. Structural materials produced, for example, by additive manufacturing processes enable property profiles that previously seemed impossible and allow entirely new degrees of freedom in the design and use of innovative products. In addition, efficient material and catalyst syntheses, new sustainable raw materials, recycling strategies, and concepts of biomimetics and bioengineering play an important role within the research of these materials science Leibniz institutes.

A new field is the development of “light-plus-matter” materials, in which novel functions based on quantum effects can be realised. Complementing this are plasma-assisted coating, printing, and surface processes, which make decisive contributions both in additive manufacturing and in the development of environmentally friendly material systems.

The goal of the research is to holistically understand the complex structure-property relationships of materials and, in a close interdisciplinary interplay of natural and engineering sciences, to traverse the entire path from molecule to material and ultimately to component and system integration – with a view to concrete applications and in the spirit of the **circular economy** through to recycling at end of life. Associated with this is the development and provision of nanoscopic and in-operando characterisation techniques and complementary theoretical-physical modelling (Computational Materials Science and Digital Surface Engineering). Particular synergies and cross-sectional added value in **materials research** arise, on the one hand, through accelerated innovations via **research data management** and through the use of **artificial intelligence**; and on the other hand, through collaboration within the Leibniz Research Alliances "Health Technologies" and "Advanced Materials Safety".

The Leibniz Research Alliance **"Advanced Materials Safety"** has set itself the goal of creating safer and **more sustainable advanced materials** by integrating a holistic assessment of the sustainability and safety of advanced materials already at the level of material design. The research alliance combines expertise from the fields of materials development and assessment of the impacts of materials on human health and the environment. The focus is in particular on materials with applications in the fields of bioanalytics, nanomedicine, and energy. The modelling of their toxicological properties, the investigation of their effects through predictive models, molecular mechanisms, and accumulation studies is complemented by integrated data management, communication, and technology transfer. In this way, the transition from a reactive to a proactive approach in the field of safe and sustainable material design is being advanced.

Optics and photonics

Light and plasma are central research tools in the natural, engineering, and life sciences, and the foundation for photonic technologies. Tailored light across broad spectral and temporal ranges has massively expanded the application possibilities of photonic methods. It makes **photonics** one of the most important key and cross-cutting technologies for the 21st century.

Photonic technologies are applied in many fields, including the geo-, space, and life sciences, medicine, communication, quantum technologies, security applications, and data storage. Photonic research and technologies are among the most important innovation drivers for modern society and the economy.

The development of novel light sources and in particular new **laser systems** benefits many areas of science and technology. These include ultra-stable lasers with narrow linewidths, lasers with ultrashort pulses, and lasers emitting in new spectral ranges. It encompasses a wide variety of technologies, including crystals, semiconductors, fibres, and waveguides on photonic chips.

As a type of **laser system**, optical frequency combs are being developed across all regions of the electromagnetic spectrum, from the terahertz to the extreme ultraviolet range. Various photonic technologies are employed, from mode-locked lasers based on crystals or doped fibres to passive and active components on photonic chips. They are used for a wide variety of precision measurements and in quantum technology, from the frequency standard and clockwork mechanism for an optical clock to sensors in spectroscopy and length measurements.

The Leibniz institutes of the section work in a field ranging from the fundamental understanding of **light-matter interaction** on extreme temporal and spatial scales to optoelectronic devices and technical systems. Light-matter interactions are used to investigate materials and components, to shape surfaces and nanostructures, and to switch their properties. A particular potential for applications lies in the coordinated joint design of light and matter, through which entirely new functionalities for applications based on quantum effects can be realised, in direct interplay between photonics and materials research. Theoretical work and mathematical methods of analysis and simulation also play an important role.

In the **terahertz range** – i.e., in the electromagnetic spectrum at the transition from long-wave infrared radiation to electronic frequencies for wireless communication – fundamental optical and electrical material properties are investigated. Various diode lasers, such as quantum cascade lasers or high-power lasers, as well as novel detectors, are synthesised at the Leibniz institutes with atomic precision, optimised by means of theoretical analyses, and validated using the latest materials characterisation methods. Translated into next-generation devices, the results open up promising applications, for example in **security technology** at airports, in the exploration of the Earth's atmosphere and outer space, and in the development of cost-effective resilience systems for the protection of our public life.

The spectral range of **X-ray radiation** offers new possibilities for studying the atomic and electronic structure of materials in a time-resolved manner, thereby understanding dynamic processes on the atomic and nanometre scale that – beyond the fundamental gain in knowledge – can in future be used as mechanisms for realising novel applications, e.g. in the field of **quantum-based sensing**. Films with nanometre resolution allow functional components to be analysed and optimised.

Optical methods can be used in a versatile manner; the Leibniz institutes of the section develop new methods and push the boundaries of what is technically possible. Dual-comb interferometry extends the limits

of precision measurement in several areas. As a spectroscopic technique, it provides insight into the structure of matter or serves sensor applications, e.g. for environmental or health diagnostics. Further applications of interferometry include dimensional metrology of macroscopic objects with sub-nanometre accuracy. In the field of astrophysics, photonic methods – so-called astrophotonics – enable new approaches in the miniaturisation of optical elements, in order to gather new insights in space missions and to carry out precision measurements in spectroscopy and interferometry.

In the field of Earth's atmosphere, the Leibniz institutes develop special procedures for the use of **lasers**, the so-called "LiDAR" (Light Detection and Ranging). LiDAR is used to investigate the thermal and dynamic structure from the Earth's surface to the uppermost layer of the atmosphere, the thermosphere. The systems developed by Leibniz institutes achieve temporal and spatial resolutions that allow new insights into the global interplay of our planet and enable scientific predictions and a global understanding of the benefits of sustainable action on the habitability of our planet. Improved LiDAR systems secure the world-leading technological position in **autonomous driving**, as they are indispensable for distance measurement.

In parallel, the development of new **photonic systems** (plasma, light) is being pursued, including for environmental analytics, the exploration of plasma- and ion-assisted technologies for precision manufacturing of surfaces for optics and photonics, through to applications in medical technology, such as in devices for medical diagnostics and new forms of therapy, as well as applications in hygiene. Cold atmospheric pressure plasmas additionally enable novel combinations of photonic and plasma-based processes.

Further important research topics include the development of analytical methods for thin films and smallest material quantities, the development of compact diode lasers with high output power, new applications of plasma and laser technology in medicine, sensing, and process engineering, as well as the monolithic integration of light sources from III–V compound semiconductors into silicon technology. New technological and materials science challenges, such as the integration of optical photonic circuits on the scalable silicon technology platform, are being actively pursued, as is the synthesis and realisation of innovative quantum light sources based on entangled photons for use in medicine and environmental analytics.

Biotechnology and living matter

Biotechnological research in the section pursues complementary approaches to the integration of biological and technical systems, developing a broad spectrum of innovative materials in the process. A key focus lies on materials that directly interact with biological systems and modulate their behaviour therapeutically or functionally. These include responsive and adaptive polymer coatings for controlling cell adhesion and signal transduction, ions implanted in biomaterials for targeted modulation of the cellular microenvironment, and crosslinked functional hydrogels at interfaces suitable for tissue engineering, as dynamic cell niches, or as controlled release systems for bioactive molecules. These developments are complemented by new prosthetic materials with optimised mechanical performance and improved biocompatibility, used in regenerative medicine, as implant surfaces, or as intelligent drug depots.

Complementary to this, the section is increasingly focusing on living materials (Engineered Living Materials), in which bioprogrammed cells are embedded in materials and endow them with entirely novel properties. Through their biological component, these materials integrate functions such as adaptivity, growth, self-organisation, or metabolic activity. In the biomedical field, this gives rise to living therapeutic materials that continuously or on-demand produce and release therapeutic substances directly on site – self-refilling depots for sustainable, patient-individualised drug delivery. In parallel, living materials for sensing and structural applications are being developed, offering both novel bioprogrammed properties and sustainability advantages.

Both material worlds – synthetic materials for integration into biological systems, as well as materials programmed with living cells – complement each other and are being further developed towards application together with clinical and industrial partners.

Biomedical research and health technologies

Biophotonic and **bioanalytical technologies** open up new pathways for detecting biological changes precisely and at an early stage. They provide both detailed molecular information and high-resolution spatial and functional insights into tissues and cells. In doing so, they improve diagnostics, enable more accurate assessment of disease progression, and support well-founded prognoses. Overall, they strengthen the development of modern, personalised approaches in health technologies.

Biophotonics, with its focus on optical imaging and spectroscopy, concentrates on the development of application-oriented photonic methods with which biological structures and processes can be captured in a highly specific, sensitive, and non-invasive manner. Central are optical imaging and spectroscopic methods – from label-free spectroscopy (e.g. Raman/IR) through fluorescence and lifetime imaging to multimodal approaches – which are standardised and clinically evaluated, for both centralised and decentralised applications.

Bioanalytics has a focus on application-oriented method development to characterise biological processes more precisely at the molecular level, thereby enabling significant advances in health technologies with applications in the diagnostics, prognostics, and ideally prevention of diseases. A central area comprises high-resolution methods for the analysis of various molecular classes that contribute to the phenotype. Molecular imaging (imaging mass spectrometry) contributes significantly to visualising the spatial distribution of hundreds of different molecules at cellular resolution and to gaining a new perspective on the emergence of disease processes.

A particular profile of the section is the linking of these molecular and imaging methods into multimodal measurement strategies that combine chemical information with spatial and functional data. In addition, approaches to data integration are being developed to evaluate complex multi-omics and imaging data and to identify new diagnostic markers. In application-oriented projects, these technologies are used to better understand the mechanisms of cardiovascular diseases, inflammatory processes, tumour development, and infections.

Overall, the section contributes to providing innovative diagnostic procedures, improved progression analyses, and more precise prognostic instruments for medicine. At the same time, these new approaches for personalised medicine are to be transferred into clinical routines. The Leibniz institutes of the section develop standards, reference materials, and data pipelines for the transfer of prototypes into clinically validated instruments.

The section's research on the integration of biological and technical systems aims, among other things, to generate data for **modelling and simulation** – e.g. through the tailored evaluation of mass spectrometric, molecular (Next Generation Sequencing), massively parallel microarray data, and optical-spectroscopic data, including in point-of-care systems. Modelling and simulation allow experiments to be designed – or even avoided. They enable the prediction of experimental results in environmental and climate research and in medicine.

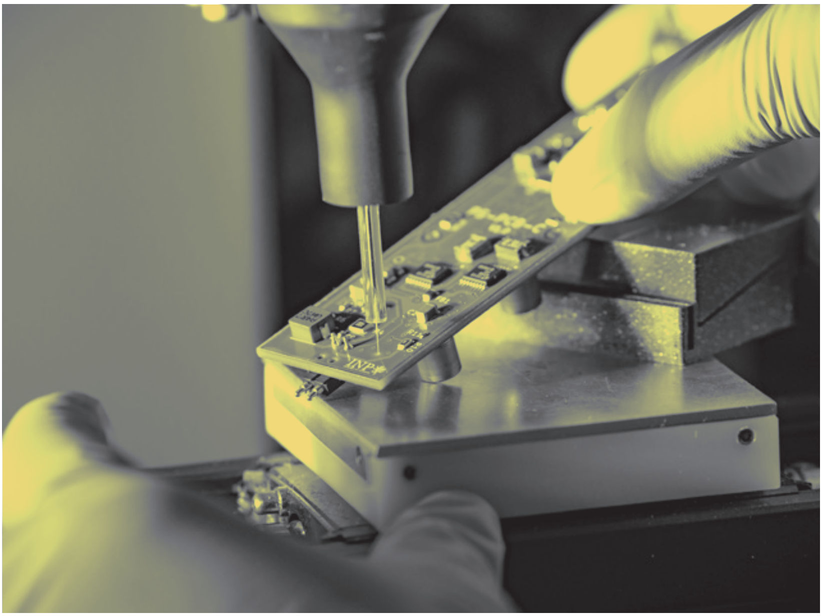
In order to bring research results to the health market more easily and quickly, the Leibniz institutes cooperate not only with other sections of the Leibniz Association, but also with clinical partners and frequently directly with companies. Together with Leibniz institutes from the sections "Economics, Social Sciences, Spatial Research" and "Life Sciences", they have furthermore founded the Leibniz Research Alliance "Health Technologies". This interdisciplinary exchange platform makes it possible to promote innovations in health technologies from basic research through to commercialisation, thereby accelerating **translation**. At the same time, accompanying research allows risks to be identified at an early stage.

The Leibniz Research Alliance "Health Technologies" is dedicated to five fields of competence. It researches and develops:

- reliable, cost-effective optical/photonic and non-photonic **point-of-care technologies** and screening methods for rapid diagnostics, such as for cancer, as well as risk assessment of age- and lifestyle-related diseases,
- more precise optical/photonic methods for highly specific and highly sensitive imaging,
- technologies for the detection of **biomarkers** for the early detection of lifestyle- and age-related diseases, such as cardiovascular or oncological diseases, differential diagnostics in multimorbidities, and the assessment of therapy progression,
- the use of plasma medicine, UV disinfection, and their combination with further optical technologies for **personalised treatment and therapy options** and prevention, whereby plasma sources for dermatological, oncological, and respiratory applications are transferred into the healthcare sector in close cooperation with clinical partners,

- new materials for tissue regeneration, real-time diagnostic, and personalised therapeutic applications.

Health technologies are established in the profile of the section, and the technologies and services of the participating Leibniz institutes hold great potential for life science and clinical research. They can help to treat and care for patients more effectively and to create a more efficient and effective healthcare system.



Astrophysics and Earth's atmosphere

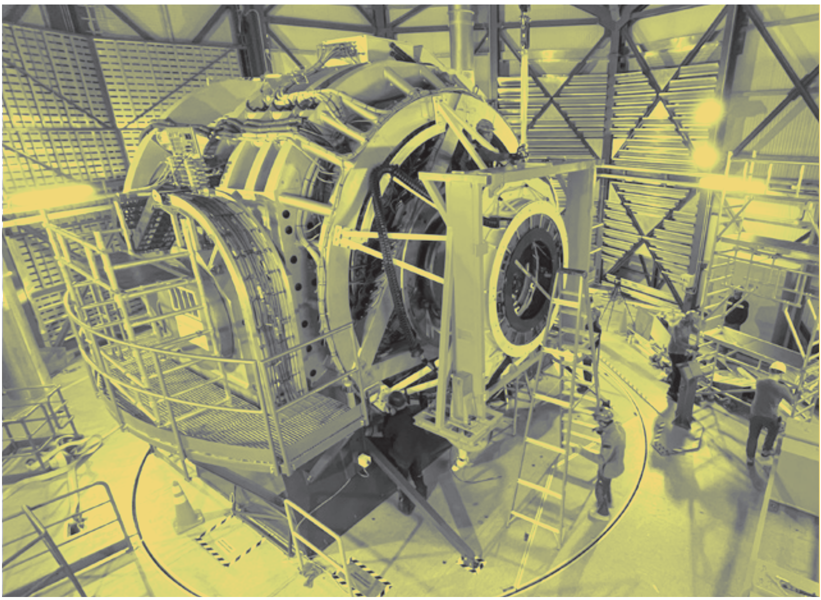
The exploration of **near-Earth space and the cosmos** illuminates largely uncharted territories of human knowledge about physics. Its scope ranges from the upper layers of the atmosphere as the interface of our planet with space to the boundaries of the observable universe. Research is dedicated to the dynamics of the upper Earth atmosphere, the structure of the large-scale distribution of matter in the universe, the structure of our Milky Way, and the stars, including our Sun.

Two Leibniz institutes of the section serve as a link between these fundamental topics and the application-oriented areas of the section. They develop and maintain internationally renowned **research infrastructures**. In doing so, they drive the development of methods and technologies, particularly in **optics and photonics** and **mathematical modelling**. These advances require both the use of novel methods in observation and modelling, as well as high-performance technologies and materials beyond today's standards. As a result, the Leibniz institutes of the section are well embedded here within the broad materials and technology science base.

In **atmospheric physics**, the dynamics of the upper atmospheric layers between approximately 50 and 200 km are investigated. These layers form the boundary between the Earth's atmosphere and space and are therefore governed by both typical atmospheric and solar-terrestrial processes. Experimental and theoretical methods thus face particular challenges. This altitude range of the atmosphere is gaining increasing importance due to growing **satellite operations** and satellite-based information and communication. Understanding its dynamics and the impact of climate change on it is therefore of fundamental importance.

The magnetism of stars fundamentally influences their state and evolution. The highly complex processes it triggers are still largely not understood. Concentrations of magnetic fields on the Sun trigger spontaneous eruptions. This can result in intense interactions with the Earth's magnetic field and the upper Earth atmosphere. Their influence on the technological infrastructure of our modern civilisation is – through space weather – clearly perceptible.

Gravitation and electromagnetism and their interplay determine the structure and evolution of the **cosmos** and its objects (stars and galaxies) even on the largest scales. They are measured with the largest telescopes and with spectrographs that simultaneously capture the light of very many sources with precision. With them, scientists can recognise the physical state of the light sources and its evolution. In no terrestrial laboratory can those processes be replicated that arise from the interaction of astrophysical plasmas with magnetic fields, or through the action of hitherto unknown substances such as dark matter and dark energy. The close kinship with the plasma physics of terrestrial systems creates bridges here between basic and applied research. New, fundamental insights into physics can sometimes only be gained through the observation of the universe.



Mathematics and modelling

Mathematics influences our lives, even if often unnoticed. In our highly technologised world, hardly any field can do without it. As a cornerstone of quantitative communication in natural science and technology, it constitutes the medium for innovations. Mathematical modelling, data analysis, **artificial intelligence**, computer-aided solutions, and the optimisation and control of processes shape **all aspects of modern innovation processes** in all domains of science.

Modelling translates scientific questions into the language of mathematics, in order to make them accessible to analysis and numerical solution methods. In a further step, real-world situations can be “played through” in simulations using modern computing technology.

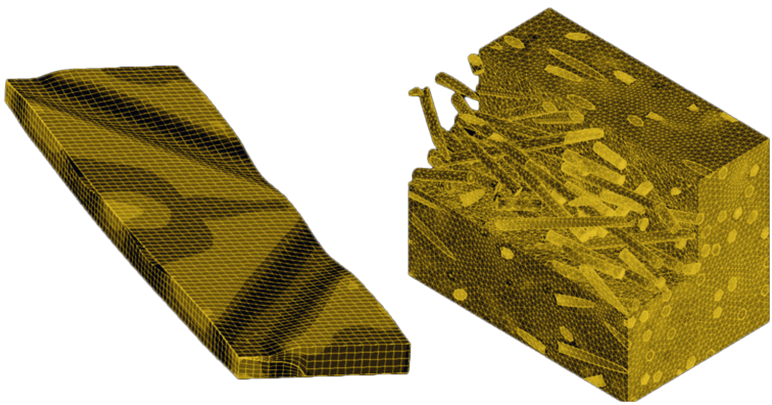
Modern methods of **mathematical modelling and simulation** (MMS) are indispensable for a location of cutting-edge technology. Through them, expensive, energy- and time-intensive, or environmentally burdensome experiments can be minimised or even entirely avoided. They enable virtual laboratories in which realistic digital twins of complex reality can be generated and analysed. MMS enable insights at spatial and temporal scales that cannot be captured with a conventional experimental approach. When experiments are dangerous or not feasible, they allow predictions and shape climate and environmental research or medicine. MMS can also be used to assess risks, for example when deploying new technologies. In many cases, the application of MMS significantly reduces costs, shortens development cycles, and simultaneously increases quality. Furthermore, the influence of random (stochastic) events can be analysed and made usable.

In addition to classical numerical methods, MMS increasingly encompasses data-driven and hybrid approaches: deep learning-based surrogate models, physics-informed neural networks (PINNs), differentiable simulation, Bayesian inference, and uncertainty quantification. These methods accelerate inverse problems, enable real-time predictions, and couple domain knowledge with learning models – for example in plasma processes, materials, and biophotonics simulations.

The section uses MMS to investigate processes from the atomic level through the nano- and microscale to cosmic structures. These are typically highly complex and require the use of state-of-the-art numerical methods and techniques running on high-performance computing platforms. Newly developed efficient simulation tools address the associated challenges.

For many projects of the Leibniz Association, **mathematical modelling and simulation** are of the highest relevance. In order to create synergies, the cross-sectional Leibniz Research Network "MMS" was therefore established. This also includes complex multiscale simulations of plasma processes and surface modifications, which through data-driven approaches and **artificial intelligence** enable new insights into nonlinear systems and their applications.

The internationally renowned **conference venues and meeting centres** of the section furthermore provide space for scientific networking and the development of new ideas and concepts. The conferences span a broad thematic range, from theoretical foundations through mathematical modelling to numerical mathematics, simulation technology, complexity analysis, algorithmics, and software technology.



Artificial intelligence

Artificial intelligence (AI) has developed in recent years into a key technology that permeates virtually all scientific and societal domains. For the section "Mathematics, Natural Sciences, Engineering", AI is a central cross-cutting topic that encompasses both methodological basic research and diverse fields of application.

The Leibniz institutes of the Section develop and analyse novel methods of machine learning (ML), pattern recognition, and data-driven modelling. They research efficient and trustworthy AI methods capable of evaluating large, complex datasets in the natural, engineering, and life sciences. Transparency, robustness, and traceability, as well as the quantification of uncertainty, are at the forefront – in order to build trust in AI systems, secure their societal acceptance, and accelerate the transfer of AI methods and their results into industrial application. In this regard, the scientific meeting centres of the Section and the mathematically oriented Leibniz institutes address various aspects of basic research in AI and ML.

An important focus lies in the linking of AI with other research areas of the section:

- **Materials and process research**: AI-assisted modelling, simulations, optimisation, and data analyses accelerate the development of new materials and substances and improve the prediction of properties and life cycles.
- **Health technologies**: AI methods enable more precise diagnoses, personalised therapies, and the evaluation of complex biomedical data.
- **Communication and information technologies**: Intelligent algorithms increase the efficiency of networks, improve data security, and support new forms of human-machine interaction.
- **Astrophysics and atmospheric research**: AI-assisted analysis and solution methods help to evaluate vast amounts of data from telescopes and atmospheric measurements, to master different scales in space and time, and to gain new insights into cosmic and planetary processes.

In addition to specialised ML methods, Large Language Models (LLMs) are gaining in importance – as domain-specific research LLMs and in Retrieval-Augmented Generation (RAG) architectures, for example for chemistry and spectroscopy databases, laboratory knowledge management, and method assistants for evaluation pipelines. Transparency, traceability, evaluation, and secure operation (e.g. data/model governance) are at the forefront.

At the same time, AI plays a key role in **research data management** and **digitalisation.** It supports the organisation, linking, and sustainable use of large data holdings and opens up new possibilities for open science.

The Leibniz institutes of the section actively advance the **interdisciplinary and responsible use of AI**. Through their close collaboration in national and international research consortia and through cooperations with industry and policy, they make significant contributions to Europe‘s technological sovereignty.

Digital transformation, research data management and infrastructures

Digital transformation, which is proceeding at a rapid pace, opens up new opportunities while simultaneously giving rise to new challenges – in private life as well as in the world of work, in culture and education, and to a particular degree in science, research, and the economy.

In the natural and technical sciences, digital tools and processes have long been playing an increasingly important role. **Research data** are increasingly generated only in digital form and in ever greater volumes. Advances in information technology make it possible to store, analyse, visualise, and make these data volumes available in the long term. Teams are increasingly working location-independently in virtual research environments and accessing networked digital data resources. Digital transformation accelerates research processes and promotes international and transdisciplinary cooperations. Yet many questions regarding sustainability, quality assurance, data protection, AI compliance, and data security remain open, particularly against the backdrop of technological and political sovereignty.

With the aspiration to promote **Open Access**, **Open Data**, and **Open Science**, digital research data and their legally secure management are coming into the focus of science policy and research funders. Effective management of research data is the key to innovations and holds high value creation potential.

Central to this is the long-term availability of data. Through it, research processes and results remain traceable in the future. Furthermore, it enables reuse in entirely different, new contexts. This opens up the possibility of unlocking new horizons of knowledge and research spaces, as well as new forms of scientific work.

Increasingly, data themselves are becoming publications. Scientists must be able to rely on a powerful **information infrastructure** that encompasses external and supra-regional resources and services, and for which corresponding dedicated research must be conducted. Only then can the growing volumes of digital data and publications be made usable efficiently, with quality assurance, and in a legally secure manner.

Within the Leibniz Association, there exists the unique potential to jointly develop innovative scenarios that are exemplary for the successful interplay of science and information infrastructure. Scientific performance and efficient **research data management** go hand in hand.

In particular, the section “Mathematics, Natural Sciences, Engineering”, with its data-intensive research approaches and highly developed information infrastructures, can set the benchmarks for the future here. One example is the specialist repository INPTDAT, developed specifically for plasma technologies and serving as a blueprint for domain-specific research data management. In addition, Leibniz institutes operate domain-specific repositories such as VibSpecDB for vibrational spectroscopic data (e.g. Raman/IR) – including structured metadata, quality assurance, and interfaces for AI-assisted evaluation. Leibniz institutes of the section are involved in 17 consortia of the **National Research Data Infrastructure (NFDI)**, in the Mathematical Research Data Initiative (MaRDI), NFDI4Chem, NFDI4Cat, and NFDI4Biochem as the lead institution. The section is also represented on the steering committee of the BMFTR initiative “Material-Digital”. Through the technical and organisational NFDI involvements in the section, robust bridges exist to all other sections – extending into the humanities research infrastructures.

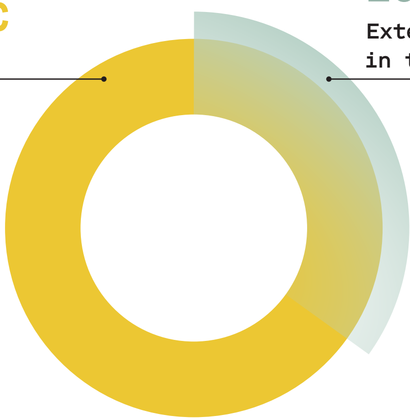
The Leibniz institutes of the section also participate in major national initiatives for research infrastructures. In the national prioritisation process for new, large-scale research infrastructures, they are involved, for example, as partners in the initiatives for the Einstein Telescope or LEGEND-1000. They are likewise engaged in the establishment of the German Centre for Astrophysics (DZA) or are shareholders in the Leibniz Centre for Photonics in Infection Research (LPI).

The Section “Mathematics, Natural Sciences, Engineering” in Figures

Last Update: May 2026

585 Mio €
Budget in total

204 Mio €
External funding in total



2,157 | 41 %
Women in total

5,283
Staff in total

The Section "Mathematics, Natural Sciences, Engineering" in Figures

Last Update: May 2026

3,033

Researchers in total

977 | 32 %

Female researchers

1,370 | 45 %

International researchers

865

Doctoral researchers in total

449

Researchers in executive positions in total

316 | 37 %

Female doctoral researchers

106 | 24 %

Female researchers in executive positions

23 Leibniz Institutes of the Section “Mathematics, Natural Sciences, Engineering”

		BADEN-WÜRTTEMBERG
●	**FIZ KA**	FIZ Karlsruhe – Leibniz Institute for Information Infrastructure
●	**MFO**	Mathematisches Forschungsinstitut Oberwolfach
		BERLIN
●	**FBH**	Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Berlin
●	**IKZ**	Leibniz-Institut für Kristallzüchtung, Berlin
●	**MBI**	Max-Born-Institute for Nonlinear Optics and Short Pulse Spectroscopy, Berlin
●	**PDI**	Paul Drude Institute for Solid State Electronics, Berlin
●	**WIAS**	Weierstrass Institute for Applied Analysis and Stochastics, Berlin
		BRANDENBURG
●	**AIP**	Leibniz Institute for Astrophysics Potsdam
●	**IHP**	Leibniz Institute for High Performance Microelectronics, Frankfurt (Oder)
		BREMEN
●	**IWT**	Leibniz Institute for Materials Engineering, Bremen
		LOWER SAXONY
●	**TIB**	TIB – Leibniz Information Centre for Science and Technology and University Library, Hanover
		MECKLENBURG-VORPOMMERN
●	**IAP**	Leibniz Institute of Atmospheric Physics at the University of Rostock
●	**INP**	Leibniz Institute for Plasma Science and Technology, Greifswald
●	**LIKAT**	Leibniz Institute for Catalysis e. V. at the University of Rostock
		NORTH RHINE-WESTPHALIA
●	**DWI**	DWI – Leibniz Institute for Interactive Materials, Aachen
●	**ISAS**	Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund und Berlin
		RHINELAND-PALATINATE
●	**IVW**	Leibniz-Institut für Verbundwerkstoffe, Kaiserslautern
		SAARLAND
●	**INM**	INM – Leibniz Institute for New Materials, Saarbrücken
●	**LZI**	Schloss Dagstuhl – Leibniz Center for Informatics, Wadern
		SAXONY
●	**IFW**	Leibniz Institute for Solid State and Materials Research Dresden
●	**IOM**	Leibniz Institute of Surface Engineering, Leipzig
●	**IPF**	Leibniz Institute of Polymer Research Dresden
		THURINGIA
●	**IPHT**	Leibniz Institute of Photonic Technology, Jena

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