NICPB in 2020: development plan and overview of the institute

Contents

1 Introduction

The document contains hyperlinks to other documents, CV-s of personnel and projects. Please follow these links to further details. The summary of the development of NICPB until February 2019 is available in previous activity reports.

This year NICPB celebrated the 40th anniversary: it was established on February 16, 1980 as an institute of the Estonian Academy of Sciences.

In the spring of 2020 we updated the NICPB Development Plan 2021 – 2026 and our strategic research programmes. Both documents were discussed by the Science Council of the institute in June, where it was suggested to send the documents to the science departments of the four main Estonian universities for comments. The documents were finally approved by the Science Council in September and are included in the current activity report.

The final sections of the document contain a short overview of the state of the institute at the end of 2020.

2 Development Plan 2026

2.1 Introduction

National Institute of Chemical Physics and Biophysics (NICPB) acts in the benefit of knowledge-based Estonia. As the only research institution in public law in Estonia, NICPB diversifies the science landscape and enhances the international competitiveness of Estonian science. NICPB is characterised by comprehensive interdisciplinary research programmes and co-operation with leading research centres of the world. Knowledge created by excellent research as well as movement of new ideas and highly educated young people from academia to different fields of society and industry are key to knowledge-based economy both in Estonia and the world. Success of NICPB is founded on attractive working environment valuing academic freedom and offering development opportunities.

The current Development Plan (DP) addresses the problems and challenges facing NICPB in a 10-year perspective.

2.2 Mission

NICPB is an independent research institution in public law where the main task of the scientists is research based on academic freedom.

NICPB is a positively evaluated research institution that carries out fundamental and applied research and engages in the development (R&DI) of novel directions in physical, technological and biomedical sciences[1].

NICPB helps to educate new generation of scientists pursuant to the association and other agreements with the universities and other academic institutions. All level students can start their scientific career and to perform their research in the Laboratories of the Institute.

NICPB participates actively in shaping national science policies, in the organisation of the activities of Estonian scientists and R&D institutions and in solving the challenges facing the society.

2.3 Common Values

The Common Values of NICPB are **Openness**, **Science-Based Action**, **Interdisciplinarity** and **Orientation to the Future**.

NICPB is a research institution open to Estonian and international science community and to Estonian society. It is an institution where academic freedom and quest and development of new ideas are valued.

NICPB promotes knowledge-based development and harnesses its competences not only to further scientific research but to solve problems facing the society in general.

Co-operation and interdisciplinarity within NICPB, in Estonia and in the world broadly is the only way to sustainable excellent research.

NICPB is oriented to future – new knowledge created by us will be used in the future and we are open to new developments and trends in our research.

[1] Common European Research Classification Scheme (CERCS)

2.4 Current Situation and Challenges

The DP originates from the NICPB Act and reckons that NICPB is a strategic partner to Estonian universities in advancing the cutting-edge science in all our fields of science, i.e. physics, materials science, astrophysics and cosmology, chemistry, biology, ecology, energetics and information technology.

An inseparable part of our research is co-operation with universities, their graduate and undergraduate students carry out their research in our laboratories. Our researchers, on the other hand, lecture at the universities and supervise thesis works of the students. Also, two Centres of Excellence housed by NICPB, numerous joint grants and projects and common Estonian Science Roadmap objects are good examples of the co-operation.

A public state-owned high school will soon be built next to us. That opens new possibilities to acquaint high school students with cutting edge natural science and hopefully paves way to more conscious career choices. In a long run that will help to shape future knowledge-based generations and to popularise sciences.

NICPB participates through national, European and other research programmes, grants, agreements, etc. in domestic and international R&D. The Institute supports and participates actively in current R&D programmes and in shaping future R&D programmes of local, national and international priorities. NICPB is highly visible research centre both domestically and internationally and is a valued and sought partner to the Estonian state in matters concerning R&D.

NICPB prioritises fields of science related to its strategic research programmes (SRP) and pays appropriate attention to possible applications. Co-operation with industry in the development of fuel cells for H_2-energetics, acquainting the domestic industry with the possibilities of CERN, coordination of CERN-oriented activities in Estonia and in the Baltics serve as an example. Development of nanoparticle based anti-bacterial coatings for surfaces and textiles in co-operation with both industry and universities has been intensified due to the outbreak of the COVID-19 pandemic.

The single greatest threat to sustainability of the Institute is the predominantly short-term, project-based funding (soft money) of science in Estonia. This impediment was brought up during the regular evaluation of Estonian science in 2017 but also and already by the reports of the International Science Advisory Board (ISAB) of NICPB of 2012 and 2016. An important priority of the Institute is improvement of the national system of financing of science. Toward that end NICP communicates actively with other R&D institutions, relevant ministries and Riigikogu (Estonian Parliament).

To maintain the high quality and overall sustainability of the Institute it is essential to find both new people and new ideas. A Development Fund has been set up in the Institute to open and support new research fields. The Institute works systematically both domestically and abroad to present its attractive and dynamic environment as a place to further one's scientific career.

2.5 Strategic Research Programmes (SRP)

The research in NICPB is based on fields science set forth in the NICPB Act, covering key areas of Estonian and European priorities and is fundamentally based on national and international co-operation. The R&D in the Institute is implemented through Strategic Research Programmes that converge different areas of research and fields of science and are integrated with one another. As a rule, a SRP covers full chain of logical cognition, mathematical description and creation and use of technical toolkit to solve a scientific problem. In comparison with other domestic R&D institutions, our Programmes are more comprehensive, covering both fundamental and applied research and being interdisciplinary. In 2020 NICPB has four such Programmes:

- Environmental Toxicology and Nanosafety;
- Physical Chemistry and Chemical Biology;
- Physics, Materials Science and Energy Technologies;
- High Energy Physics and Theoretical Physics.

2.6 Competences

The basic competences (in no order) of NICPB include:

- Nanoecotoxicology
- Environmental Chemistry
- Fundamental and Applied Bioenergetics
- Investigation of Physical Properties of Materials, including
    - High Resolution and Solid-State multinuclear NMR
    - Terahertz-Spectroscopy
    - Non-linear Optics
    - Quantum Chemical Calculations
    - Magnetic, electric and thermodynamic properties of materials in a broad range of temperatures and magnetic field strengths
    - Synthesis & Characterisation of (Nano)Materials
- Energy technologies, including
    - Investigation of Fuel Cells and H_2-energetics
    - Safety of Nuclear Power
- Experimental Particle Physics and CERN
- Theoretical Physics, Cosmology and Gravitation
- IT-applications and development of scientific computing
- Theory of Complex Systems

2.7 Vision 2026

NICPB is highly visible both in domestic and international research and development.

NICPB is effective and efficient independent R&D institution where all its academic and non-academic members sense the opportunities and responsibilities in achieving Institute's goals. The administration is transparent and intelligible and provides attractive working environment.

The success and reputation of NICPB is based on excellence in research, on competences, on initiation of innovative fields of research and on development of science infrastructure for both national and international co-operation.

NICPB is a leading national laboratory at least in 2 to 3 fields of R&D. NICPB houses several internationally renowned research teams, co-operates actively on international level and is an attractive employer for both domestic and foreign researchers.

The graduate studies (though NICPB is not a degree-awarding institution) provide pertinent qualification for scientific research and ensure critical accrual of early-stage researchers (ESR) in the Institute. NICPB has established an international network to support ESR's in the circulation of ideas, science and scientists.

2.8 Strategic Goals 2026

1. Internationally recognised research in all research topics. Status of a Regional and/or European centre with at least two Strategic Programmes.
2. National Centre of Expertise in at least two fields according to public order and in keeping with our competences in particle physics, nuclear energy, analytical spectroscopy, quantum chemical modelling, functional materials, hydrogen energetics and nano- and ecotoxicology.
3. Sustainable financing of the Institute to pursue its vision and goals has been secured through different national and international financing sources and instruments.
4. The sustainability of research teams and the accession of Early-Stage Researchers has been secured. The Institute is known for its attractive working environment and all employees are satisfied and highly motivated.
5. NICPB engages vigorously in pursuing the Goals of the "Knowledge–based Estonia" programme, it is highly visible in the society and is a highly rated R&D institution.

2.9 Milestones and Activities

2.9.1 Organisation and Management

The organisation structure and the management of the Institute are transparent, dynamic and efficient. Strategic decisions are made by the Institute's Science Board, the implementation of the strategy and everyday management is carried out by the administration. Both the Science Board and Administration follow the advices of the Institute's International Science Advisory Board.

Activities to achieve efficiency:

(1) the relation of in-house and purchased (ancillary) services is kept optimal;
(2) the number of support staff is kept optimal to ensure the provision of the support services;
(3) state-of-the-art IT solutions (document and personnel management, accounting, etc.) are used;
(4) an attractive working environment and efficient support services have been created.

The research is carried out in scientific units of the Institute, the laboratories. A laboratory assembles research teams working on related topics and houses the necessary (research) infrastructure. Laboratory is chaired by the Head of the laboratory, who's main task is the development of the Lab in concert with the Institute's strategic plan.

2.9.2 Research and Development

The main fields of the R&D are defined as the Strategic Research Programmes. Due to the competition-based financing of science in Estonia, they can be funded from personal research grants of the researchers. From Institute's point of view, it is instrumental to introduce and develop new fields. Therefore, promising young researchers are supported at the outset of their careers until they have obtained their own grants and gained enough momentum. Also, the principal investigators in Institute's main fields of research are guaranteed a permanent salary.[2]

[2] Permanent salary for PI's is our goal that depends on the Estonian science funding system. It is still not possible in 2021.

Milestone 1 International level research in all fields

Activities

(1) Research fields that are possible candidates for regional or European centre status will be defined. The named fields will be manned with researchers with great potential of success and researchers will be guided and supported to achieve their ambitions.
(2) Regular inventory and renewal of the SRPs, opening of new research areas in co-operation with universities.
(3) Recruitment and keeping of researchers with great potential of success.
(4) Support of innovation, knowledge transfers and start-ups.
(5) Initiation of new activities with the help of NICPB's Development Fund.

Milestone 2 National Centres of Expertise

Activities

(1) Mapping of the demand for Centres of Expertise together with state agencies and agreement on the permanent funding of the Centres.
(2) Launching of the Centres (personnel, infrastructure, procedures, accreditations).

Milestone 3 Sustainable Funding

Activities

(1) Permanent and positive co-operation with legislators and participation in the shaping of (national) science policy. Motivation of the researchers to develop their ideas and to participate in funding calls.
(2) Introduction of tenure track model for all research professors of the Institute.

2.9.3 People

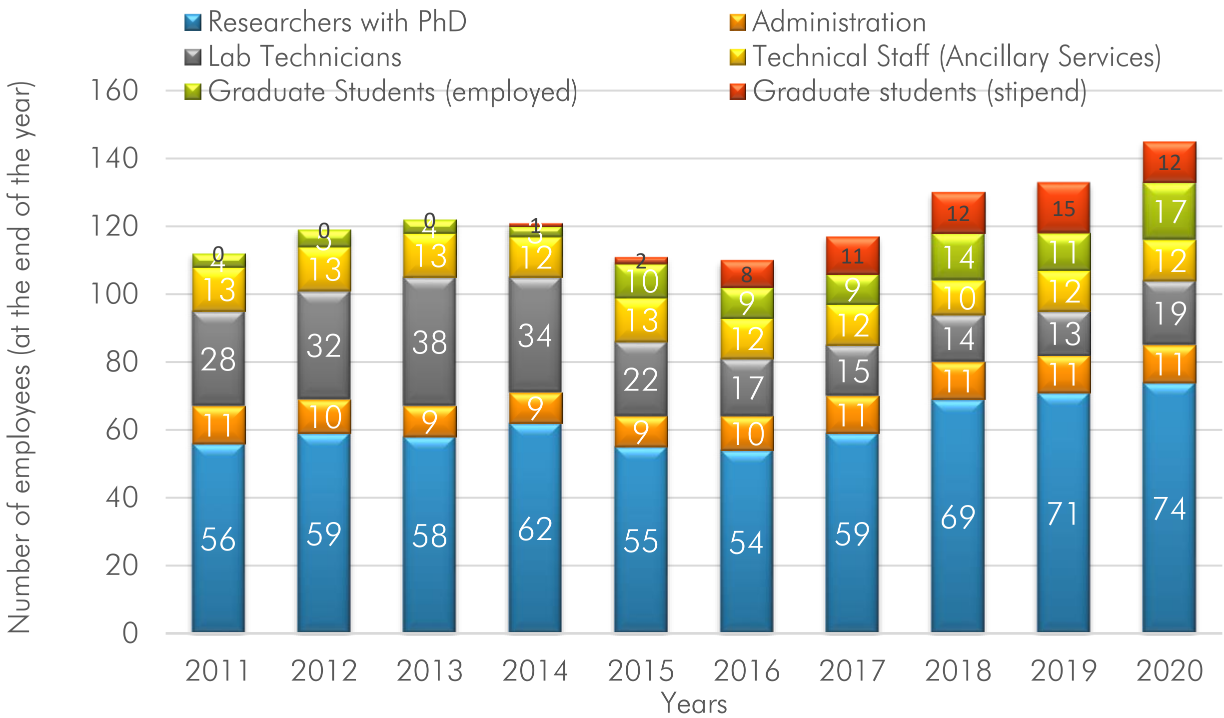

Figure 1. Researchers and graduate students who worked at the NICPB at the end of each year.

At the end of November 2020 there worked 74 PhD researchers, 29 graduate students and 19 lab technicians at the Institute. The Administration consisted 11 people and we also had 12 workers (cleaners, keepers, etc.) who provided ancillary services.

According to the Web of Science, Essential Science Indicators database 9 researchers (S. Bhowmik, A. Carvalho, J. Ellis, A. Ivask, M. Kadastik, A. Kahru, K. Kasemets, M. Raidal, C. Veelken) of the Institute belong to the top 1% most cited scientists in their respective field in the world as of May 2020.

Two researchers (A. Kahru and M. Raidal) are the members of the Estonian Academy of Sciences and two (E. Heinsalu – Past President, M. Kadastik – President) are members of the Estonian Young Academy. Three of our scientists (A. Kahru, I. Kruusenberg and T. Rõõm)) are members of the Evaluation Board of the Estonian Research Council.

Milestone 4.1 Sustainability of the research teams and accretion of researchers

Activities

(1) NICPB is in an orderly manner involved in the teaching at several universities and in supervising students' work at the Institute's own laboratories.
(2) NICPB participates in international learning mobility of students and young researchers.
(3) A tenure track career model will be introduced, including:
    1) scholarships or employment contracts to master and graduate students;
    2) support of Postdoctoral studies abroad, as a rule;
    3) support of young PhD researchers during up to 3 years to obtain their own grants;
    4) younger researchers are rapidly brought into PI status and then into leadership roles within the Institute.
(4) Coordinated and systematic approach to introduce the possibilities and advantages of NICPB to students.
(5) Annual awarding of Scholarships to students for working at the Institute.
(6) Securing accrual of researchers in critical or strategic fields (to match and exceed expected retirements) is an important task of the Heads of the Laboratories.

Milestone 4.2 Contentment and High Motivation of researchers

(1) High motivation and contentment are ensured through support of the development of employers and through creating excellent working environment.
(2) Different training courses are hold regularly to support personality development. All-Institute and Lab-based seminars oriented especially to master and graduate students and ESRs are held regularly.
(3) A fund will be set up to finance training necessary to promote researcher's career and a mechanism is created to target individual training needs.

Milestone 5 Knowledge-based society, visibility and high rating

(1) Active participation in the fulfilment of the Estonian R&D&I strategy "Knowledge-based Estonia" according to Institute's competences.
(2) Participation in solving the challenges facing the society, especially in energetics, biomedicine and environmental toxicology.
(3) Active standing in problems facing the society, participation in social debates and representative bodies of scientists.

3 Strategic Research Programmes of NICPB

The strategic research programmes form a part of the development programme of NICPB.

3.1 Environmental Toxicology and Nanosafety

Research on environmentally hazardous materials – toxic substances that are released by human activity and are harmful to ecosystems as well as to people – is a field that involves biology, physics, chemistry, material science and healthcare. An interdisciplinary institution such as NICPB is therefore highly suitable for the successful development of this field of research and environmental studies continue to be one of the central research strategies of NICPB.

The research in environmental toxicology in NICPB, especially the studies of the environmental hazard of metal oxide nanoparticles initiated in 2004 were ground-breaking as reflected by the number of citations, highly cited papers as well as successful participation in the EU FP6, FP7 and H2020 projects.

The strategic goal of the environmental toxicology program is to elucidate the hazard of (industrial) chemicals that are already in the environment or have the potential to end up there. This goal will be approached by answering the following questions: is it toxic, to whom and how toxic, why toxic and how to assess the toxicity comprehensively and cost-effectively. According to the chemicals regulation in the European Union (REACH) all chemical substances produced in excess of 1 ton per year (estimated number of these substances exceeds 100 000) have to be characterized for their potential hazard for the human and environment. It is a considerable burden for the European chemical industry (including Estonian chemical industry), since the responsibility of hazard assessments lies on the manufacturer or importer.

A new class of chemicals – synthetic nanoparticles i.e. particles with at least one dimension below 100 nm – are already produced in large scale in a variety of compositions, shapes and sizes. Compared to conventional materials, the nanosize particles have novel properties, exploitation of which may lead to breakthroughs in many technologies starting from energy production and ending with medicine. However, the novel properties may also lead to adverse effects for humans and the environment. To avoid this, it is crucial to have the infrastructure and the scientific expertise for conducting the respective safety studies. On the other hand, the targeted use of the toxic characteristics of some of the materials can be harnessed for creation of novel antimicrobial materials (textiles and surface coatings) to fight against the spread of microbial and viral infections and the emergence of drug resistant bacteria.

To summarize, the Laboratory of Environmental Toxicology currently holds the key competence and infrastructure in Estonia for evaluating the adverse effects of chemicals (including nanomaterials and microplastics) and ecotoxicity of e.g., waste waters, solid wastes, polluted soils and sediments. The Laboratory has the facilities, test organisms and know-how on ecotoxicological analysis with crustaceans, algae, protozoa, bacteria etc. Majority of the assays are done in compliance with the OECD and/or ISO standards. In the laboratory, the GLP (good laboratory practice) principles are followed to guarantee the quality as well as the reliability of the studies.

One direction of the strategic program is the development of test systems that enable efficient assessment of biological effects of chemicals and nanomaterials. Attention is focused mostly on in vitro tests that allow the assessment of adverse effects and toxicity mechanisms of chemicals and nanomaterials. As a rule, the toxicity of chemicals is related to adverse effects on cell membranes and processes of basal metabolism, which can be predicted using in vitro assays (including tests with e.g. bacteria, protozoa and invertebrates) with enough prediction power. Thus, in addition to the existing competence in environmental chemistry, NICPB has developed the unique and necessary competence for Estonia in ecotoxicology. That has been used and will be used for the environmental safety assessment of solid wastes from the oil shale industry (incl. energy production) with the special emphasis of their sustainable re-use. As an example, the earlier research initiated by NICPB scientists led to the reclassification of one of the most important solid waste of the oil shale industry – fresh semi coke – as hazardous waste in 2003, resulting in the change of its deposition according to the rules of the European Union. This research is currently continued by (i) ecotoxicological studies of Purtse river contaminated sediments within the framework of the EU LIFE IP CleanEST project (2018-2028) conducted by the Estonian Ministry of the Environment and (ii) environmental safety of potential use of oil shale fly ash in e.g., granulated fertilizers and asphalt. In addition, a new topic of environmental aspects of rare earth metals has been recently started as these technologically critical elements are increasingly used in top-technologies worldwide and in Sillamäe (Estonia) there is one of the largest rare earth metal manufacturers in Europe - the NPM Silmet AS.

3.2 Physical Chemistry and Chemical Biology

3.2.1 Fundamental and applied bioenergetics

Recent advances in bioenergetics (the study of energy metabolism in living organisms) have become increasingly important in the fields of biology, medicine, and environmental protection.

Modern science has means for describing the cell structure, its components, and the signal transduction pathways. But we are not yet able to understand and quantify the individual cell or the organism as a whole system, including the precise mechanisms of the disease development. Systems biology-based research is trying to bridge this gap. The laboratory of Chemical biology follows those principles. The key point is to consider the properties of the biological system, arising from the interactions of the different components that cannot be identified in an isolated state. Systems should, therefore, be examined as comprehensively as possible, combining biology, biophysics, and medicine.

The strategic goal is to scrutinize highly organized and coordinated systems such as intracellular energy transfer networks in muscle and tumor cells and to identify changes in bioenergetics underlying the development of the disease.

Skeletal and cardiac muscles are energy-demanding tissues, so disturbances in energy supply due to aging or pathologies cause a serious decline in people's quality of life. For example, mitochondrial diseases, myopathies, and many heart diseases are associated with changes in cellular bioenergetics. The mechanisms underlying these disorders are related to the reprogramming of cellular bioenergetics, changes in substrate pathway preferences, and deregulation of metal metabolism. High-resolution respirometry in combination with various fluxomic approaches makes it possible to determine the exact points of change in the pathways of energy production and transfer. This knowledge provides new information to improve diagnostic processes or to make recommendations for targeted treatment.

Another direction of the program is to elucidate functional changes in mitochondria in cancer cells. Primary targets of the research are breast and colorectal cancers as one of most common tumors found in humans. We have shown that disturbances in energetic regulation are one of the early signals of pathological changes in cells. Rapid and accurate determination of this pre-malignant stage increases chance of survival and reduces treatment burden for both the patient and the healthcare system.

Cancer cells reorganize energy metabolism to maintain intense proliferation even under adverse conditions. Specific differences in bioenergetics of malignancies have not been systematically studied in a well-defined patient population. A sub goal of the program is to confirm whether mitochondrial oxidative phosphorylation is the main "driver" that contributes to the growth of malignant tissue in highly aggressive cancers. It is also not yet clear how cancer cells reorganize energy transfer pathways and how the balance between glycolysis, glutaminolysis and mitochondrial oxidative phosphorylation is regulated.

The elucidation of these mechanisms provides better understanding of tumor development and the causes of metastatic progression. The program helps to extend our knowledge on mitochondrial mechanisms in malignancies and possibly contribute to development of predictive/prognostic biomarkers and lead treatment decisions.

The third goal is to develop supporting cell culture models (tumors, muscles, neurons) based on the principles of systems biology. Their use is necessary for better identification and control of metabolic mechanisms, which will accelerate the development of novel and more specific treatment options.

The laboratory is planning to expand into neurodegenerative disease research. Recent years have shown accumulating evidence indicating the central role of altered bioenergetics in this group of diseases. The causative mechanisms are related to de-regulation of cell metabolism and changes in the regulation of metal homeostasis.

Taken together, the program provides a theoretical basis for understanding and measuring pathologies in bioenergetics systems driving diseases in muscle cells, many neurodegenerative diseases, and cancers.

The Laboratory of Chemical biology brings together high-level researchers with diverse backgrounds in chemistry, physics, biochemistry, and systems biology. The group combines multidisciplinary knowledge and modern methodologies in energy metabolism research in different cell types. We aim to integrate and expand knowledge on key fundamental aspects of the cell bioenergetics.

3.2.2 Chemistry and Spectroscopy

The development of chemistry and spectroscopic techniques are strongly intertwined – chemistry studies molecules and intermolecular interactions, while spectroscopy comprises various physical-chemical analytical techniques to probe these molecules and interactions. NICPB has been in the forefront of the development of the most versatile spectroscopic technique – nuclear magnetic resonance spectroscopy (NMR) – for years. Our NMR laboratory is the most versatile NMR laboratory in the Baltics, conducting solution and solid-state NMR research to study molecular structures and mixtures. NICPB also has competence and long traditions in the development of solid-state NMR detectors. Today, the NICPB NMR laboratory is involved in efforts towards solving the largest bottleneck of NMR, poor sensitivity, by nuclear hyperpolarization techniques. We were one of the first laboratories in the world were hyperpolarization techniques were successfully applied to biological mixtures, allowing to detect biomolecules that would otherwise go undetected.

Solid state NMR is particularly important for material sciences and solid-state physics, it carries a good potential for collaboration companies operating on these fields. Clear targets and actions towards these goals will have to be defined in the beginning of the decade. Solution NMR is important for most chemical and biochemical research fields and is already routinely offering services to the chemical and food industries. Further commercialization of our competence will be achieved through incorporating the NICPB NMR laboratory into the Estonian the Estonian Centre of Analytical Chemistry (ECAC/AKKI).

The first and foremost challenges for the NMR laboratory for the starting decade is maintaining its high reputation and international visibility, assuring a steady influx on students and young personnel to assure long term viability, as well as developing new applications and staying in touch with the field in general. Its important to assure the existence and viability of our solid-state NMR capability, which is unique in the region and has high potential for industrial collaborations and is important for a wide range of engineering and natural sciences research fields. Efforts will be made to maintain NICPB as the outstanding contact point and centre of excellence in NMR analysis in the region that serves industrial partners and academic researchers alike. To that end we must be professional and fast acting analysis partners for our present and future collaborators. To achieve this, the laboratory will take an active role in developing the national chemical analysis infrastructure, maintaining existing competences and setting up new techniques.

We see a lot of potential in engaging in omics research that is quickly gaining popularity worldwide. Omics techniques can be described as methods for the simultaneous detection of many biomolecules and methods for processing and analysing the resulting data with the aim on assessing the state and the health of an organism. NMR is one of the two main metabolomics techniques (the research field that concentrates on detecting metabolites). Our NMR laboratory will develop methods and protocols for metabolomics research, diagnostics, for the discovery of biomarkers, surveys of food safety of transportation fuel quality and other applications that involve complex mixtures. Achieving these goals requires active collaboration with partners with various interests and competences important for metabolomics analysis, including medical research, food safety, environmental protection, statistics, data processing and many others.

3.2.3 Supramolecular Chemistry

Supramolecular chemistry includes organic synthesis, X-ray diffraction and NMR experiments. In NICPB, cyclic compounds, macrocycles, are synthesized, and these can form complexes with other molecules or ions through weak interactions and do not require covalent bonds. Additionally, it is possible to form organized aggregates in solution and in the solid state. Macrocycles and their aggregates can be used, for example, as drug carriers in the human body, as sensors, as a catalytic medium for reactions, and as molecules that capture toxicants in the environment, e.g., from drinking water. NICPB's strategic direction in supramolecular chemistry involves, firstly, the development of new macrocycles, starting with the synthesis and determining their structures, and, secondly, the development of NMR experiments and methods to characterize new macrocycle complexes with important molecules and ions. Variable temperature experiments in NICPB form a large part in the supramolecular chemistry direction since they allow to study the kinetics and thermodynamics of macrocycle complexes. These experiments show how the macrocycles and their complexes or aggregates change their shape and conformation in solution and therefore help to develop better methods for the use of the macrocycles. In supramolecular chemistry, attention is paid to developing collaborations with Estonian and foreign working groups; NICPB's competence enables to perform NMR experiments and to characterize supramolecular chemistry systems developed in other Estonian or foreign research institutions and universities. On the other hand, experiments on macrocycles that are synthesized in NICPB are performed in collaboration with other research groups, which enhance their complexation properties in solution and the solid state

3.3 Physics, Materials Science and Energy Technologies

Modern physics of condensed phases and material science focuses on substances with novel electric, magnetic, optical and thermal properties. The functionality of those compounds is highly unpredictable either due to strong electron correlation (magnetism, ferroelectricity, charge order etc) or due to extremely complicated structure (huge unit cells of intermetals and oxides, composites), and more often, due to both reasons. The current Programme offers three approaches to facilitate better understanding of the complex quantum matter and its design – better synthesis and control, state-of-the-art experimental (analytical) techniques and novel theoretical methods.

3.3.1 New Spin Materials and Superconductors

Spin is a fundamental property of an elementary particle that is described properly only by laws of quantum mechanics. Spin has practical implications in material science due to its quantum nature. Nuclear magnetic resonance uses nuclear spin as a local probe of structure and dynamics of materials at the atomic level. Permanent magnets and giant magnetoresistive effects are caused by the coherent action of many electron spins. Even more, in multiferroics it is possible to reorient the spins with electric fields. This reduces the amount of Joule heating of write operations in magnetic memories. Magneto-electric interaction between spin and polarization waves in multiferroics is a cornerstone for new THz devices. The driving force of the exploration of quantum phase transitions in materials with strong electron correlations and Bose-Einstein condensation of magnons (spin waves) has been superconductivity and magnetism

Superconductivity arises when electrons with spin ½ form pairs with integer spin, which can only be excited by an energy that exceeds a critical threshold. That threshold in the excitation spectrum of superconductors can be studied with THz spectroscopy. Breaking the time reversal symmetry in unconventional superconductors causes the Kerr effect, rotation of the plane of polarization of the reflected light. Thus it is possible to experimentally verify different models describing the unconventional superconductors by the time reversal symmetry or the order parameter.

The research programme on new spin materials aims at studying fundamental physical phenomena in materials that may have high-tech applications. Spin materials are studied with nuclear magnetic resonance, THz and Raman spectroscopy methods, all contributing to the understanding of structure and structure-function relationship. The quantum nature of material properties requires application of high magnetic fields and low temperatures.

3.3.2 Endohedral atoms and molecules in fullerenes

Fullerene C_{60} is a remarkable molecular cage with a 4 Ångström size cavity. This cavity is large enough to accommodate atoms and small molecules without having a chemical bond with the fullerene carbons. These endohedral complexes are known as $A@C_{60}$, where *A* is an atom or a molecule, for example $He@C_{60}$ or $H_2O@C_{60}$. Endohedral complexes are stable and are destroyed only if heated to several hundred degrees of Celsius. It is possible to grow crystals out of them or to dissolve them in liquids. Because there is no chemical bond between *A* and C_{60}, the internal degrees of freedom, rotations and molecular vibrations of *A*, are retained. However, the translational motion is quantized by the surrounding molecular cage. Some new phenomena – translation-rotation coupling – can be observed if *A* is not spherical. Thus, it is possible to study small molecule dynamics as it was in the gas phase but at very low temperatures where *A*, if not shielded by C_{60}, usually condenses into liquid or solid phase. The information about vibrational, rotational and translational motion of *A* can be obtained with THz and infra-red spectroscopy. The aim is to use these molecular rotors in combination with ortho-para conversion and optical pumping for the enhancement of nuclear magnetic resonance and tomography sensitivity.

3.3.3 Investigation of Structure, Dynamics, and Properties at Different Magnetic Field Strengths and at Various Temperatures

NMR spectroscopy is based on high-precision measurement of nuclear spin energy levels in a magnetic field. Fine structure of the spectra depends on local interactions, generated by chemical bond and other nuclei. Different magnetic field strength and various temperatures allow for increased sensitivity and/or to alter the states and functionality of the sample at hand.

Using NMR as an analytical tool in chemistry, biology and solid state physics forms an essential part of the program. Structural analyses and control of syntheses of enantiomers, diastereoisomers and other sophisticated molecules is addressed as an issue of basic chemistry. The goal of the molecular biology part is to determine protein mobility and interactions, regarding also quantum- and tunnelling effects, and also to develop studies on membrane and transport proteins (Cf also Bioenergetics). High accuracy cell metabolite measurement will be used for malignancy diagnostics in collaboration with central hospital.

In solid state physics the programme is strongly coupled and quintessential to both the spin materials programme (see above) and to the energy materials' programme (see below). Towards that end super-fast rotation techniques at extreme temperatures will be developed. High resolution and sensitive measurements at temperatures ranging from 10°K (new spin materials) up to 1200°K (energy materials) open qualitatively new possibilities for detailed study of the structure and dynamics of molecular interactions and facilitate the development of new technological materials.

3.3.4 Precision spectroscopy of two-photon absorption (2PA) of organic fluorophores in condensed media

The nonlinear-optical phenomenon of two-photon absorption (2PA constitutes the basis for a number of applications in cell biology, medicine, materials science and, more recently, new information technologies based on quantum optics. The practical properties of 2PA are primarily due to the peculiarities of the quantum mechanical probability of the nonlinear excitation process, which distinguish it from the conventional i.e. linear or single photon absorption (1PA) process. On the one hand, this feature manifests in terms of quadratic dependence of transition probability on the flux density of the incoming photons, and on the other hand, it allows the use of near-infrared wavelengths for excitation of visible transitions, which is an important advantage in microscopy of biological objects, including tissue- and cell structure studies. NICPB conducts experimental and theoretical research on the 2PA phenomenon in view of several closely related strategic long-term goals. Our starting point is the fact that the efficiency of 2PA applications depends not only on the properties of the light source or the laser beam, but at least equally, if not more, on the structure and spectroscopic parameters of the molecular absorbers or 2PA fluorophores. It should be noted here that although 2PA has been in use for many years, including commercial instrumentation such as fluorescence microscopes, determining 2PA molecular cross-section spectrum of needed fluorophores and other specialized materials is rather limited, mainly due to the lack of an adequate methodology. In essence, labs carrying out such measurements around the world often produce contradictory and poorly reproducible outcomes. One of the tasks of the NICPB Working Group on Nonlinear Spectroscopy is to develop such accurate measurements and methods, with the aim of bringing them to a level comparable to the widely used 1PA quantitative photometry and metrology. Among other things, we have set ourselves the goal of becoming a centre for the accurate measurement of 2PA recognized in the European Union, with an important component of success based on involvement of the relevant expertise in optical metrology.

In addition to enhancing known technologies, the above 2PA precision measurements allow performing new and unique fundamental spectroscopic studies and experiments. Second key area of interest for our Working Group is therefore the determination of the constant electrical dipole moments of chromophores based on 2PA spectroscopy, which in turn is closely related to determining the local- or intermolecular electric field acting on the scale of a few nanometers between- and around individual molecules. The latter is known to be one of the key factors in shaping properties of complex functional materials, including proteins, DNA and other biopolymers. It is safe to say that, despite the great progress made in recent years in determining the atomic and molecular structure of living matter and other complex substances, it is not yet possible to detect with enough accuracy and specifically the intermolecular electrostatics forces. The aim of the basic research planned at NICPB is to engage the best experimental and computational methodology to find access to direct measurement of the local electrostatic interactions on the nanometer scale, incl. in biological molecular structures. If successful, this would ultimately allow us to better understand the physical principles of life itself.

Third, we aim to develop an experimental capability for nonlinear quantum optics to measure the interaction between a light-absorbing substance and entangled- or biphoton states of light. Since this constitutes an entirely new direction for our group, we hope to achieve success by capitalizing on our expertise in advanced conventional 2PA materials, spectroscopy and photo detection. Biphotons have interesting high-potential applications in information technology, and our long-term goal is to develop spectroscopy of the corresponding specialized nonlinear-optical materials, multiphoton fluorophores, etc.

3.3.5 Energy technologies

Research of energy materials is of utmost importance to the energy production and storing in the next generation fuel cells, Li-ion batteries, and supercapacitors. The programme focuses on solid oxide fuel cells making use of our unique capacity and competences to do optical, electrochemical impedance, thermogravimetric measurements of those compounds, to say nothing about solid state NMR studies at extremely low (10°K) and high (1200°K) temperatures.

We are also active in the development of commercially usable SOFC elements and their stacks with our commercial partner Elcogen Ltd.

The carbon nanomaterials are important in fuel cells and hydrogen energy. We are experimenting in employing novel techniques to produce carbon by electrolysis and studying the electrochemical production of fuels. In addition, different carbon-based catalyst materials are synthesized and tested for low-temperature fuel cells and metal-air batteries. This also includes valorisation of lignin and other biomass-based waste materials. Research on low-temperature fuel cells and on their different components is carried out in collaboration with PowerUP Fuel Cells.

Lithium-ion batteries (LIBs) powered appliances have grown rapidly in recent years and, with this process showing no sign of abating, the quantity of spent LIBs (SLIBs) that will emerge soon is substantial. As LIBs contain graphite and different valuable materials (the cathode layer holds Li, Co, Ni, Mn, Al and the anode layer graphite and Cu), the recycling of SLIBs is economically and environmentally beneficial. Thereby working group of Energy Technologies is focusing on development of methods and technology for complete and sustainable recycling of Li-ion batteries.

Given the need for development of nuclear energy related competence in Estonia a Nuclear Science and Engineering (NSE) research group has been established in the High Energy and Computational Physics laboratory. NSE group is carrying out high-quality research in the fields of reactor physics, reactor technology and nuclear power safety to provide technical expertise in power and non-power applications of nuclear technology. Clear understanding of the nature of nuclear power is a key element in the development of Estonian nuclear energy strategy as well as to inform public debates on the wise use of nuclear technologies to overcome the challenges fighting the climate change.

3.4 High Energy Physics and Theoretical Physics

The most important open questions in contemporary elementary particle physics are the origin of mass and the physical mechanisms determining the state of the Universe (including Dark Matter and Energy). This program includes both theoretical work and numerous international experiments in particle physics and cosmology. The strategy of the Institute is to be involved in both: in the development of new theories and in their experimental testing in forthcoming experiments.

3.4.1 Experimental High Energy Physics

In the experimental side NICPB is a member of the CMS collaboration at the Large Hadron Collider at CERN. NICPB is the coordinator of Estonian scientists and various other programs at CERN including summer students.

As a required tool for large scale distributed data analysis the Institute also houses a Tier-2 computing centre, which is one of the biggest computing centres for the CMS experiment in Europe.

The physics program of the experimental group has been tied mostly to the Higgs boson and top quarks in the initial state with leptons in the final state and with special emphasis on the tau lepton. The group has been extremely active in tau related final states and leading in various top and Higgs subgroups in that regard. The current analysis effort is finalizing measurements at the LHC Run II for ttH final state and is moving forward with di-Higgs searches in preparation for Run III.

In parallel the group is also expanding closer to hardware through contributions to the Level 1 and High-Level Trigger efforts. Those include both software and algorithms, but also their implementation in hardware. In this regard the group is in active collaboration with the Tallinn Technical University to leverage their FPGA expertise.

Recently the group has also started initial studies of tau lepton related studies at the next large accelerator concept, the FCC-ee. These studies are at this point very preliminary, but a required effort to extend the knowledge to e^+e- colliders and prepare the next generation of experimentalists who will help design, build and operate the next accelerator and related detector programs.

3.4.2 Theoretical Physics, Astrophysics and Cosmology

The direction of the theoretical work in NICPB is phenomenological and relies on the availability of experimental data. The research topics developed at the NICPB are related to the interpretation of various high- and low energy particle physics experiments as well as to the developments in astrophysics and in cosmology. In addition, there exist statistical physics and gravity groups carrying out the related research.

In theoretical particle physics the researchers of NICPB interpret both the LHC data as well as the data from low energy experiments. We develop new physics theories to be tested using Higgs boson and other LHC data which could explain the existence of dark matter of the Universe. In this moment there are important developments in astrophysics and in cosmology which are related to explaining the dark matter and dark energy of the universe, and in physics of gravitational waves and black holes. Today the nature and origin of the dark matter and dark energy are unknown. The discovery of gravitational waves opened a new avenue in this research – the multimessenger astronomy – which allows one to study properties of astrophysical objects and physical processes using new gravitational wave data. The researchers of NICPB contribute to this development. The studies of cosmology in the NICPB are dominated by the studies of various dark matter candidates starting from theoretical model building, predicting their properties and performing computer simulations for their cosmological behaviour. Another priority topic of theoretical research is relating inflation to new theories of gravity, in particular to Palatini gravity, and to the dark matter. Due to the discovery of gravitational waves it become possible to test particle physics phenomena in the early Universe, such as phase transitions, as well as the extensions of gravity beyond General Relativity. Those new theories may be tested in precision studies of black holes or in new behaviour of gravitational waves. For example, the researchers of NICPB have contributed to studies of primordial black hole dark matter starting from their production in inflation, their abundance and their tests using multi-messenger astronomy. All those topics in theoretical particle physics, astrophysics and cosmology form one logical problem which the researchers of the NICPB attack from all possible angles. To help this approach to research, the NICPB is leading Centre of Excellence

"The Dark Side of the Universe" which coordinates this research with the University of Tartu and with the Tartu Observatory.

In the field of statistical physics, the researchers of NICPB study different problems of physics and complex systems. Among others, different diffusion processes (normal and anomalous diffusion, classical and quantum Brownian motion) and their relevance in and influence on the behaviour of various complex systems. Diffusion processes are important for the functioning of cells, in condensed matter theory, astrophysics as well as in sociology, economy, ecology, language dynamics etc. Often one must consider interaction processes specific to the system under study, considering various forces as well as through exchange processes (the researchers of NICPB study for example kinetic wealth exchange models applied to some economic systems, analogously to the kinetic energy exchange models of gases), competition (language dynamics and ecological systems) or different frameworks. During recent years it has become clear that also the heterogeneity of the subsystems or individuals is important for the system behaviour and the researchers of NICPB have contributed in this understanding; for example, the mechanism of the power-law in heterogeneous systems has been proposed. A new research line concerns the use of Bayesian statistics in the semiotic and language naming games relevant for the modelling and understanding of human learning processes as well as for applications in the artificial intelligence.

4 Laboratories

4.1 Laboratory of High Energy Physics and Computational Physics

The research activities of the laboratory covers theoretical physics, astrophysics, cosmology, experimental high energy physics and as a new topic nuclear reactor technology and safety. The head of the laboratory M. Raidal.

The Laboratory has been growing, maybe even too rapidly. There are enough students, including PhD students, but the number of postdoctoral researches is a bit too high. The quality of the PhD students varies across the research groups and finding good postdoctoral researchers is a problem in the group of experimental particle physics. As of November 2020, the Laboratory employs 29 researchers and postdocs with PhD, including two top researchers. They supervise 8 doctoral students and 1 master student in different Estonian universities. Those researchers have been successful in grant applications.

Funding of research groups is covered by current projects but starting from 2022 we need to secure new team grants from the Estonian Science Agency, the most likely source of funding for basic research in Estonia.

The laboratory is active in solving problems theoretical and experimental particle physics on international level. According to Essential Science Indicators the group had several top papers in 2020. And one can always do better. Several new topics have been started recently. After the discovery of gravity waves we started to investigate their possible origins, how they can be created and how the gravity waves related are to particle physics. The most important new task in experimental particle physics is participation in building the new trigger for the CMS upgrade. As a completely new direction for the institute we have started a group to study the nuclear safety, a topic that can be very important in future when Estonia must decide on the possible use of nuclear energy to reduce CO_2 emissions.

The working conditions in the lab are good, the experimentalists moved to the newly renovated offices on the 5th floor of the downtown building. There is a problem with the roof of the building that leaks with heavy rain and wind from certain direction.

4.1.1 Grants, budget in 2020

In 2020 the budget of the laboratory consists mostly of research grants: team grants 47%, personal grants 10%, top researcher's grants 20% and CERN research contract 18%.

- Centre of Excellence, Institutional and team grants[3] totalling
  - TK133 "Dark Side of the Universe", M. Raidal (2016 – 2022)
  - IUT39-1 "The role of diversity in complex systems" (2015 – 2020), E. Heinsalu
  - PRG434 "Multimessenger astronomy as a probe of new physics" (2019 – 2023), K. Kannike
  - PRG445 "Study of Higgs boson production in the decay channel to tau leptons" (2019 – 2023), C. Veelken
  - PRG780 "Preparing the CMS experiment for high luminosity operations through trigger improvements" (2020 – 2024), M. Kadastik (NICPB) in partnership with Tallinn Technical University
  - PRG803 "Multi-Messenger Probes of Dark Matter" (2020 – 2024), M. Raidal
- Top Researchers Grants
  - MOBTT5, "Beyond the Standard Model of Particle Physics" (2017 – 2022), J. Ellis
  - MOBTT86, "Probing the Higgs sector at the LHC and beyond" (2018 – 2022), A. Djouadi
- Personal Grants
  - Marie Skłodowska-Curie grant 78564 "Early Universe Vacuum Stability and Beyond the Standard Model Physics" (EUVSBSMP, 2019 – 2021), T. Markkanen
  - PUT1356 "Dynamics of languages: Models and methods from complex systems theory" (2017 – 2020), M. Patriarca
  - MOBJD323 "Cosmological impacts of the electroweak vacuum instability" (2018 – 2020), T. Markkanen
  - MOBJD381 "Dynamically induced Planck, dark matter, neutrino and electroweak mass scales" (2018 – 2020), A. Karam
  - MOBJD527 "Searching Higgs particle and developing trigger algorithm in the CMS detector at LHC, CERN Switzerland" (2019 – 2021), S. Bhowmik
  - MOBTP135, "Physics of boson stars and its implications for new physics", (2019 – 2021), H. Veermäe
  - MOBTP176, "Passive cooling during severe accidents in small modular reactors", (2020 – 2022), M. Jeltsov
- CERN research contract

4.1.2 Up to 10 important publications

1. Arcadi, Giorgio; Djouadi, Abdelhak; Raidal, Martti, Dark Matter through the Higgs portal, **Physics Reports-Review Section of Physics Letters** Volume: 842 Pages: 1-180 Published: FEB 3 2020
2. CMS Collaboration, Extraction and validation of a new set of CMS pythia8 tunes from underlying-event measurements, **European Physical Journal C** Volume: 80 Issue: 1 Published: JAN 3 2020

[3] PRG356 "Gauge gravity: unification, extensions and phenomenology (2019 – 2023)", T. Koivisto, is hosted by Tartu University in collaboration with NICPB

3. By: Vaskonen, Ville; Veermaee, Hardi, Lower bound on the primordial black hole merger rate, **Physical Review D** Volume: 101 Issue: 4 Article Number: 043015 Published: FEB 19 2020
4. CMS Collaboration, Study of excited Lambda(0)(b) states decaying to Lambda(0)(b)pi(+)pi(-) in proton-proton collisions at root s=13TeV, **Physics Letters** B Volume: 803 Article Number: 135345 Published: APR 10 2020
5. Fabbrichesi, Marco; Gabrielli, Emidio, Dark-sector physics in the search for the rare decays K+ -> pi(+)nu(nu)over-bar and K-L -> pi(0)nu(nu)over-bar, **European Physical Journal C** Volume: 80 Issue: 6 Article Number: 532 Published: JUN 13 2020
6. Kannike, Kristjan; Loos, Kaius; Raidal, Martti, Gravitational wave signals of pseudo-Goldstone dark matter in the Z(3) complex singlet model, **Physical Review D** Volume: 101 Issue: 3 Article Number: 035001 Published: FEB 3 2020

4.2 Laboratory of Chemical Physics

The laboratory of chemical physics is led by Dr. R. Stern, the research programs are categorised as mostly physics (section 3.3 Physics, Materials Science and Energy Technologies) and mostly chemistry (3.2.2 Chemistry and Spectroscopy, 3.2.3 Supramolecular Chemistry).

As of November 2020, the Laboratory employs 22 researchers and postdocs with PhD. They supervise 15 doctoral students mostly from Tallinn University of Technology and one MSc student. Most of the PIs have been successful in grant applications, they have new ideas, there PhD students and postdocs in their groups. The fastest growing has been the energy technology group of Ivar Kruusenberg who have found themselves within the rapidly evolving field of hydrogen energetics, they can increase the institute's visibility where practical impact on economy is expected. An emerging talent in developing liquid state NMR experiment techniques to increase the sensitivity is Indrek Reile. High-resolution solid-state NMR at the same time has lost some of its novelty and is struggling to find funding.

The laboratory runs the largest infrastructure of the institute, the Tallinn branch of the Estonian Magnet Laboratory that has several nuclear magnetic resonance (NMR) instruments, THz spectroscopy and low temperature physics setups, all backed by the in-house helium liquefier. While the Estonian Magnet Laboratory is a completely informal structure NICPB is a partner in the Horizon2020 project "ISABEL"[4].

In 2020 an ERC advanced grant proposal by Girsh Blumberg got funding, he plans to start from July 2021.[5]

On the national level NICPB is making laboratory's instruments available within a broader scientific infrastructure network, the Estonian Center of Analytical Chemistry which is a distributed interdisciplinary scientific research infrastructure for the development and application of modern analytical methods as well as the quality assurance of chemical measurements in research, surveillance and industry laboratories. In collaboration with Tallinn Technical University the 500 MHz liquid state NRM spectrometer was upgraded from an outdated Bruker console with a refurbished last generation Agilent console that made it usable again. Several chemistry labs were also renovated with new fume hoods, etc.

[4] ISABEL - Improving the sustainability of the European Magnetic Field Laboratory: Development And Long-Term Sustainability of New Pan-European Research Infrastructures H2020-INFRADEV-2018-2020_topic: INFRADEV-03-2018-2019

[5] ERC-2019-ADG number 885413 – Kerr, https://cordis.europa.eu/project/id/885413

Working conditions are good in general, but some of the labs should be renovated and more office space should be added.

4.2.1 Grants, budget in 2020

About 50% of laboratory's budget is covered by team grants, 21% by personal grants, 14% by several smaller contracts and the institute covers 15% of expenses in 2020 to support high-resolution solid-state NMR:

- Centre of Excellence and team grants
    - TK134 "Emerging orders in quantum and nanomaterials (2015 – 2023)", U. Nagel
    - PRG4 "Emerging Novel Phases in Strongly Frustrated Quantum Magnets (2018 – 2022)", R. Stern (NICPB)/A. Tamm (UT)
    - PRG661 "Femtosecond multiphotonics: From quantitative spectroscopy to quantum optics" (2020 – 2024)", A. Rebane
    - PRG736 "Sub-THz range polar Kerr spectroscopy of chiral superconductors (2020 – 2024)", U. Nagel
- Personal Research Grants
    - PSG11 "Quantitative detection of cancer biomarkers in urine by hyperpolarized NMR (2018 – 2021)", I. Reile
    - PSG312 "Metal Oxide-based Catalyst Materials from Recycled Li-ion Batteries for Metal-air Battery and Fuel Cell Applications (2019 – 2022)", I. Kruusenberg
    - PSG317 "Quantitative sensing of intramolecular electric fields by DNA-intercalating organometallic two-photon probes (2019 – 2022)", C. Stark
    - PSG400 "Functional cavitands for drug discovery and delivery (2020 – 2023)", J. Adamson
    - MOBTP128 "Nonlinear-optical metrology (2018 – 2020)", M. Sildoja
    - MOBJD449 "Unconventional superconductivity in the $Mo_nGa_{(5n+1)}$ intermetallics (2018 – 2020)", V. Verchenko
- Several research contracts with companies

4.2.2 Up to 10 most important publications from 2020:

1. K. Amelin, Y. Alexanian, U. Nagel, T. Room, J. Robert, J. Debray, V. Simonet, C. Decorse, Z. Wang, R. Ballou, E. Constable, and S. de Brion. "Terahertz magneto-optical investigation of quadrupolar spin-lattice effects in magnetically frustrated $Tb_2Ti_2O_7$". **Physical Review B**, 102(13), OCT 20 2020.
2. K. Amelin, J. Engelmayer, J. Viirok, U. Nagel, T. Room, T. Lorenz, and Z. Wang. "Experimental observation of quantum many-body excitations of E-8 symmetry in the Ising chain ferromagnet $CoNb_2O_6$." **Physical Review B**, 102(10), SEP 24 2020.
3. K. Kaare, E. Yu, A. Volperts, G. Dobele, A. Zhurinsh, A. Dyck, G. Niaura, L. Tamasauskaite-Tamasiunaite, E. Norkus, M. Andrulevicius, M. Danilson, and I. Kruusenberg. "Highly Active Wood-Derived Nitrogen-Doped Carbon Catalyst for the Oxygen Reduction Reaction". **ACS Omega**, 5(37):23578-23587, SEP 22 2020.
4. A. M. Kantola, P. Lantto, I. Heinmaa, J. Vaara, and J. Jokisaari. "Direct magnetic-field dependence of NMR chemical shift". **Physical Chemistry Chemical Physics**, 22(16):8485{8490, APR 28 2020.
5. K. Kukli, M. Mikkor, A. Sutka, M. Kull, H. Seemen, J. Link, R. Stern, and A. Tamm. "Behavior of nanocomposite consisting of manganese ferrite particles and atomic layer deposited bismuth oxide chloride film". **Journal of Magnetism and Magnetic Materials**, 498, MAR 15 2020.

6. L. G. Lukasiewicz, M. Rammo, C. Stark, M. Krzeszewski, D. Jacquemin, A. Rebane, and D. T. Gryko. "Ground- and Excited-State Symmetry Breaking and Solvatofluorochromism in Centrosymmetric Pyrrolo[3,2-b]pyrroles Possessing two Nitro Groups". **Chemphotochem**, 4(7):508{519, JUL 2020.
7. D. Opherden, N. Nizar, K. Richardson, J. C. Monroe, M. M. Turnbull, M. Polson, S. Vela, W. J. A. Blackmore, P. A. Goddard, J. Singleton, E. S. Choi, F. Xiao, R. C. Williams, T. Lancaster, F. L. Pratt, S. J. Blundell, Y. Skourski, M. Uhlarz, A. N. Ponomaryov, S. A. Zvyagin, J. Wosnitza, M. Baenitz, I. Heinmaa, R. Stern, H. Kuhne, and C. P. Landee. "Extremely well isolated two-dimensional spin-1/2 antiferromagnetic Heisenberg layers with a small exchange coupling in the molecular-based magnet Cu-POF". **Physical Review B**, 102(6), AUG 28 2020.
8. R. Rasta, I. Heinmaa, K. Kimura, T. Kimura, and R. Stern. "Magnetic structure of the square cupola compound $Ba(TiO)Cu_4(PO_4)_4$:a ^{31}P NMR Study" **Physical Review B**, 101(5), FEB 12 2020.
9. D. Szaller, K. Szasz, S. Bordacs, J. Viirok, T. Room, U. Nagel, A. Shuvaev, L. Weymann, A. Pimenov, A. A. Tsirlin, A. Jesche, L. Prodan, V. Tsurkan, and I. Kezsmarki. "Magnetic anisotropy and exchange paths for octahedrally and tetrahedrally coordinated Mn^{2+} ions in the honeycomb multiferroic $Mn_2Mo_3O_8$". **Physical Review B**, 102(14), OCT 7 2020.
10. Z. Zhang, K. Amelin, X. Wang, H. Zou, J. Yang, U. Nagel, T. Room, T. Dey, A. A. Nugroho, T. Lorenz, J. Wu, and Z. Wang. Observation of E-8 particles in an Ising chain antiferromagnet. **Physical Review B**, 101(22), JUN 26 2020.

4.3 Laboratory of Chemical Biology

The Laboratory of Chemical Biology is the smallest laboratory of the NICPB, employing 9 PhD researchers: who supervise 2 PhD students. The head of the Laboratory is Dr. T. Käämbre. The planned research in the field of fundamental and applied bioenergetics (section 3.2.1) is ambitious and publications are of high quality.

The laboratory joins excellent scientists with various backgrounds on chemistry, physics, medicine, biochemistry and system biology. The laboratory is a member of MitoGlobal Network - a world-wide information platform for scientific mitochondrial organizations and mitochondrial research consortia. The laboratory is a member of the steering committees of two COST networks (COST MITOEAGLE and EU CARDIOPROTECTION).

The lack of funding and good people is recognized by the institute, supporting the hiring of Anton Terasmaa in September 2020 who will focus on energy metabolism studies for two types of pathology, neurodegeneration and cancer, what probably share the same biochemical changes, just in the opposite directions.

4.3.1 Funding and grants.

In 2020 the budget of the laboratory is covered by NICPB central funding and there is just one personal research grant[6].

- PUTJD963 " A new therapeutic strategy to eradicate cancer stem cells (CSCs) in breast cancer (2020 – 2022)", a post-doctoral grant of A. Klepinin for working with Prof. Michael P. Lisanti in Manchester.

4.3.2 Up to 6 most important papers from 2020

1. E Rebane-Klemm, L Truu, L Reinsalu, M Puurand, I Shevchuk, Vladimir Chekulayev, Natalja Timohhina, Kersti Tepp, Jelena Bogovskaja, Vladimir Afanasjev, Külliki Suurmaa, Vahur Valvere, Tuuli Kaambre.

[6] The lab got 1 year funding for 2021: PRG1035, PI T. Käämbre "Oncobioenergetics of breast and colorectal cancer: in vitro models and clinical material: from 'omics' to mathematical modeling" that helps to refocus the research

Mitochondrial Respiration in KRAS and BRAF Mutated Colorectal Tumors and Polyps, Cancers Volume: 12 Issue: 4 Article Number: 815 Published: APR 2020, DOI: 10.3390/cancers12040815

2. M Makrecka-Kuka, E Liepinsh, AJ Murray, H Lemieux, M Dambrova, Kersti Tepp, Marju Puurand, Tuuli Käämbre, Woo H Han, Paul de Goede, Katie A O'Brien, Belma Turan, Erkan Tuncay, Yusuf Olgar, Anabela P Rolo, Carlos M Palmeira, Neoma T Boardman, Rob CI Wüst, Terje S Larsen. Altered mitochondrial metabolism in the insulin-resistant heart, Acta Physiologica Volume: 228 Issue: 3 Article Number: e13430 Published: MAR 2020, doi: 10.1111/apha.13430
3. M Ruiz-Meana, K Boengler, D Garcia-Dorado, DJ Hausenloy, T Kaambre, . Georgios Kararigas, Cinzia Perrino, Rainer Schulz, Kirsti Ytrehus. Ageing, sex, and cardioprotection. British Journal of Pharmacology; 2020 doi: 10.1111/bph.14951
4. A Koit, N Timohhina, L Truu, V Chekulayev, S Gudlawar, I Shevchuk, . Lepik K, Mallo L, Kutner R, Valvere V, Kaambre T.. Metabolic and OXPHOS activities quantified by temporal ex vivo analysis display patient-specific metabolic vulnerabilities in human breast cancers. Front Oncol. 2020 Jun 30;10:1053. DOI: 10.3389/fonc.2020.01053
5. Klepinin A, Zhang S, Klepinina L, Rebane-Klemm E, Terzic A, Kaambre T, Dzeja P. Adenylate Kinase and Metabolic Signalling in Cancer Cells. Front Oncol. 2020 May 19;10:660, DOI: 10.3389/fonc.2020.00660
6. Tepp K, Puurand M, Timohhina N, Aid-Vanakova J, Reile I, Shevchuk I, Chekulayev V, Eimre M, Peet N, Kadaja L, Paju K, Käämbre T. Adaptation of striated muscles to Wolframin deficiency in mice: Alterations in cellular bioenergetics. Biochim Biophys Acta Gen Subj. 2020 Apr;1864(4):129523. doi: 10.1016
7. US Patent 10,753,924

4.4 Laboratory of Environmental Toxicology

The research activities of the laboratory led by academician Anne Kahru are outlined in the program of Environmental Toxicology and Nanotoxicology (section 3.1) and is pursued in two main directions (i) ecotoxicology of nanoparticles and microplastic and (ii) evaluation of efficiency and safety of antimicrobial compounds. Publications are of high quality in both directions.

We have gained funding for the next two years via national and EU research funding competitions.

The Laboratory has been growing and as of November 2020 employs 13 researchers and postdocs with PhD who supervise 4 doctoral students and 6 master students.

Working conditions have been improved and a new large laboratory room and an office room for 10 students are under renovation

4.4.1 Grants, budget

In 2020 team grants cover 53%, personal research grants cover 18% of the budget of the laboratory with various contracts totalling 23% of the budget of the laboratory.

- Team grants
  - PRG684 "Technology-critical elements: potential ecotoxicological effects of application (2020-March 2021)", I. Blinova
  - PRG749 "Antimicrobial chitosan-nanocomposites for biomedical applications: efficiency and safety (2020 – 2024)", K. Kasemets
- 3 Personal research grants
  - PUT1015 "Nanoparticle-macrophage interactions in vitro: focus on nanosafety (2016 – 2021)" O. Bondarenko
  - PUT1512 "Evaluation of the potential hazardous effects of microplastic to marine and freshwater zooplankton (2017 – 2021)", M. Heinlaan
  - PSG311 Response of algal communities to toxicants with different modes of action (2019 – 2022). V. Aruoja
  - MOBJB509 "Assessment of hazard of UV weathered microplastics in aquatic environment (UV-PLASTOX) (2020 – 2022)", Alla Khosrovyan
  - Marie Skłodowska-Curie Grant 867457 "Nanocomposite Engineered Particles for Phosphorus Recovery and Toxicological Risk Assessment for the Aquatic Environment — NanoPhosTox" (2020 – 2022), Asya Ivanova Drenkova-Tuhtan
- Other projects
  - EC Horizon 2020, H2020-MSCA-ITN-2019-859891 grant 'Best chemical risk assessment professionals for maximum Ecosystem Services benefit – PRORISK, 1.04.2020–31.03.2024. A. Kahru, M. Heinlaan, V. Aruoja,
  - partnership in the Estonian Scientific Infrastructure Roadmap Object NAMUR+ (2017 – 2021 (A. Kahru, K. Kasemets). Coordinator of the project: Dr. Vambola Kisand (Tartu University)
  - RITA1/02-10-09 research grant from the Ministry of Agriculture 'Opportunities for mitigation of bee losses' (ForBee), 2019 – 2021. A. Kahru, M. Sihtmäe, I. Blinova. Coordinator Dr Marika Mänd (Estonian University of Life Sciences)
  - COSVG16 "Novel nanoparticle-based filter materials and face masks for SARS-CoV-2 inactivation (2020 – 2021)" O. Bondarenko NICPB in collaboration Tartu University, Tallinn University of Technology and Esfil Tehno

4.4.2 Up to 10 publications from 2020

Ecotoxicology of nanoparticles and microplastic

1. Heinlaan, M., Kasemets, K., Aruoja, V., Blinova, I., Bondarenko, O., Lukjanova, A., Khosrovyan, A., Kurvet, I., Pullerits, M., Sihtmäe, M., Vasiliev, G., Vija, H., Kahru, A. (2020). Hazard evaluation of polystyrene nanoplastic with nine bioassays did not show particle-specific acute toxicity. **Science of The Total Environment**, 707, 136073. https://doi.org/10.1016/j.scitotenv.2019.136073
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3. Blinova, I., Muna, M., Heinlaan, M., Lukjanova, A., Kahru, A. (2020). Potential Hazard of Lanthanides and Lanthanide-Based Nanoparticles to Aquatic Ecosystems: Data Gaps, Challenges and Future Research Needs Derived from Bibliometric Analysis. **Nanomaterials,** 10(2), 328. https://doi.org/10.3390/nano10020328
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5 Budget of NICPB

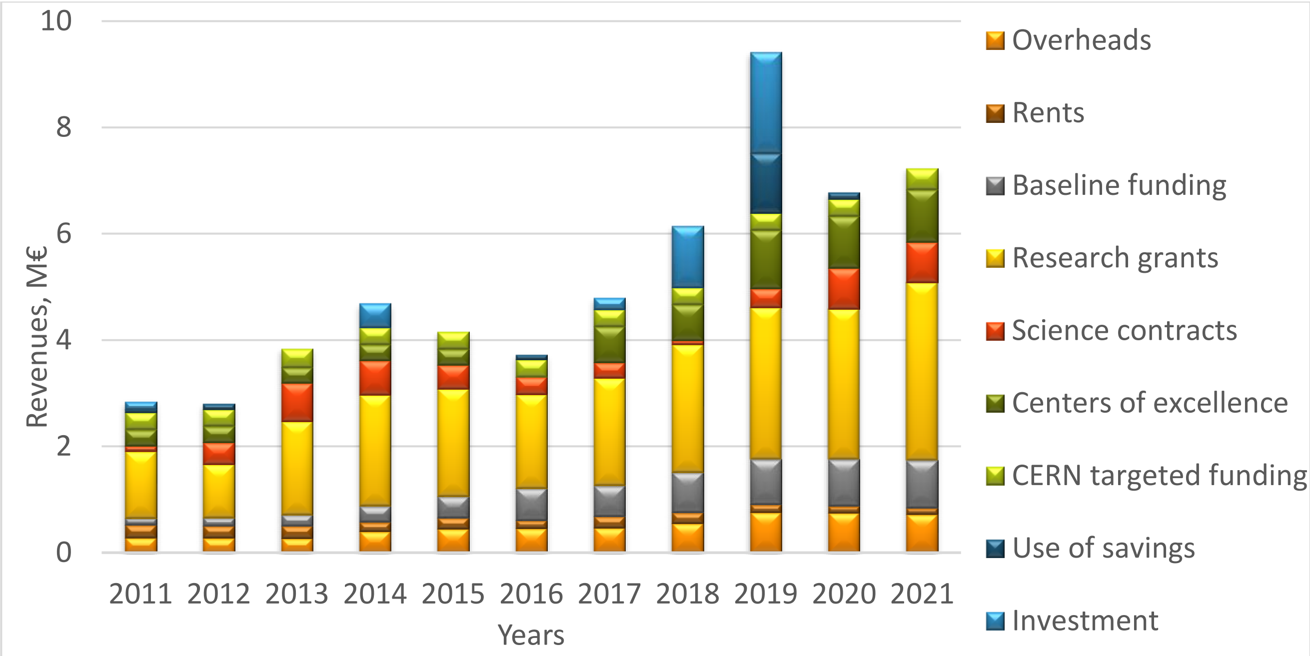


Figure 2. The budget of NICPB from 2011 to 2021 as approved by the science council.

The majority of revenues in the budget of NICPB come from various research grants of the Estonian Science Agency. The next biggest item is the Estonian centers of excellence funding, followed by baseline funding. Science contracts with companies and various EU institutions is by amount similar to the sum of all overheads. As seen from Figure 2, the budget of NICPB has increased from 2011 more than twice while the number of researchers has increased much less over the same period (Figure 1) and the number of PhD students has increased from 4 to 29. Baseline funding of the institute is calculated form the publication record, volume of research contracts, etc. over few past years and it is also a form of competitive funding, but more stable than grants.

In 2018 and 2019 we renovated the Akadeemia tee building, insulated the walls and roof, replaced windows and the heating system and installed a ventilation system. The renovation was made possible by investment through the ASTRA project that covered more than half of the costs, the rest being covered by part of the 2017, 2018 and 2019 baseline funding of the institute.

Grants are spent according to the specific rules of each grant type, following the budget of the grant. The researchers' salaries are covered by grants or by the centres of excellence.

Overheads together with rental revenues are not enough to cover the running costs of the institute (heating, electricity, salaries of administration, etc.) and we have always used part of the baseline funding to cover them, see Figure 3 for the comparison. The institute has supported the laboratories from the baseline funding over the years, but the principles have not been very stable. Generally, a laboratory has been supported if they suddenly fail to secure grant funding to pay salaries to core personnel.

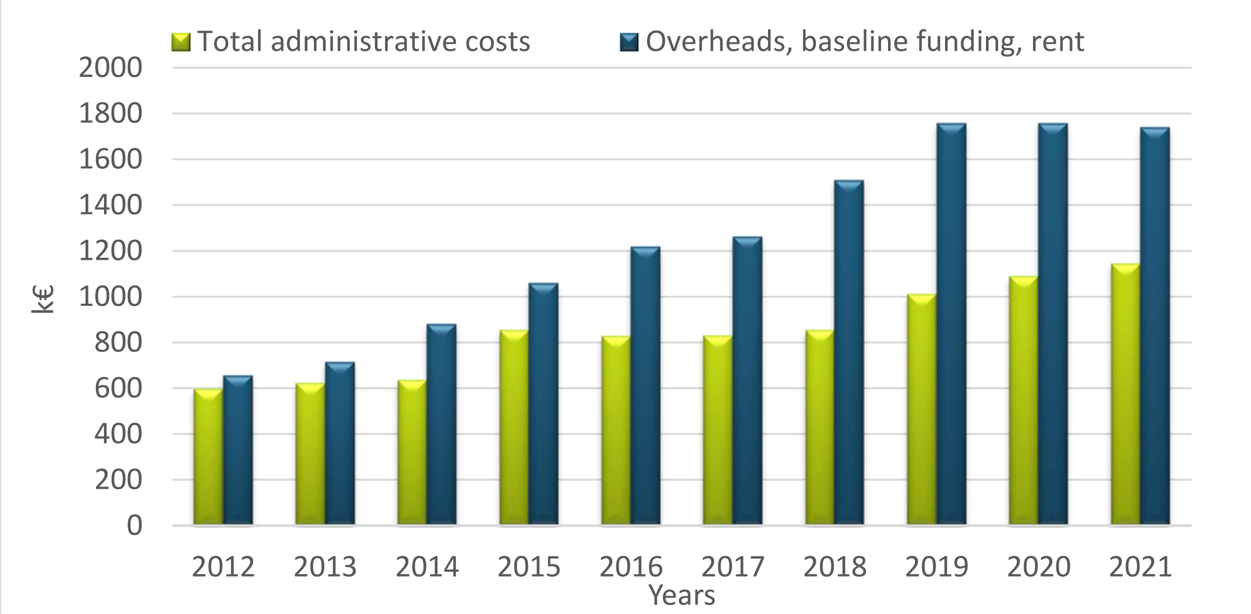


Figure 3. Administrative costs compared to the funding sources that can be used to cover them.

One of the milestones of our development plan is the introduction of a tenure track model (2.9.3). Our aim has been to obtain some additional stable funding to cover the salaries of a limited number of our core senior researchers. We have had no success so far, as the Estonian science funding model is based on competitive grants.

Nevertheless, we do have some possibilities. We see from *Figure 3* that recently we have had about 500 k€ each year that we have been able to use for the development of the institute. From that money we must renovate lab spaces, cover the self-funding costs of projects, start new topics and eventually replace aging core infrastructure that is beyond the scope of separate research projects. And we could spend some of it on salaries.

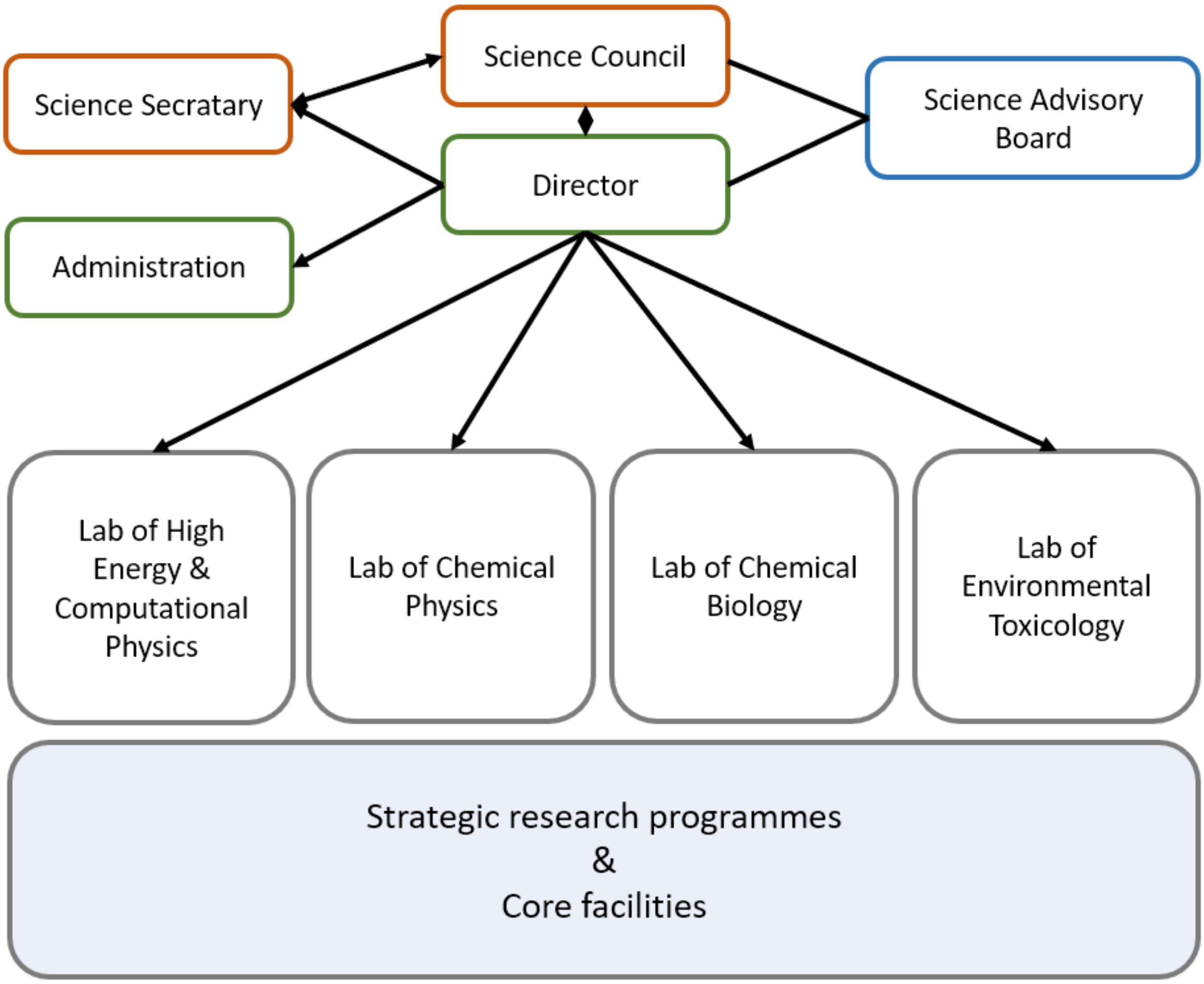
5.1 NICPB development fund

In September 2020 the institute formed an institute development fund, using the 1.4 M€ that we received from selling the Akadeemia tee 25 property to the state, as the Ministry of Education and Science wants to build a public state-owned high school with the focus on real sciences next to the campus of the technical university.

The purpose of the NICPB development fund is to promote new ideas that follow the strategic research programs by start-up funding for one year. We have elected younger researchers into the council of the development fund, one from each laboratory, together with the director and deputy director. Three projects were granted funding in 2020 with the total of about 500 k€.

6 Appendix

6.1 NICPB organization chart



6.2 NICPB administration chart