

**National Institute of  
Chemical Physics and Biophysics**



# **Activity Report 2007–2010**

**NICPB 1980–2010**

**National Institute of Chemical Physics and Biophysics**

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**Toomas Välimäe, Ed.**

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## Mission

NICPB is a professional science institution, where the main task of the scientists is research that values academic freedom.

NICPB carries out fundamental and applied research and engages in the development of the novel directions in material sciences, gene- and biotechnology, environmental technology and computer science.

NICPB helps to educate a new generation of scientists in accordance with the association contracts and other contracts with the universities and other academic institutions.

Institute introduces its work regularly in other research and degree-granting institutions, in specialised literature, scientific conferences and public media.

## Vision

NICPB is an integrated and effective scientific institution, where all employees recognise their responsibilities and possibilities in achieving the goals of the Institute. NICPB's reputation is based on high-level research, initiation of innovative topics and development of competence and scientific infrastructure at national and also international level.

## Preface

NICPB is a unique phenomenon on the scientific landscape of Estonia, most likely also in the Baltic States and maybe even in the whole Northern Europe. As the only Institute from the former Academy of Sciences surviving the wave of merges to various universities, it nowadays sets an example of purely professional scientific research institution in our country. NICPB celebrated its 30th birthday in year 2010, so this current summary serves also as an internal evaluation of our performance and success during the years of independent research Institute on the landscape shaped by several large and dominating universities. There are many reasons to be proud of the achievements of our scientists. Based on the Thomson Reuters ISI WoK database, the NICPB, while 60 times smaller than our best partner and competitor, the University of Tartu, has published only 15 times less peer refereed papers that have been cited only 8 times less than the whole production of the UT making the average citations per NICPB papers almost 2 times better than those from UT. Besides this historical remark, we recently deserved the trust of our national authorities to host 2 out of the 20 objects of the new Estonian Research Infrastructure Roadmap: The CERN-Estonian cooperation and the Estonian Magnet Laboratory. We will invest our experience and competence into the development of both of these scientific centres to strengthen further the good image of Estonia as an excellent place for R&D&I.



**Raivo Stern**  
**Director**



# I RESEARCH AND DEVELOPMENT

## Research

Scientific research in the Institute is based on strategic scientific programmes that integrate different, yet closely interrelated areas of science. According to the Strategic Plan for 2005 to 2015, the programmes are:

Bioenergetical nonlinear photonics	Macromolecular interactions
Environmental Chemistry	New spin materials and states
In vitro toxicology and 3R	Nuclear Magnetic Resonance
Ionic conductivity and catalysis	Particle physics

In practice the research follows long-term research projects funded by the targeted financing schemes that have been approved by the Minister of Education and Research.

## 1 Bioenergetics

### ***Topic: Mechanisms of regulation of integrated energy metabolism in cancerous and muscle cells***

The project is funded from the NICPB Targeted Funding Scheme SF0180114Bs08

**Principal Investigator:** Professor Valdur Saks, DSc, Member of the Academy of Sciences of Estonia  
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Web: <http://www.kbfi.ee/?id=59>

The Laboratory of Bioenergetics has actively participated in developing a new direction, Molecular Systems Bioenergetics (MSB), which is an important part of Systems Biology. The main focus of MSB are the processes of energy conversion both at molecular and cellular levels, with special emphasis on the structure and function of energy transfer and regulatory networks, mechanisms of interaction between their components, and a quantitative description of these networks by computational models.

Our earlier work described quantitatively the molecular organization, dynamics and regulation of integrated energy metabolism in adult cardiac and skeletal muscle. The existing data on regulation of mitochondrial energy conversion point to decisive role of protein-protein interactions between the cytoskeletal proteins and the mitochondrial outer membrane. This regular system with crystal-like arrangement of mitochondria is highly organized due to specific organization of the cytoskeletal system of muscle cells. During the last years we have formulated a model of regulation of respiration in a supercomplex named Mitochondrial Interactosome. In cancerous cells this complex is significantly modified.

The results of these investigations will give the basis for understanding of many cellular pathologies of heart like ischemia, heart failure, myocardial infarction, neurodegenerative diseases, bioenergetic mechanisms of cancer and mechanisms of reperfusion injury.

The Laboratory of Bioenergetics is in tight collaboration with French scientists in Bordeaux and Grenoble Universities, with Innsbruck Medical University, Daniel Swarovski Research Laboratory and with National Institutes of Health, USA.

**Researchers**

Valdur Saks, PhD, DSc

Vladimir Tšekulajev, PhD

Tiia Anmann, PhD

Natalja Timohhina, PhD student

Tuuli Käämbre, PhD

Kersti Tepp, PhD student

Peeter Sikk, PhD

Minna Varikmaa, PhD student

Igor Ševtšuk, PhD

**Associated Targeted Financing**

1. Mechanisms of integration and regulation of mitochondria and ATPases in normal oxidative muscle cell, 2003-2007, SF0182549Bs03, PI: V. Saks

**Associated Estonian Science Foundation (ETF) Grants**

1. Compartmentalized energy transfer in cardiomyocytes and mechanisms of preconditioning, 2005-2008, ETF6142, PI: V. Saks
2. Dynamics of formation of modular bioenergetic systems during differentiation of stem cells into myocytes and their degradation during ageing, 2009-2012, ETF7823, PI: V. Saks

**Scientific Degrees Defended**

1. Saaremäe, Merle. The expression of  $\beta$ -tubulin isoforms and their role in the regulation of permeability of mitochondrial outer membrane. MSc, Tallinn University of Technology, 2010
2. Varikmaa, Minna. Model systems of dopamine transporter for the pharmacological characterization of ligands. MSc, University of Tartu, 2008
3. Anmann, Tiia. Integrated and Organized Cellular Bioenergetic Systems in Heart and Brain. PhD, Tallinn University of Technology, TUT Press, 2007
4. Timohhina, Natalja. A Study Of Origination Of Characteristic Elements Of Foucault' Cardiogram. MSc, University of Tartu, 2007

**Selected Publications**

1. **Saks VA.** Molecular system bioenergetics: energy for life. 2007, Weinheim: Wiley-VCH. xxviii, 604 p.
2. Monge C, ... , **Saks VA.** Regulation of respiration in brain mitochondria and synaptosomes: restrictions of ADP diffusion in situ, roles of tubulin, and mitochondrial creatine kinase. *Molecular And Cellular Biochemistry*, 318 (1-2): 147-165
3. **Timohhina N**, et al. Direct measurement of energy fluxes from mitochondria into cytoplasm in permeabilized cardiac cells in situ: some evidence for Mitochondrial Interactosome. *J. Bioenerg. Biomembr.*, 2009, 41(3): 259-75
4. **Saks V**, et al. Structure-function relationships in feedback regulation of energy fluxes in vivo in health and disease. *Mitochondrial Interactosome. Biochim. Biophys. Acta*, 2010, 1797(6-7): 678-697

**2 Chemical Energy Technology****Topic: Energy flows at the quantum level and in ensemble thermodynamics**

The project is funded from the NICPB Targeted Funding Scheme SF0690021s09 "Chemical energy technology"

**Principal Investigator:** Professor Endel Lippmaa, DSc, Member of the Academy of Sciences of Estonia

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Research carried out during recent years in Chemical Energy Technology (T140 Energetics and T370 Fuel Technology) centred around feasibility studies of various novel approaches proposed for clean energy. The techniques used involved various forms of spectrometry such as NMR, UV-VIS and chromato-mass spectrometry and, at the other extreme, the vacuum energy studied at CERN.

As a local problem, the potentialities of the abundant black argillite shales were studied both as a source of oil and some rare metals (U, Mo, V, Re). It was shown that the Maardu-type Dictyonema shale, relatively rich in oil and poor in metals, is not the only black shale available. The other form is a very different argillite mudstone that yields practically no oil, but is reasonably rich in V, Mo and Re. It is found in Eastern Estonia with the best mines at Sillamäe. In this particular case the heavy metals are bound into porphyrine rings that form extremely stable chelates. These structural elements open new approach for the studies of black shale formation and maturation, but create also technological problems just as is the case with Canadian and Venezuelan bitumens.

The main techniques used were 800 MHz NMR and also quantum-chemical calculations of molecular associations and chemical reactivity using a very modern heavily parallel-action 96-core computer with Infiniband interconnect and the latest professional Accelrys and Gaussian software.

The TOTEM results at CERN are consistent with the absence of new particles, including Higgs and the like detectable in the accessible LHC energy range.

### Researchers

Endel Lippmaa, DSc

Risto Tanner, PhD

Ello Maremäe, PhD

Aleksander Trummal, PhD

Arno Pihlak, PhD

Alar Rummel, MSc

### Associated Targeted Financing

Spectroscopic Chemical Physics, 2003-2007, SF0222598s03, PI: T. Pehk

### Scientific Degrees Defended

Trummal, Aleksander. Computational Study of Structural and Solvent Effects on Acidities of Some Brönsted Acids. PhD, University of Tartu Tartu, Tartu University Press, 2009

### Publications

1. Chatrchyan S, **Hektor A**, Kadastik M, Kannike K, **Lippmaa E**, Müntel M, Raidal M, **Rebane L**. et al. The CMS experiment at the CERN LHC, The CERN Large Hadron Collider: Accelerator and Experiments, The CMS Collaboration, 2, CERN/LHCC, CERN, Geneva, Switzerland, 2009, 1-334
2. **Lippmaa E**, Maremäe E, Pihlak AT, Aguraiuja R. Estonian Graptolitic Argillites – Ancient Ores Or Future Fuels? Oil Shale, 2009, Volume: 26, Issue: 4, Pages: 530-539
3. Anelli G, **Lippmaa E**, **Rummel A**, **Trummal A**. et al. The TOTEM Experiment at the CERN Large Hadron Collider, The CERN Large Hadron Collider: Accelerator and Experiments, The TOTEM Collaboration, 2, CERN/LHCC, CERN, Geneva, Switzerland, 2009, 1-107
4. Antchev G, **Lippmaa E**, **Rummel A**, **Trummal A**. et al. Diffraction at TOTEM, 13th International Conference on Elastic and Diffractive Scattering (“Blois Workchop”), EDS 2009, 29th June - 3rd July 2009, CERN, Geneva, Switzerland, Proceedings of the 13th International Conference on Elastic and Diffractive Scattering (“Blois Workchop”), EDS 2009 (M. Deile, D. d’Enterria, and A. De Roeck, Eds), CERN-Proceedings-2010-002, 2010, 249-256
5. Antchev G, **Lippmaa E**, **Rummel A**, **Trummal A**. et al. The TOTEM Detector at LHC, 13th International Conference on Elastic and Diffractive Scattering (“Blois Workchop”), EDS 2009, 29th June - 3rd July 2009, CERN, Geneva, Switzerland, Proceedings of the 13th International Conference on Elastic and Diffractive Scattering (“Blois Workchop”), EDS 2009 (M. Deile, D. d’Enterria, and A. De Roeck, Eds), CERN-Proceedings-2010-002, 2010, 449-455



### 3 Environmental chemistry

#### *Topic: Environmentally friendly utilization strategy of oil shale processing solid wastes*

The project is funded from the NICPB Targeted Funding Scheme SF0690001s09

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The use of oil shale for energy generation and oil production as a common practice for Estonia started to be a strategic issue for several other countries, including US. Processing of oil shale, however, results in vast quantities of solid wastes containing carcinogenic organic compounds and toxic trace metals deposited in environment. The mobility of hazardous ingredients in wastes was investigated in laboratory and field leaching tests. The negligible release (0.1% or less) was found for V, Mn, Zn, Pb, Ni, and Co, Cu (0.5-1.0%), whereas Cr and Cd (2.5-3.1%) were the metals of medium mobility. The environmental impact of these wastes was found to be essential. There are both economical and ecological needs to convert these wastes into a resource. However, the utilization of oil shale wastes should include treatment of material to eliminate toxic ingredients or decrease their mobility.

The special treatment strategy of oil shale ash for syntheses of geopolymers was found to be promising. The silicon in the original ash was converted into Calcium-alumino-silicate hydrates, e.g., into tobermorite structures with long silicate chains and a small number of bridging sites. A non-destructive technique, solid state MAS  $^{31}\text{Si}$  NMR spectroscopy, was used for the investigation of the interaction of pyrogenic matter with soil and compost. Chemical methods including solid phase micro extraction (SPME) were used to extract and isolate the soluble part of the mixture followed by chromatographic analysis.

Using the preparations with catalytic and adsorbent activity, made on the bases of some ash fractions, the toxic trace compounds could be removed from the system.

Thus, for the safe recycling of oil shale solid wastes, the leaching of trace elements from the system could be avoided by pre-treatment of waste to a geopolymeric material by alkaline hydrothermal reagents.

#### **Researchers**

Uuve Kirso, DSc	Kelly Joa, MSc
Natalya Irha, PhD	Jekaterina Jefimova (Panova), PhD student
Janek Reinik, PhD	Gary Urb, Ph student
Erik Teinemaa, PhD	Jasper Adamson, Ph Student
Margit Lassi, MSc	Reelika Mägi, MSc

#### **Associated EU and other International Projects**

1. BioSpinno2 project No 19222, 2005-2007, Enterprise Estonia (EU structural funds), PI: U. Kirso
2. European SF Scientific Programme (Interdisciplinary Tropospheric Research: from the Laboratory to Global Change), 2003-2009, European SF, PI: U. Kirso

#### **Associated Targeted Financing**

1. Speciation and distribution of priority pollutants in Estonian environment, 2003-2007, SF0222597s03, PI: U. Kirso

#### **Associated ETF Grants**

1. The investigation of methods of recycling of solid waste of oil shale processing, 2006-2009, ETF6828, PI: U. Kirso



### Scientific Degrees Defended

1. Mägi, Reelika. Application of a new analytical method for analysis of environmental discharges of oil shale processing. MSc (Second prize in category of master thesis), Tallinn University of Technology, 2010
2. Adamson, Jasper. Fluoride-Free Cross-Coupling Methodology Using Disiloxanes: Synthesis of Terminal Aryl Acetylenes and Biaryl Compounds. MSc, Magdalene College, University of Cambridge, UK, 2009
3. Panova, Jekaterina. The Fenton chemistry and its combination with coagulation for treatment of dye solutions. MSc, Tallinn University of Technology, 2007

### Selected Publications

1. Adamson J, Irha N, Adamson K, Steinnes E, Kirso U. Effect of oil shale ash application on leaching behavior of arable soils: an experimental study. *Oil Shale*, 2010, 27(3), 250-257
2. Joa K, Panova E, Irha N, Teinemaa E, Lintelmann J, Kirso U. Chemical analysis of Polycyclic aromatic hydrocarbons (PAHs) in oil shale processing wastes practice and new trends. *Oil Shale*, 2009, 26 (1), 59-72
3. Reinik J, Heinmaa I, Mikkola J. P, Kirso U. Synthesis and characterization of calcium-alumino-silicate hydrates from oil shale ash – Towards industrial applications. *Fuel*, 2008, 87, 1998-2003
4. Kirso U, Irha N, Reinik J, Urb G, Laja M. The role of laboratory and field leaching tests in hazard identification for solid materials. *ATLA*, 2007, 35, 1, 119 -122

## 4 In vitro toxicology and 3R

### Topic: In vitro toxicology and (nano)ecotoxicology

The research is part of the NICPB Targeted Funding Scheme SF0690063s08: “Mechanisms and interactions in toxicology and toxinology: *in vitro* models”

**Principal Investigator:** Anne Kahru, PhD, leading research scientist, Head of the Laboratory of Molecular Genetics, Chair-person of the Estonian Society of Toxicology

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Following the evolution of research priorities worldwide, the Laboratory of Molecular Genetics has since 2006 developed a new research direction in NICPB - the studies of potential hazardous effects of synthetic nanoparticles. This change of priorities was supported by the renovation and updating of the facilities for ecotoxicological, microbiological, molecular biology and cellular biology research during 2005-2007.

Currently the group is first in Estonia and one of the few groups worldwide who started ecotoxicological studies of metal oxide nanoparticles (<http://sciencewatch.com/dr/fbp/2009/09augfbp/09augfbpKahr/>). We have developed a novel approach based on a combination of traditional ecotoxicological methods (comparing the ecotoxic effects of nanosize metal oxides with their bulk analogues and soluble salts) and metal-specific recombinant biosensors. This combined approach allows differentiating the toxic effects of metal oxide NPs per se and solubilised metal ions. Since 2007 our group participates in FP6 IP OSIRIS with 31 partners in developing high-throughput *in vitro* toxicity screens and QSARs (quantitative-structure-activity relationships) and has created a web-database E-SovTox from Russian toxicity data sources (<http://kbfi-databases.eu/database/>) (see also: Scientific Collections, pp 23-24). In a new FP7 project, NA-NOVALID, with 35 partners we lead a WP on toxicological profiling of synthetic nanoparticles that merges knowledge on high-throughput toxicity screening, environmental chemistry, physiology of various aquatic organisms and construction of mechanism-based recombinant sensor bacteria.

Our earlier work preceding to nanotoxicological research focused on development of *in vitro* test batteries of biotests and recombinant biosensors for the analysis of harmful effects of major environmental pollutants of human relevance (heavy metals, phenols, PAHs). This *in vitro* testing strategy contributes to the 3R (Reduction, Replacement, Refinement) strategy that allows to significantly reduce laboratory animal use.

The research of Laboratory of Molecular Genetics is contributing to the NICPB strategic programme “*In vitro* toxicology and 3Rs”.

The Laboratory of Molecular Genetics collaborates actively with all main Estonian Universities via co-supervision of PhD students (Profs M. Lopp, T. Paalme, R. Kuusik, E. Truve, K. Sepp, R. Munter) and joint research projects and/or publications (Drs U. Maran, K. Orupõld, A. Tuvikene, L. Bitjukova). We have strong international connections with scientists from Clemson University and University of California Los Angeles (USA), Liverpool John Moore University and Teesside University (UK), Francois Rabelais University (France) and the University of Ljubljana (Slovenia), to name a few.

### Researchers

Anne Kahru, PhD	Villem Aruoja, PhD student
Irina Blinova, PhD	Monika Mortimer, PhD student
Margit Heinlaan, PhD	Mariliis Sihtmäe, PhD student
Angela Ivask, PhD	Imbi Kurvet, PhD student
Kaja Kasemets, PhD	Olesja Bondarenko, PhD student
Heiki Vija, MSc	Aleksandr Käkinen, PhD student

### Associated EU and other International Projects

1. OSIRIS (Optimized Strategies for Risk assessment of industrial chemicals through integration of non-test and test information) EU FP6 Integrated Project, 2007-2011. NICPB PI: A. Kahru
2. NANOVALID (Development of reference methods for hazard identification, risk assessment and LCA of engineered nanomaterials, FP7 Large-scale integrating Collaborative Project, 2011-2014. NICPB PI: A. Kahru
3. Environmental impact of oil shale combustion ashes on topsoils in Narva Powerplants region: combined geochemical and ecotoxicological approach. EMP45 Grant. Joint project between TUT and NICPB, 2008-2010. PIs: L. Bitjukova (TUT) and A. Kahru (NICPB).
4. Bioavailability of key environmental pollutants in different environmental matrices: from quantification to mechanisms. Maj ja Tor Nessling Foundation, 2007-2009. PI: A. Ivask
5. Risk Management and Remediation of Chemical Accidents (RIMA). Interreg IV A Programme, 2010-2013 PI: I. Blinova

### Associated Targeted Financing

1. Toxicological risk assessment in vitro, 2003-2007, SF0222601Bs03, PI: A. Kahru

### Associated ETF Grants

1. Bioavailability and (eco)toxicity of metal oxide nanoparticles: effects and mechanisms, 2007-2010, ETF 6956, PI: A. Kahru
2. Mechanism-based study of toxicity: recombinant microbial models, 2007-2010, ETF 6974, PI: A. Ivask
3. In vitro toxicity of metal oxide nanoparticles: eukaryotic models, 2008-2011, ETF 7686, PI: K. Kasemets
4. Bioavailability of contaminants in Estonian lakes and rivers, 2009-2012, ETF 8066, PI: I. Blinova
5. Ivask, Angela. High throughput bacterial screening for the characterization of toxicity of nanosized particles and materials, 2010-2012, ETF Post-Doc Grant MJD67

### Scientific Degrees Defended

1. Heinlaan, Margit. Ecotoxicological Evaluation of Synthetic Nanoparticles and Particulate Environmental Samples. PhD, Estonian University of Life Sciences, 2010
2. Kurvet, Imbi. Natural and recombinant bioluminescent bacteria for high throughput toxicity screening. MSc, Tallinn University of Technology, 2009



### Selected Publications

1. **Heinlaan M, Ivask A, Blinova I, Dubourguier H-C, Kahru, A.** Toxicity of nanosized and bulk ZnO, CuO and TiO<sub>2</sub> to bacteria *Vibrio fischeri* and crustaceans *Daphnia magna* and *Thamnocephalus platyurus*. Chemosphere, 2008, 71:1308-1316. (Essential Science Indicators SM of Thomson Reuters listed this paper in Aug 2009 as Fast Breaking Paper in Environment/ Ecology) (<http://sciencewatch.com/dr/fbp/2009/09augfbp/09augfbpKahr/>)
2. **Kahru A, Dubourguier H-C, Blinova I, Ivask A, Kasemets K.** Biotests and Biosensors for Ecotoxicology of Metal Oxide Nanoparticles: A Minireview. Sensors, 2008, 8: 5153 - 5170.
3. **Kahru A, Dubourguier H-C,** From ecotoxicology to nanoecotoxicology. Toxicology, 2010, 269(2-3): 105-119. (Most downloaded paper from „Toxicology“ from Science Direct, Jan-June 2010 (<http://top25.sciencedirect.com>))
4. **Ivask A, Bondarenko O, Jepihhina N, Kahru A.** Profiling of the reactive oxygen species-related ecotoxicity of CuO, ZnO, TiO<sub>2</sub>, silver and fullerene nanoparticles using a set of recombinant luminescent *Escherichia coli* strains: differentiating the impact of particles and solubilised metals. Anal. Bioanal. Chem, 2010, 398:701–716
5. **Aruoja V, Dubourguier H.C., Kasemets K, Kahru A.** Toxicity of nanoparticles of CuO, ZnO and TiO<sub>2</sub> to microalgae *Pseudokirchneriella subcapitata*. Sci. Total. Environ, 2009, 407, 1461-1468

## 5 Ionic conductivity and catalysis

### Topic: Development of Solid Oxide Fuel Cells

The Project is commissioned by Elcogen Ltd, Estonia

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Solid Oxide Fuel Cells (SOFC) is an emerging technology for electricity production for small and medium sized stationary applications. High temperature fuel cell technologies like SOFC have potential for high electrical efficiency, 55-60%, and total efficiency up to 90% for Combined Heat and Power (CHP) units combined with low emissions. The main development challenges related to the commercialization of SOFC technology are in the reduction of its cost and increasing its lifetime. Also, the electrical efficiency of SOFC systems needs to be improved to increase their competitiveness.

These challenges motivate our involvement in fuel cell development. We are active, on one hand, in the development of usable SOFC elements with our commercial partner Elcogen. On the other hand, we are investigating the atomic level structure of ceria based oxides, including ceria-zirconia mixed oxides, and its connection to oxygen dynamics in these lattices that is necessary for optimization of SOFC resistance and longevity.

In SOFC the aliovalently doped ceria can be used as an electrolyte, a barrier layer between zirconia electrolyte and cathode, or an anode catalyst to suppress coke forming from carbon containing fuels. As an electrolyte, it has higher ionic conductivity than stabilized zirconia at low temperatures, but it develops electronic conductivity and morphological instability at low anodic oxygen activities, limiting its use as a single layer electrolyte. On the other hand, it has better compatibility with efficient cathode materials than zirconia and can be used as a barrier layer between thin zirconia electrolyte and cathode. Here ceria tends to form a lower conductivity mixed oxide with zirconia, limiting efficiency of produced fuel cell. As an anode catalyst, its functioning depends again on its interactions with other anode materials, zirconia and nickel. Both ion conductivity and catalytic properties depend on atomic short range order that we do not understand well enough in these materials.

Our capability to do combined optical, electrochemical impedance, thermogravimetric and solid state NMR studies of these compounds gives us unique possibilities that we are eager to use. We have estab-

lished a complicated activated lattice dynamics in lanthanum doped ceria through temperature dependent NMR relaxation studies [1], and are currently expanding our work to different dopants.

### Researchers

Juhan Subbi, PhD

Jüri Pahapill, MSc

Helgi Kooskora, MSc

Tõnu Tolk, senior engineer

### Associated EU and other International Projects

1. Development of Solid Fuel Cells 2005-2007, Elcogen Ltd, PI: J. Subbi
2. Development of Solid Fuel Cells II, 2008-2010, Elcogen Ltd, PI: J. Subbi

### Associated Target Financing

1. Spectroscopic Chemical Physics, 2003-2007, SF0222598s03, PI: T. Pehk
2. Physics, Chemistry and Technological Applications of Condensed Phases, 2008, SF0690176s08, PI: T. Pehk
3. New Developments and Applications of Nuclear Magnetic Resonance Techniques, 2009-2014, SF0690034s09, PI: I. Heinmaa

### Selected Publications

1. **Heinmaa I, Joon T, Kooskora H, Pahapill J, Subbi J.** Local structure and oxygen dynamics in La doped ceria:  $^{17}\text{O}$  NMR study. *Solid State Ionics*, 2010, 181: 1309 - 1315.

## 6 Macromolecular interactions

### Topic: Toxinology

The project is part of the NICPB Targeted Funding Scheme SF0690063s08 “Mechanisms and interactions in toxicology and toxinology: *in vitro* models”

**Principal Investigator:** Jüri Siigur, PhD  
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Snake venoms are a rich source of peptides and proteins of pharmacological importance. The main area of interest has been the study of structure and function of snake venom components affecting haemostasis, cell adhesion, apoptosis, and angiogenesis. The venom proteins are also attractive tools for protein-protein interaction studies and some of them are useful as diagnostics. The specific and effective snake venom components are novel and ideal lead structures to generate potential antibacterial, antithrombotic, anti-cancer therapeutics. Some venom components may be potent therapeutics in regulating tissue regeneration and wound healing.

Molecular cloning and characterization of activities of individual snake venom proteins is crucial for understanding envenomation (general toxic effects) and targeted effects (blood, nervous system, immune system, etc) as well as for developing novel agents for diagnostic and therapeutic purposes. Characterization of snake venom components structurally and functionally (venomics) needs using a lot of methods of protein chemistry, molecular biology, bioinformatics, cell culture systems and animal models.

We have isolated different proteins and peptides from *Viperidae* and *Elapidae* venoms and studied their biological function. Using *Vipera Lebetina* venom gland cDNA library different venom components were cloned and sequenced. However, the biological effects of myriad of venom components (proteins, peptides) need still to be elucidated.





We plan structural studies of newly discovered proteins (peptides) in cooperation with the laboratory of chemical physics using new NMR facility of NICPB. Structural information of these venom proteins together with recombinant technology might promote the construction of new drugs.

The research group's competence in the field of snake venom biochemistry has been used at the Tallinn Pharmaceutical Plant in producing drugs from snake venoms.

The Laboratory of Bioorganic Chemistry collaborates primarily with the Department of Gene Technology of the Tallinn University of Technology (L. Järvekülg, V. Paalme, K. Tomson, P. Kogerman, K. Vanatalu), and with Protein Chemistry Research Group and Core Facility, Institute of Biotechnology, University of Helsinki (N. Kalkkinen).

### Researchers

Jüri Siigur, PhD

Katrin Trummal, PhD

Anu Aaspõllu, PhD

Küllü Tõnismägi, MSc

Mari Samel, PhD

Heiki Vija, MSc

Ene Siigur, PhD

Olga Vassiljeva, MSc student

### Associated Target Financing

1. Functional proteomics-structure-activity relationships and molecular recognition in natural protein systems, 2003-2007, SF0222603s03

### Associated ETF Grants

1. L-Amino acid oxidases: isolation, primary structure, cellular interactions, 2003-2007, ETF5938, PI: E. Siigur
2. Biomedically important proteins and peptides from snake venoms, 2007 – 2010, ETF7251, PI: J. Siigur
3. Protein-protein interactions with the snake venom nerve growth factor, 2008 – 2011, ETF7694, PI: E. Siigur

### Scientific Degrees defended (2007-2010)

1. Trummal, Katrin. Purification, Characterization and Specificity Studies of Metalloproteinases from *Vipera lebetina* Snake Venom. PhD, Tallinn University of Technology, 2007
2. Tõnismägi, Külli. Comparative study of snake venom l-amino acid oxidases. MSc, Tallinn University of Technology, 2008
3. Vija, Heiki. Separation of toxic peptides from *Amanita phalloides* and *Amanita virosa*. MSc, Tallinn University of Technology, 2008

### Selected Publicationsä

1. Vija H, Samel M, Siigur E, Aaspõllu A, Trummal K, Tõnismägi K, Subbi J, Siigur J. Purification, characterization, and cDNA cloning of acidic platelet aggregation inhibiting phospholipases A(2) from the snake venom of *Vipera lebetina* (Levantine viper). *Toxicon* 2009, 54:429-439
2. Vija H, Samel M, Siigur E, Aaspõllu A, Tõnismägi K, Trummal K, Subbi J, Siigur J. VGD and MLD-motifs containing heterodimeric disintegrin viplebedin-2 from *Vipera lebetina* snake venom. Purification and cDNA cloning. *Comp. Biochem. Physiol. B, Biochem. Mol. Biol.* 2009, 153:253-260
3. Paalme V, Trummal K, Samel M, Tõnismägi K, Järvekülg L, Vija H, Subbi J, Siigur J, Siigur E. Nerve growth factor from *Vipera lebetina* venom. *Toxicon* 2009, 54:329-336
4. Siigur J, Siigur E. Activation of Factor X by Snake Venom Proteases, Chapter 26, in "Toxins and Hemostasis. From Bench to Bedside" Eds. Kini RM, Clemetson KJ, Markland FS, McLane MA, Morita T. 2010, Springer, pp. 447-464

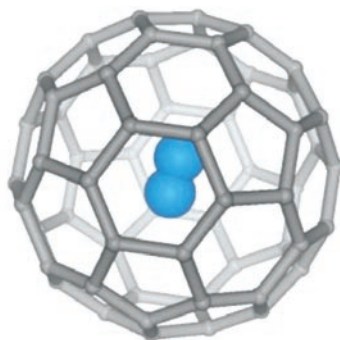
## 7 New spin materials and states

### Topic: Spectroscopy of functional materials

The project is funded by the NICPB Targeted Funding Scheme SF0690029s09

**Principal Investigator:** Toomas Rõõm, PhD  
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Functions of materials are caused by collective action of their constituent atoms and electrons, quantum properties of these particles, and their mutual interaction. Understanding the functioning is an iterative process between theory and experiment. Our main tools are terahertz, infrared and nuclear magnetic resonance spectroscopy which help to map different aspects of material properties and thus improve the theoretical understanding.



$H_2@C_{60}$  is a molecular complex where the simplest molecule, diatomic hydrogen, is trapped in the most symmetric molecule, buckminster fullerene  $C_{60}$ .  $H_2$  behaves like a rotor moving inside the spherical cavity [1, 2]. The orbiting frequency of  $H_2$  inside  $C_{60}$  is 6THz. Another carbon compound, graphite with calcium atoms between the carbon layers, is a superconductor below  $T_c=12K$ . The size of the superconducting gap of this material can be measured directly from the THz reflection spectra [3].

The highest  $T_c$  of non-copper-based superconductors, to date, belongs to recently discovered iron pnictides. IR reflection spectra evidence strong interaction between charge carriers and bosons in the normal state of an iron pnictide [4]. In the superconducting state the conventional theory of superconductivity fails to count for the excess normal charge carriers as revealed by the low frequency optical conductivity [5].

Magnetic excitations may experience Bose-Einstein condensation similar to the condensation of Cooper pairs in a superconductor or atoms in ultra-cold gases. A spatial modulation of condensed boson density in a spin-gap material  $BaCuSi_2O_6$  was discovered in the collaborative NMR study where very high magnetic fields and very low temperatures were needed [6]. The high magnetic field THz spectroscopy studies show, for the first time, the complexity of magnetic excitation spectra in a spin gap material  $Sr_{14}Cu_{24}O_{41}$  [7] and in multiferroic  $LiCu_2O_2$  [8].

#### Researchers

Toomas Rõõm, PhD

Dan Huvonen, PhD, post-doc at ETH Zürich

Urmas Nagel, PhD

Min Ge, PhD, post-doc

Raivo Stern, PhD

Mukesh Chandra Dimri, PhD, post-doc

#### Associated EU and other International Projects

1. Collaboration Agreement “Far Infrared Spectral Analysis Software”, 2001-2020, Sciencetech Inc, Canada, PI: U. Nagel

#### Associated Targeted Financing

1. Spectroscopic Chemical Physics, 2003-2007, SF0222598s03, PI: T. Pehk



### Associated ETF Grants

1. Singlet-triplet transitions in terahertz spectra of spin-gap materials, 2005-2008, ETF6138, PI: U. Nagel
2. Optical spectroscopy of frustrated magnets in magnetic field, 2007-2010, ETF7011, PI: T. Rõõm
3. Ge, Min. Infrared spectroscopy of endohedral hydrogen-fullerene and calmodulin-peptide complexes, 2009-2011, ETF Post-Doc Grant JD187
4. Infrared Study of the Dynamics of Endohedral Hydrogen-Fullerene Complexes, 2010-2013, ETF8170, PI: U. Nagel
5. Chandra, Mukesh. Magnetic studies on doped dielectric oxides (ZrO<sub>2</sub> and TiO<sub>2</sub>) for spintronic applications, 2010-2013, ETF Post-Doc Grant MJD65

### Scientific Degrees Defended

Hüvonen, Dan. Terahertz Spectroscopy of Low-Dimensional Spin Systems. PhD, Tallinn University of Technology, 2008

### Selected Publications

1. Mamone S, **Ge M**, **Hüvonen D**, **Nagel U**, Danquigny A, Cuda F, Grossel M C, Murata Y, Komatsu K, Levitt M H, **Rõõm T**, and Carravetta M. Rotor in a cage: Infrared spectroscopy of an endohedral hydrogen-fullerene complex. *J. Chem. Phys.* 2009, **130**, 081103
2. Carravetta M, Danquigny A, Mamone S, Cuda F, Johannessen O G, **Heinmaa I**, Panesar K, **Stern R**, Grossel M C, Horsewill A J, **Samoson A**, Murata M, Murata Y, Komatsu K, Levitt M H. Solid-state NMR of endohedral hydrogen-fullerene complexes. *Phys. Chem. Chem. Phys.*, 2007, **9**, 4879
3. **Nagel U**, **Hüvonen D**, **Joon E**, Kim J S, Kremer R K, **Rõõm T**. Far-infrared signature of the superconducting gap in intercalated graphite CaC<sub>6</sub>. *Phys. Rev. B*, 2008, **78**, R041404
4. Yang J, **Hüvonen D**, **Nagel U**, **Rõõm T**, Ni N, Canfield P C, Bud'ko S L, Carbotte J P, Timusk T. Optical Spectroscopy of Superconducting Ba<sub>0.55</sub>K<sub>0.45</sub>Fe<sub>2</sub>As<sub>2</sub>: Evidence for Strong Coupling to Low-Energy Bosons. *Phys. Rev. Lett.*, 2009, **102**, 187003
5. Lobo R. P. S. M, Dai Y M, **Nagel U**, **Rõõm T**, Carbotte J P, Timusk T, Forget A, D. Colson D. Optical signature of subgap absorption in the superconducting state of Ba(Fe<sub>1-x</sub>Co<sub>x</sub>)<sub>2</sub>As<sub>2</sub>. *Phys. Rev. B*, 2010, **82**, R100506
6. Krämer S, **Stern R**, Horvatić M, Berthier C, Kimura T, Fisher I R. Nuclear magnetic resonance evidence for a strong modulation of the Bose-Einstein condensate in BaCuSi<sub>2</sub>O<sub>6</sub>. *Phys. Rev. B*, 2007, **76**, R100406
7. **Hüvonen D**, **Nagel U**, **Rõõm T**, Haas P, Dressel M, Hwang J, Timusk T, Wang Y-I, Akimitsu J. Magneto-optic far-infrared study of Sr<sub>14</sub>Cu<sub>24</sub>O<sub>41</sub>: Triplet excitations in chains. *Phys. Rev. B*, 2007 **76**, 134418
8. **Hüvonen D**, **Nagel U**, **Rõõm T**, Choi Y J, Zhang C L, Park S, Cheong S-W. Magnetic excitations and optical transitions in the multiferroic spin-1/2 system LiCu<sub>2</sub>O<sub>2</sub>. *Phys. Rev. B*, 2009, **80**, R100402

## 8 Nuclear Magnetic Resonance

### Topic: New Developments and Applications of NMR Techniques

The project is funded by the NICPB Targeted Funding Scheme SF0690034s09

**Principal Investigator:** Ivo Heinmaa, PhD

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Nuclear magnetic resonance (NMR) is a unique analytical tool giving in principle most comprehensive information about short range atomic topology in condensed matter. Unlike other analytical methods, it demands not only appropriate hardware, but also significant competence to design measurement methods and to interpret data.

Despite great potential, NMR-studies of many important problems remain beyond sensitivity and temperature range. Problem is aggravated by low natural abundance of spin-carrying nuclei in main build-

ing elements of organic and ceramic materials. Another limit to the magic angle sample spinning (MAS) solid state NMR is comparatively narrow temperature interval, typically from  $-150^{\circ}\text{C}$  to  $+250^{\circ}\text{C}$ . Recent progress in NICPB involves development of CryoMAS technique and building of CryoMAS probe. We are currently able to carry out MAS NMR experiments with fast spinning of the sample from room temperature down to  $T=10^{\circ}\text{K}$ .

Within the current programme we aim both to develop various NMR tools and to implement them in materials science. Projected advances in NMR technology expand measurement temperature range towards high temperatures, improve sensitivity and resolution and make spectral information more comprehensible. Research fields include ionic conduction and structure of fuel cell components, localization of charge carriers in superconductors, distribution of zeolite reaction centres, syntheses of materials from products of oil shale industry and mechanism of protein aggregation.

Our high field high resolution NMR is focused to configuration (relative and absolute) and conformation studies of various chiral molecules and diastereoisomers, bio- and synthetic polymers.

### Researchers

Ivo Heinmaa, PhD

Jüri Jarvet, PhD

Jaan Past, PhD

Tõnis Pehk, DSc

Ago Samoson, PhD (currently Tallinn University of Technology)

Priit Sarv, PhD

### Associated EU and other International Projects

1. A coordinated Approach to Access, Experimental Development and Scientific Exploitation of European Large Infrastructures for High Magnetic Fields (EuroMagNET), 2005-2008, Stichting Katholieke Universiteit, EC 6<sup>th</sup> Framework Programme, PI: R. Stern
2. European Network of Research Infrastructures for providing Access and Technological Advancements in bio-NMR, 2006-2010, EC 6<sup>th</sup> Framework Programme, PI: I. Heinmaa

### Associated Targeted Financing

1. Spectroscopic Chemical Physics, 2003-2007, SF0222598s03, PI: T. Pehk
2. Physics, Chemistry and Technological Applications of Condensed Phases, 2008, SF0690176s08, PI: T. Pehk

### Associated ETF Grants

1. Multiquantum correlations under conditions of dynamic- and hyperrotation, 2005-2008, ETF6143, PI: A. Samoson
2. Fast Magic Angle Spinning at Cryogenic Temperatures, 2006-2009, ETF6846, PI: I. Heinmaa
3. The studies of steric interactions by high field NMR multinuclear spectroscopy, 2006-2009, ETF6778, PI: T. Pehk
4. NMR studies of heterostructural nanocomposites, 2007-2010, ETF7232, PI: P. Sarv
5. Sensitivity enhancement of the solid state MAS-NMR technique, 2010-2013, ETF8198, PI: I. Heinmaa

### Selected Publications

1. **Heinmaa I, Joon T, Kooskora H, Pahapill J, Subbi J.** Local structure and oxygen dynamics in La doped ceria:  $^{17}\text{O}$  NMR study. *Solid State Ionics*, 2010, 181: 1309 - 1315
2. Davis L J M, **Heinmaa I**, Goward G R. Study of Lithium Dynamics in Monoclinic  $\text{Li}_3\text{Fe}_2(\text{PO}_4)_3$  using  $^6\text{Li}$  VT and 2D Exchange MAS NMR Spectroscopy. *Chemistry of Materials*, 2010, 22: 769 - 775
3. Perálvarez-Marín A, Wahlström A, Lind J, Hugonin L, **Jarvet J**, Mäler L, Barth A, Gräslund A. Amyloid-like Misfolding Of Peptides By Membrane Mimicking Environments. *Biophysical Journal*, 2009, 96(3): 93a
4. Kropman D, Mellikov E, Öpik A, Lott K, Volobueva O, Kärner T, **Heinmaa I**, Laas T, Medvid A. Strain



relaxation mechanism in the Si-SiO<sub>2</sub> system and its influence on the interface properties. *Physica B: Condensed Matter*, 2009, 404: 5153 - 5155

5. Kanger T, Kriis K, Laars M, Kailas T, M  urisepp A-M, **Pehk T**, Lopp M. Bimorpholine-Mediated Enantioselective Intramolecular and Intermolecular Aldol Condensation. *Journal of Organic Chemistry*, 2007, 72: 5168 - 5173
6. Pashkova V O, **Sarv P**, Derewinski M. Composite porous materials containing zeolitic domains prepared by controlled partial recrystallization of amorphous aluminosilicates. Xu R, Gao Z, Chen J, Yan W (Eds). *Studies in Surface Science and Catalysis*, 2007, vol. 170A: 289 – 296, Elsevier
7. Massad T, **Jarvet J**, **Tanner R**, Tomson K, Smirnova J, Palumaa P, Sugai M, Kohno T, Vanatalu K, Damberg P. Maximum entropy reconstruction of joint phi, psi-distribution with a coil-library prior: the backbone conformation of the peptide hormone motilin in aqueous solution from phi and psi-dependent J-couplings. *Journal of Biomolecular NMR*, 2007, 38(2): 107 - 123

## 9 Particle physics

### *Topic: High Energy and Theoretical Physics*

The project is funded by the NICPB Targeted Funding Scheme SF0690030s09

**Principal Investigator:** Martti Raidal, PhD

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The successful start up of the Large Hadron Collider (LHC) at CERN has been the most important event in particle physics in the 21st century. The unprecedented centre-of-mass energy of collisions gives a chance to look for the Higgs boson and physics beyond the Standard Model.

Our team is collaborating with the Compact Muon Solenoid detector group at CERN. We host the biggest Grid clusters in Estonia and use it to analyse fresh data from the LHC. We have studied the production of double-charged Higgs, predicted by one of the main neutrino mass models, at the LHC. The search for H<sup>++</sup> has become one of the priority searches in CMS Higgs group as the current world limits on H<sup>++</sup> are such that fresh data from LHC can produce new results already early next year.

Astronomical observations show that the nature of about 80% of all matter in the universe – dark matter – is unknown. While it cannot be seen directly, dark matter has played a major r  le in the formation of cosmic structures at large scales. Recently there has been a surge in interest of dark matter models due to intriguing satellite data (PAMELA and others) hinting at annihilating or decaying dark matter. In addition, direct detection experiments are on the verge of finding dark matter passing through the solar system.

Our group has been tackling dark matter from several directions.

We have built a model of scalar dark matter where the matter parity stabilising dark matter arises from breaking a U(1) subgroup of the SO(10) Grand Unified symmetry group. In the model, dark matter is also connected to the electroweak symmetry breaking that together with GUT scale conditions puts heavy constraints on the parameter space. The model predicts that dark matter will be seen in next generation detectors and produced at the LHC if it is light enough.

We have worked on model-independent constraints on dark matter annihilation and decay modes from PAMELA and FERMI satellite data. We have put bounds on reactions with different end products, e.g. dark matter annihilation into electrons is virtually excluded. We have confronted possible production of gamma rays from dark matter annihilation with FERMI data, being among the first to take correctly into account the inverse Compton scattering.

We continue to build models of physics beyond the Standard Model and confront them with new data from the LHC, dark matter detection experiments and cosmic ray data from satellites.



### Researchers

Martti Raidal, PhD

Els Heinsalu, PhD

Andi Hektor, PhD

Mario Kadastik, PhD

Kristjan Kannike, PhD

Yuji Kajiyama, PhD

Mait Müntel, PhD

Marco Patriarca, PhD

Antonio Racioppi, PhD

Liis Rebane, PhD student

Alessandro Strumia, PhD

### Associated EU and other International Projects

1. EU FP6 project Baltic Grid, 2005-2008, EC 6<sup>th</sup> Framework Programme, PI: M. Raidal
2. EURATOM Association European Fusion Development Agreement, 2007-2009, EURATOM, PI: A. Hektor
3. Research Training Course in Detector Technology, 2008-2009, Nordic Council of Ministers, PI: M. Raidal
4. NordForsk project LHC and beyond, 2008-2010, Nordic Council of Ministers, PI: M. Raidal
5. Scientific and educational cooperation with CERN, 2008-2014, Estonian Ministry of Education and Research, PI: M. Raidal
6. Semantic Business Processes Based On Software-As-A-Service And Cloud Computing (SITIO), 2009-2011, Enterprise Estonia, EUREKA, PI: I. Livenson
7. EGI – European Grid Initiative 2009-2012, EC 7<sup>th</sup> Framework Programme, PI: M. Raidal

### Associated ETF Grants

1. Spectroscopic Chemical Physics, 2003-2007, SF0222598s03, PI: T. Pehk
2. Leptogenesis, supersymmetry and LHC Physics, 2005-2008, ETF6140, PI: M. Raidal
3. Modern methods of statistical physics: applications to diffusion processes in complex systems, 2008-2011, ETF7466, PI: M. Patriarca
4. Racioppi, Antonio. Phenomenology of Anomalous Z', 2009-2012, ETF Post-doc Grant JD164
5. Searching for New Physics at LHC, 2009-2014, ETF8090, PI: M. Raidal
6. Scientific calculus in computer cloud and grid, 2010-2015 ETF TAP-5, PI: M. Raidal
7. Experimental high-energy physics, 2010-2013, ETF8499 PI: M. Kadastik
8. Hektor, Andi. Data mining in the CMS experiment at CERN, 2010-2013, ETF Post-doc Grant MJD52
9. Kannike, Kristjan. Properties of Dark Matter, 2010-2013, ETF Post-doc Grant MJD140
10. Strumia, Alessandro. Astro particle physics and the Large Hadron Collider, 2010-2015, ETF Top Researcher Grant MTT8

### Scientific Degrees Defended

1. Heinsalu, Els. Normal and anomalously slow diffusion under external fields. PhD, University of Tartu, 2008
2. Hektor, Andi. Neutrino physics beyond the Standard Model. PhD, University of Tartu, 2008
3. Kadastik, Mario. Doubly charged Higgs boson decays and implications on neutrino physics. PhD, Tallinn University of Technology, 2008
4. Kannike, Kristjan. Implications of Neutrino Masses. PhD, University of Tartu, 2008
5. Müntel, Mait. Detection of doubly charged Higgs boson in the CMS detector. PhD, University of Tartu, 2009

### Selected Publications

1. Kadastik M, Raidal M, Strumia A. Enhanced anti-deuteron Dark Matter signal and the implications of PAMELA. Physics Letters B, 2010, 683: 248 - 254.
2. Kadastik M, Kannike K, Racioppi A, Raidal M. EWSB from the soft portal into Dark Matter and prediction for direct detection. Physical Review Letters, 2010, 104(20): 201301
3. Hütsi G, Hektor A, Raidal M. Implications of the Fermi-LAT diffuse gamma-ray measurements on annihilating or decaying dark matter. Journal of Cosmology and Astroparticle Physics, 2010, 07: 008



4. Ellis J, Lola S, **Raidal M**. Supersymmetric Grand Unification and Lepton Universality in  $K \rightarrow l \nu$  Decays. Nuclear Physics B, 2009, 812: 128 - 143
5. Chatrchyan S, **Hektor A, Kadastik M, Kannike K, Lippmaa E, Müntel, M, Raidal M, Rebane L**, et al. The CMS experiment at the CERN LHC. Amos Breskin and Rüdiger Voss (Eds). The CERN Large Hadron Collider: Accelerator and Experiments (1 - 334), 2009, CERN, Geneva, Switzerland: CERN/LHCC
6. **Raidal M, Hektor A, Kadastik M, Kajiyama Y, Müntel M, Rebane L**. Flavour physics of leptons and dipole moments. European Physical Journal C, 2008, 57(1-2): 13-182

## Development

### MAS Systems Ltd

NICPB is the founder (2006) and sole owner of MAS Systems Ltd. MAS Systems is focused on development and production of solid-state NMR probes.

Relevant shifts in Zeeman transition, observed in Nuclear Magnetic Resonance (NMR) experiment, can be of the order of a fraction of a Hertz to about several hundred kHz. This frequency range can be attained also by periodic mechanical motion of macroscopical objects. Mechanical reorientation of the sample brings about change of direction of the strong magnetic field relative to e.g. internuclear space vector, giving us a powerful tool for manipulating the content of the spectral information.

Our state of the art probeheads permit rotation of the sample at speeds up to 70,000 Hz and acceleration up to 1,000,000 Hz/s for motion of sample around single axis (MAS). For simultaneous rotation about two axes (DOR) speeds 10,000/2,000 Hz have been reached.

The applicable temperature range for MAS sample spinning at present stretches from 10 K to 700 K, which is quite sufficient for optimum temperature studies of many important solid state phenomena from superconductivity to petrochemical zeolite catalysis.

General Manager: Andres Reinhold  
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## Core Facilities

### Estonian Magnet Laboratory

#### Nuclear Magnetic Resonance Spectroscopy

Contact persons:

Ivo Heinmaa, PhD (ivo.heinmaa@kbfi.ee) – solid state NMR  
 Jüri Jarvet, PhD (Jyri.jarvet@kbfi.ee) – bioNMR  
 Tõnis Pehk, DSc (tonis.pehk@kbfi.ee) – HR NMR

The Laboratory has four research grade Bruker NMR spectrometers that cover a range of frequencies, nuclei and a diversity of applications.

AVANCE III 800MHz (18.8T magnetic field) spectrometer capable of performing advanced multidimensional experiments

Features:

- Triple resonance  $^1\text{H}/^{13}\text{C}/^{15}\text{N}$  PFG probehead
- Dual  $^1\text{H}/^{13}\text{C}$  PFG probehead
- Solid state triple resonance  $^1\text{H}/^{13}\text{C}/^{15}\text{N}$  probehead
- QCI CryoProbe

AVANCE II 600MHz (14.1 T magnetic field) instrument capable of performing advanced multidimensional experiments

Features

- Triple resonance  $^1\text{H}/^{13}\text{C}/^{15}\text{N}$  PFG probehead
- Solid state probes 1-6 mm and DOR probehead

AMX 500 (11.7T magnetic field)

Features:

- Liquid  $^1\text{H}/^{13}\text{C}$  probehead

CXP 360 spectrometer attached to 8.5T or 4.7T WB-magnets

Features:

- Solid state/low temperature MAS

The Lab has access to cryogenic liquids and compressed He gas for low temperature work.

### Team

Jaan Past, PhD

Tiit Tuherm, senior engineer

Andres Reinhold, senior engineer

## Terahertz spectroscopy and Low Temperature Physics

Contact persons:

Urmas Nagel, PhD (Urmas.Nagel@kbfi.ee) – THz, optics

Toomas Rõõm, PhD (Toomas.Room@kbfi.ee) – THz, optics

Raivo Stern, PhD (Raivo.Stern@kbfi.ee) – NMR, PPMS

THz spectrometer SPS-200

Features:

- 3 – 200  $\text{cm}^{-1}$  with 0.3K bolometer
- Sample temperature 2-200K
- Magnetic field 0-12T
- Reflection (Faraday configuration) and transmission (Faraday and Voigt)

Bruker Fourier spectrometer Vertex 80v

Features:

- Two sample cryostats: cold finger 5-300K, exchange gas 2-300K
- Transmission and reflection
- 10 – 50 000  $\text{cm}^{-1}$

Quantum Design PPMS

Features:

- 14T magnet
- Sample temperature 1.8-400K
- VSM magnetometer with oven (up to 1000K)
- Heat capacity measurement with He-probe (down to 300mK)
- Electrical and thermal transport measurements

### Team

Min Ge, post-doc

Himani Khanduri, PhD student

Mukesh Chandra, Dimri, post-doc

Taaniel Uleksin, PhD student

## Optics

Contact person:

Aleksander Rebane, PhD (sassrebane@gmail.com)

The Laboratory has a Mode-locked femtosecond Titanium Sapphire (Ti:S) laser Mira 900 pumped with 10 W frequency-doubled neodymium-doped vanadate (Nd:YVO<sub>4</sub>) laser Verdi V-10, both from Coherent, Inc.

The laser system generates 100 fs pulses at 76 MHz repetition rate and may be tuned in the spectral range 705 – 975 nm.

The Ti:S laser output average power is 0.5 – 1.5 W depending on the wavelength.

This laser system is ideally suited for two-photon absorption spectroscopy of organic and biological chromophores.

### Team

Georg Liidja, DSc

Jüri Pahapill, MSc

Girsh Blumberg, PhD

## Estonian Tier 2 Computing Centre and Grid & Cloud Computing

Contact persons:

Mario Kadastik, PhD (mario.kadastik@cern.ch) - Group leader

Ilja Livenson, MSc (ilja.livenson@kbfi.ee) - Support and R&D

The computing centre has developed from the need of participation in the Large Hadron Collider (LHC) Compact Muon Solenoid (CMS) experiment where experimental data analysis requires using a distributed computing model. Our computing centre is Estonian Tier 2 centre for CERN Worldwide LHC Computing Grid facility. Over the years the centre has grown to facilitate not only CMS analysis, but also to support dark matter and cosmology calculations as well as various other computational genres. We are at the forefront of distributed computing resource management with our participation in Grid projects since 2004 as well as recent frontline tests and usage of computing Cloud technologies.

The centre is marked on Estonian Science Roadmap and participates in building the nationwide infrastructure for scientific computing. It is one of three centres in the country featuring computational resources and large scale storage capacity in the years 2012-2015 and onwards.

Features in 2010

- more than 1 200 compute cores
- 280TB of data storage facilities
- switching fabric that guarantees reasonable data transfer rates to every compute core.
- Grid interfaces for remote job submissions
- Cloud instances for dynamic resource reservation
- Ca 100 kW of cooling capacity

## Quantum Chemistry High Performance Computing Facility

Contact persons:

Endel Lippmaa, DSc (elippmaa@nicpb.ee) – quantum chemistry, quantum computing, high energy physics

Aleksander Trummal, PhD (aleksander.trummal@kbfi.ee) – quantum chemistry, HPC

Alar Rummel, MSc (alar.rummel@kbfi.ee) – quantum chemistry, catalysis

The hardware for high performance parallel computing features optimized combination of high SMP scalability and low latency/high bandwidth communication between SMP nodes to satisfy diverse requirements for both shared memory and MPI application performance associated with various quantum chemical and other codes:

#### DELL 96-core server

- Features:
- Four PowerEdge R905 AMD 8435 SMP nodes
  - Mellanox Infiniband interconnect between SMP nodes
  - Peak theoretical performance 1.6 TFLOPS
  - Precision 3500 console workstation

#### SGI 24-CPU SMP server

- Features:
- Three Origin R10000 SMP modules
  - NUMALink interconnect between CPUs, nodes, and modules
  - O2 console workstation

#### Supermicro 16-CPU server

- Features:
- Eight X5DP8-G2 Intel Xeon 3.06GHz SMP nodes
  - Myrinet2000 interconnect between SMP nodes

#### Major quantum chemistry software packages:

Accelrys Materials Studio Dmol3 server and Visualize  
Gaussian and GaussView  
MOPAC

QCHPCF provides dedicated secure platform for running professional quantum chemistry codes. The computers have no connection to Internet, GRID or Cloud, are completely virus-free and use only licensed professional software.

## Cryo Unit

#### Contact person:

Enno Joon, PhD (enno.joon@kbfi.ee) – Low Temperature Physics, Solid State Physics, Superconductivity, Magnetism, Nanotechnology and Cryogenic Engineering

Cryo Unit as a part of NICPB is responsible for cryogenic services of superconductive magnets installed at the institute. The services involve filling the magnets with liquid nitrogen and liquid helium, compensating for everyday evaporation of the named liquids. For this purpose about 50-60 tons of commercial liquid nitrogen and around 6 000 litres of liquid helium are used. The annual production of the liquid He despite of the long exploitation time of the liquefier (28 years) is growing: 4245 l (2007), 5890 l (2008), 7700 l (2009), 6070 l (3/4 of 2010). This amount of liquid He covers the needs of PPMS, low temperature NMR, infrared optics and Raman spectroscopy research. We also provide liquid He for SC magnet at the Tallinn University of Technology. The evaporated He gas is recovered to gas bags and compressed to high pressure storage. Liquid nitrogen is also used for precooling He liquefier, He gas cleaning, biochemical research and keeping biological samples cold.

#### He liquefier CTi-1410 (1979)

- Features: piston detander working with two piston compressors, 20 kW each

Productivity: 20 l liquid He per hour using pure gas and 15 lph using impure recovered gas, which is prepurified during the same procedure.

Cryo Unit provides the maintenance and repairing of cryo and vacuum apparatus and devices as well.





The team

Ain Toim, senior engineer

Tõnu Tolk, senior engineer

Andres Reinhold, senior engineer

Vambola Kivisaar, technician

## Scientific Collections and Databases of NICPB

### Scientific Collections

Contact person: Anne Kahru, PhD (anne.kahru@kbfi.ee)

The scientific collections of the NICPB were established in 1980 when the biological research was started. During 2004-2008 the development of the collections has been supported by the “National Programme on Scientific collections” in a project “Scientific collections in cell biology and toxicological research” (HLK04-4, PI Dr. A. Kahru). Currently, the NICPB collections consist of microbial cultures (bacterial and yeast strains and collection of plasmids), cell lines, venoms and environmental samples (soils, sediments, oil-shale industry solid wastes).

The database on scientific collections in the National Institute of Chemical Physics and Biophysics is available at <http://kbfi-databases.eu/ecotox/>. The scientific collections of NICPB are continuously upgraded.

The development of the microbial collection of NICPB has been focusing on construction of new recombinant heavy metal sensor microbes and knock-out mutants that allow studying mechanisms of toxic action of chemicals. The collection of environmental samples (about 600 samples) includes soils and sediments with various type of pollution (Zn, Cd, Pb, PAHs, phenols) and unique set of soils and solid wastes from Estonian oil-shale industry region. The environmental samples have been characterized both chemically and ecotoxicologically. The microbial strains and environmental samples are used in scientific research projects of NICPB (including MSc and PhD studies). More information on this collection can be obtained from Kaja Kasemets [kaja.kasemets@kbfi.ee](mailto:kaja.kasemets@kbfi.ee). The recombinant microbial strains constructed in NICPB have been and will be distributed free of charge to other research laboratories upon written and signed agreement (enquiries: Angela Ivask [angela.ivask@kbfi.ee](mailto:angela.ivask@kbfi.ee)).

### References

1. **Ivask A**, Rõlova T, **Kahru A**. A suite of recombinant luminescent bacterial strains for the quantification of bioavailable heavy metals and toxicity testing. *BMC Biotechnology* 2009, 9:41 (8 May 2009), doi:10.1186/1472-6750-9-41 <http://www.biomedcentral.com/1472-6750/9/41/abstract>
2. Leedjärv A, **Ivask A**, Virta M. The interplay of different transporters in the mediation of divalent heavy metal resistance in *Pseudomonas putida* KT2440. *J. Bacteriology*, 2008, 190 (8): 2680-2689
3. **Kahru A**, **Põllumaa L**. Environmental hazard of the waste streams of the Estonian oil-shale industry: an ecotoxicological review - *Oil Shale*, 2006, 23 (1): 53-93

### ***E-SovTox - An Online Database of the Main Publicly available Sources of Toxicity Data Concerning REACH-relevant Chemicals Published in the Russian Language***

While FP6 project OSIRIS was prepared, our partners proposed to the consortium to compose a database of the main publicly available sources of toxicity data concerning REACH-relevant chemicals published in the Russian language. By evaluators, this was one of the novel aspects of OSIRIS. REACH is a new EU chemical policy (Registration, Evaluation, Authorisation and Restriction of Chemicals). The database contains information selected mainly from scientific journals published during the Soviet Union era and that are available as hard copies in Estonian libraries. Currently the E-SovTox database contains toxicity data selected from more than 500 papers covering more than 600 chemicals. The user is provided with the main toxicity information, as well as abstracts of these papers in Russian and in English (given as provided in the original publication). The search engine allows cross-searching of the database by the name or CAS

number of the compound and the author of the paper. The E-SovTox database can be used as a decision-support tool by researchers and regulators for the hazard assessment of chemical substances. The database is hosted by the Laboratory of Molecular Genetics (MGL), National Institute of Chemical Physics and Biophysics, Tallinn, Estonia. The MGL is in charge of data collection and editing, database maintenance and dissemination. The online E-SovTox database is designed for scientists and regulators to provide them with (eco)toxicological data from literature published in Russian informative for the hazard assessment of chemical substances.

The database was created by the late H.C. Dubourguier, M. Sihtmäe, I. Blinova and A. Kahru. Bibliographical assistance was provided by E. Saar and S. Mae. Database was programmed by N. Legrand (Protopro-websites OÜ, [www.dynameeks.com](http://www.dynameeks.com))

#### Characterisation of the Database

- Name of the Database: E-SovTox;
- Web address: <http://kbfi-databases.eu/>;
- Cost: Free after registration;
- Year of availability of the demo-version: 2010;
- Hardware and software required: Any computer with Internet capabilities;
- Programming language: HTML/PHP/MySQL;

## Workshop

#### Contact persons:

Andres Reinhold, senior engineer ([reinhold@kbfi.ee](mailto:reinhold@kbfi.ee))

Tiit Tuherm, senior engineer ([tuherm@kbfi.ee](mailto:tuherm@kbfi.ee))

#### The workshop has the following machine tools:

Lathe Weiler Matador, accuracy 0,005mm

Milling machine ALG-100, accuracy 0,005mm

CNC KERN HSPC 2522, accuracy 0.001mm

## II EDUCATION AND CO-OPERATION

All research groups and Laboratories of the Institute actively collaborate with all main Estonian universities – University of Tartu, Tallinn University of Technology, Tallinn University of Life Sciences, – either via common curricula and co-supervision of PhD students or as external examiners of thesis works.

The facilities of the Institute are used for graduate and postgraduate training in the fields of biochemistry and –technology, environmental chemistry and chemical physics.

Thesis Works Defended by co-workers of NICPB

<b>Thesis</b>	<b>2007</b>	<b>2008</b>	<b>2009</b>	<b>2010</b>	<b>Total</b>
MSc	2	3	2	2	9
PhD	2	5	2	1	10
<b>Total</b>	<b>4</b>	<b>8</b>	<b>4</b>	<b>3</b>	<b>19</b>

In addition to the above universities, the Institute has joint research projects and/or publications with a number of domestic and international academic institutions like Clemson University and University of California Los Angeles, National Institutes of Health (USA), Liverpool John Moore University, Southampton University, Teesside University and Warwick University (UK), Bordeaux and Grenoble Universities, Francois Rabelais University (France), Institute of Biotechnology and Helsinki University (Finland), Innsbruck Medical University (Austria), Forschungszentrum Jülich (Germany), University of Ljubljana (Slovenia), University of Lund (Sweden), ETH Zürich and CERN (Switzerland), to name a few.

## III EVALUATIONS

### Evaluations of 2000-2001

Evaluation of the Laboratory of Chemical Physics was carried out on February 14, 2001 under the „Evaluation of Estonian Research in Physical, Inorganic and Analytical Chemistry“ by an international team consisting of Pekka Pyykkö (Chairman), Jorma Hölsä, Irene Montenegro and Jarl B. Rosenholm appointed by the Estonian Higher Education Accreditation Centre. The committee ranked the Laboratory as Excellent / Good.

The Laboratories of Bioenergetics and of Molecular Genetics were jointly evaluated in the fall of 2000 under the „Research Evaluation on Genetics, Physiology, Microbiology and Molecular Biology“.

Finally, the Laboratory of Bioorganic Chemistry was evaluated in January and February of 2001 under the „Evaluation of Estonian Research in Organic and Bioorganic Chemistry and Biochemistry“. The overall ranking for the Laboratory was satisfactory.

### Evaluation of 2010

The most recent evaluation was carried out by the orders of the Estonian Minister of Education and Science by a 16-strong international team headed by Ronald Axtmann, Professor at the Sussex University (GB) in May, 2010. The team also included as the heads of subcommittees Professor Hans Brix (Aarhus University, DEN), Professor Kenneth Douglas (Manchester University, GB) and Professor Eric Gregoire (D'Artoise University, FRA).

The evaluation was carried out in three fields of scientific research: Biosciences and Environment, Health and Natural Sciences and Engineering. The process included assessments in three categories: 1) the volume and level of R&D activities in comparison to international criteria; 2) R&D infrastructure; 3) Qualification of researchers in comparison to international criteria.

The NCIPB was evaluated as „positive“ in all fields and by criteria and sub-criteria, with a final assessment as „positive“. The results of the evaluation were approved and confirmed by Minister's decree on July 6, 2010.



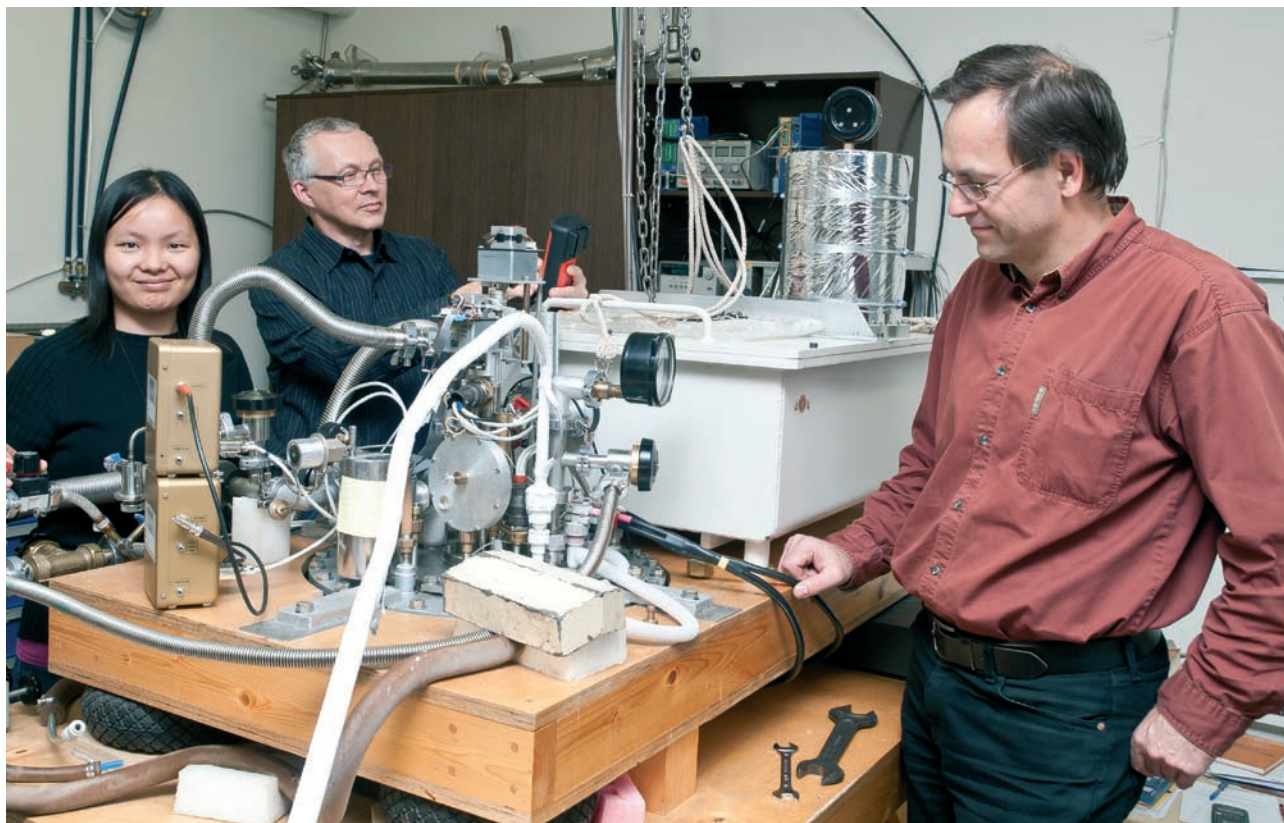


*Senior Researcher Tuuli Käämbre (left) and PhD student Kersti Tepp measuring the oxygen consumption of biosamples.*



*EUREKA! Senior Researcher Kaja Kasemets (from left) and PhD students Olesja Bondarenko and Imbi Kurvet.*





*Post-doc Min Ge (from left) and Senior Researchers Urmas Nagel and Toomas Rõõm with a FIR spectrometer setup.*



*Post-doc Mukesh Chandra Dimri operating a PPMS.*





*Leading Researcher Jaan Past (front) and Senior Engineer Tiit Tuherm tuning a home-built MAS NMR probehead.*



*Senior Researcher Ivo Heinmaa with a home-built cryo-MAS NMR probehead.*





*Post-doc Andi Hektor is maintaining the high performance computing servers at the computing centre of the NICPB.*



*Senior Researcher Enno Joon in front of the helium liquefier in the Cryo unit.*

## IV ORGANISATION AND ADMINISTRATION

The organisation and administration of the NICPB – a legal person under public law - are governed by the “National Institute of Chemical Physics and Biophysics Act” of 1998 (Estonian text: <https://www.riigiteataja.ee/ert/act.jsp?id=215551>, English translation see: <http://www.kbfi.ee/?id=27>) and the Statute of the NICPB.

According to the Act, the directing bodies of NICPB are the Director and the Scientific Board.

### Scientific Board

The Scientific Board is the collegiate decision-making body of NICPB which consists of 19 members. The Scientific Board includes the Director, Deputy Directors, Scientific Secretary and leading scientists of NICPB and from related fields.

The Scientific Board, among other activities, approves the main directions of the activities of NICPB, approves the Statutes of NICPB, approves the budget of NICPB and elects the Director of NICPB. The Board is headed by a Chairperson.

The sessions of the Scientific Board take place as necessary, but at least once in every three months. A meeting is called by the Chairman of the Scientific Board.

The Scientific Board on October 31, 2010

Member	Affiliation
Professor Jaak Aaviksoo, Chairman of the Board	Member of the Estonian Academy of Sciences, Minister of Defence
Jüri Jarvet, PhD, Deputy Chairman	NICPB
Professor Peeter Burk	Dean of the Faculty of Science and Technology, University of Tartu
Ivo Heinmaa, PhD	NICPB
Anne Kahru, PhD	NICPB
Marco Kirm, PhD	Director of the Institute of Physics, University of Tartu
Tuuli Käämbre, PhD	NICPB
Professor Ülo Niinemets	Estonian University of Life Sciences
Tõnis Pehk, DSc	NICPB
Martti Raidal, PhD	NICPB
Toomas Rõõm, PhD	NICPB
Valdur Saks, DSc	NICPB
Tiit Saluvere, PhD	NICPB, Deputy Director
Jüri Siigur, PhD	NICPB, Scientific Secretary
Raivo Stern, PhD	NICPB, Director
Erik Teinemaa, PhD	Estonian Environmental Research Centre
Professor Rein Vaikmäe	Institute of Geology, Tallinn University of Technology
Toomas Välimäe, PhD	NICPB, Deputy Director

## Director

The Director takes care of the expedient management of research and development, represents NICPB in all legal acts, approves all internal regulations and rules of house, concludes employment contracts, etc. The Director is also in charge of preparing the draft budget and ensures the implementation of the budget.

The Director is elected by the Scientific Board for a five year period and he/she is accountable before the Scientific Board.

The Director of the NICPB since 2006 is Raivo Stern, PhD.

## Deputy Directors

The Deputy Director on Administrative affairs is responsible for the Institute's administration and finances together with all administrative services and maintenance of the premises. Mr Tiit Saluvere, PhD. has served as Deputy Director since 1980.

The Deputy Director on Strategic Planning is responsible for the strategic development and financial planning including budgeting. Together with the Director they hold responsibility for the achievement of Institute's long-term goals. The Deputy Director is Toomas Välimäe, PhD.

## The International Science Advisory Board

The International Science Advisory Board evaluates periodically the current research programmes of the NICPB and advises the Scientific Board to open new programmes and/or to terminate existing programmes. The Advisory Board also evaluates scientific and administrative capacities of the candidates to the posts of the Director and/or the heads of Laboratories and working groups.

The sessions of the Scientific Board take place as necessary and they are called by the Director. Members of the Science Advisory Board are:

Member	Affiliation
Professor Peter Littlewood, Chairman	Cavendish Laboratory, University of Cambridge (UK)
Professor Dmitri Basov	Department of Physics, University of California, San Diego (USA)
Professor Carlos Ibáñez	Laboratory of Molecular Neurobiology, Karolinska Institute (SWE)
Professor Robert Kaptein	Bijvoet Centre for Biomolecular Research, Utrecht University (The Netherlands)
Professor Tapio Niinikoski	CERN
Professor Mart Saarma	University of Helsinki (FIN)
Professor Hanna Tähti	FICAM, University of Tampere (IN)
Professor Marten Wikström	Institute of Biotechnology, University of Helsinki (FIN)



## Structure

According to the Statute, the structure of NICPB includes scientific, administrative and economic units. Currently there are no other units except scientific ones.

The scientific units are laboratories of:

### ***Chemical Physics (CP)***

Head: Tõnis Pehk, DSc

tonis.pehk@kbfi.ee

Phone +372 6398 319

### ***Bioorganic Chemistry (BOC)***

Head: Jüri Siigur, PhD

juri.siigur@kbfi.ee

Phone +372 6398 360

### ***Molecular Genetics (MG)***

Head: Anne Kahru, PhD

anne.kahru@kbfi.ee

Phone +372 6398 373

### ***Bioenergetics (BE)***

Head: Professor Valdur Saks, DSc

vsaks@ujf-grenoble.fr

Phone +372 6398 383

The actual scientific research is carried out by informal research groups comprising of co-workers of different laboratories (see also the Organisation Chart on p 54).

# V STATISTICS

## Finances

### *Outline of the financing of science in Estonia*

The financing of (public) scientific institutions consists of a number of financing instruments.

**Targeted financing**, which is used to fund the activities of research groups from research institutions, is the most important financing instrument in Estonian scientific research. State budgetary resources are allocated for this purpose through the budget of the Ministry of Education and Research (MER). Proposals regarding the targeted financing of research topics of R&D institutions are submitted by the Estonian Research Council acting as an advisory body to the Minister of Education and Research. Targeted financing is used to fund evaluated R&D institutions' research topics (both basic and applied research).

**Baseline financing** involves the financing of R&D institutions that have received positive evaluations with the aim of realizing strategic development goals, co-financing foreign and domestic projects and opening up new research directions. Baseline financing is intended to guarantee the stability of financing and increases the sense of security, initiative, and responsibility of research institutions in planning their R&D activities. Thus, baseline financing makes it possible for the institutions to focus more on their main activities, and thereby achieve better results. Baseline financing is provided from the state budget through the budget of the MER. Baseline financing is also a performance-based instrument, as 50% of the sum is divided between the recipients according to their respective share of publications in the Thomson Reuters Web of Science database.

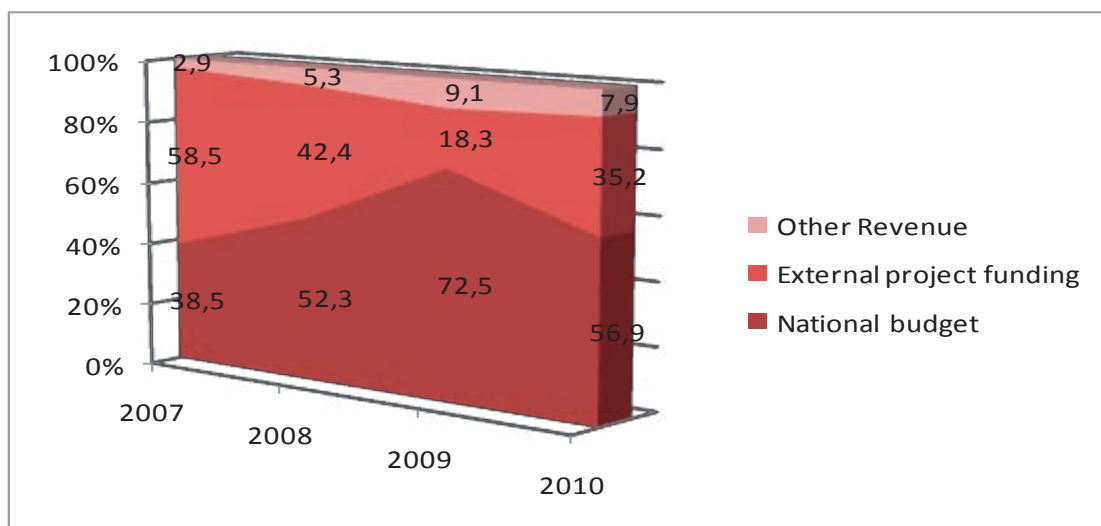
Resources are provided from the state budget through the MER budget in order to support the **covering of infrastructure costs** incurred by R&D institutions operating as legal persons governed by public law or as establishments thereof.

**Research grants** are available to individuals as well as research groups who have to undergo a research project financing competition. Annual public grant competitions, funded from the state budget through the budget of the MER, are conducted by the Estonian Science Foundation.

The implementation of EU Structural Funds for supporting research and development activities is governed by the MER and takes place through the Archimedes Foundation's Implementing Agency of Structural Support. The total cost of the most important **measure - measure for modernizing research equipment and devices** (together with co-financing and value added tax) comes to 115 million EUR, of which over 86 million EUR is provided from the Structural Funds.

**Table 1 Funding of the NICPB in 2007-2010**

Source	2007		2008		2009		2010	
	EUR	%	EUR	%	EUR	%	EUR	%
National budget	1 425 556	38,5	1 649 636	52,3	1 582 917	72,5	1 823 517	56,9
External project funding	2 164 663	58,5	1 338 426	42,4	400 311	18,3	1 128 421	35,2
Other Revenue	108 650	2,9	168 464	5,3	198 970	9,1	252 375	7,9
GRAND TOTAL	3 698 869	100,0	3 156 526	100,0	2 182 197	100,0	3 204 312	100,0



**Table 2 Financing from National Budget 2007-2010**

Source	2007		2008		2009		2010	
	EUR	%	EUR	%	EUR	%	EUR	%
Targeted financing (TF)	711 030	49,9	468 472	28,4	923 581	58,3	849 514	46,6
Baseline financing	229 750	16,1	265 578	16,1	189 072	11,9	145 642	8,0
TF of Infrastructure	250 150	17,5	250 150	15,2	246 969	15,6	244 047	13,4
TF of equipment	0	0,0	0	0,0	0	0,0	372 391	20,4
TF of renovation		0,0	121 432	7,4	0	0,0		0,0
ESF grants	221 205	15,5	245 152	14,9	223 295	14,1	211 923	11,6
Other TF	13 421	0,9	11 248	0,7	0	0,0	0	0,0
Non-earmarked financing		0,0	287 602	17,4	0	0,0	0	0,0
National budget total	1 425 556	100,0	1 649 636	100,0	1 582 917	100,0	1 823 517	100,0

**Table 3 External Project Funding 2007-2010**

Source	2007		2008		2009		2010	
	EUR	%	EUR	%	EUR	%	EUR	%
Enterprise Estonia <sup>1</sup>	0	0,0	0	0,0	0	0,0	499 867	44,3
European Union <sup>2</sup>	1 742 862	80,5	873 110	65,2	0	0,0	0	0,0
R&D <sup>3</sup>	421 801	19,5	465 316	34,8	400 311	100,0	628 553	55,7
Total	2 164 663	100,0	1 338 426	100,0	400 311	100,0	1 128 421	100,0

<sup>1</sup> – Enterprise Estonia funding for purchase of scientific equipment

<sup>2</sup> – EU Structural Funds for purchase of scientific equipment and development of infrastructure

<sup>3</sup> – R&D grants from and contracts with various institutions

## Personnel

**Table 4 Personnel of NICPB (total number), November 1, 2010**

Staff Category	Number	Percentage	% of women
Researchers incl graduate students	61	54,0	37,7
Laboratory technicians (undergraduate students)	26 (2)	23,0 (1.8)	43.5 (0.0)
Administration	11	9,7	54,5
Technical staff (ancillary services)	15	13,3	60,0
Total	113	100,0	44,2

**Table 5 Personnel of NICPB (person years), November 1, 2010**

Staff Category	Person Years	Percentage
Researchers incl graduate students	52,0	54,6
Laboratory technicians (undergraduate students)	21,2 (1,5)	22,2 (1,6)
Administration	10,3	10,7
Technical staff (ancillary services)	11,9	12,5
Total	95,3	100,0

**Table 6 Proportions of staff categories (%) in person years in 2007-2010**

Staff Category	2007	2008	2009	2010
Researchers incl graduate students	60,3	56,3	56,8	54,6
Laboratory technicians	14,9	20,5	21,3	22,2
Administration	11,2	9,5	10,6	10,7
Technical staff (ancillary services)	13,6	13,7	11,3	12,5
Total	100,0	100,0	100,0	100,0
Total Person Years	96,3	97,4	96,5	95,3
Total employees	118	120	118	113

**Table 7 Proportion of PhDs and foreign researchers among researchers (Person Years)**

Staff Category	2007	2008	2009	2010
Number of Researchers	58	55	55	52
Number of PhDs	39	40	43	43
Proportion of PhDs	66,2%	73,6%	79,0%	82,2%
Number of foreign researchers (PY)	3	7	6	6
Proportion of foreign researchers	4,3%	11,9%	10,0%	11,1%

## Staff

The Staff of the Institute in 2010, including

### Leading Researchers

Kahru Anne  
Kirso Uuve  
Past Jaan

Pehk Tõnis  
Saks Valdur<sup>1</sup>  
Siigur Jüri

Dubourguier Henri-Charles<sup>2</sup>

### Senior Researchers

Aaspõllu Anu<sup>1</sup>  
Anman Tiia  
Blinova Irina  
Blumberg Girsh<sup>1</sup>  
Heinmaa Ivo  
Irha Natalja  
Ivask Angela<sup>6</sup>  
Jarvet Jüri  
Joon Enno  
Kajiyama Yuji  
Kasemets Kaja  
Kesvatera Tõnu  
Käämbre Tuuli<sup>1</sup>

Liidja Georg<sup>1</sup>  
Lippmaa Endel  
Maremäe Ello-Ragne  
Nagel Urmas  
Patriarca, Marco  
Pihlak Arno-Toomas<sup>1</sup>  
Raidal Martti  
Põllumaa Lee<sup>2</sup>  
Rebane Aleksander<sup>1</sup>  
Reinik Janek  
Rõöm Toomas  
Samel Mari  
Samoson Ago<sup>2</sup>

Sarv Priit<sup>1</sup>  
Siigur Ene  
Sikk Peeter<sup>1</sup>  
Strumia Alessandro<sup>1, 2</sup>  
Subbi Juhan  
Ševtšuk Igor  
Tanner Risto  
Teinemaa Erik<sup>1</sup>  
Tiivel Toomas<sup>2</sup>  
Trummal Aleksander  
Trummal Katrin

### Researchers

Adamson Jasper<sup>2</sup>  
Anupõld Tiit<sup>2</sup>  
Aruoja Villem<sup>1</sup>  
Chandra Mukesh<sup>3</sup>  
Ge Min<sup>3</sup>  
Heinsalu Els  
Hektor Andi<sup>4</sup>  
Hüvonen Dan<sup>1, 5</sup>  
Joa Kelly

Kadastik Mario  
Kannike Kristjan<sup>7</sup>  
Kriisa Annika<sup>2</sup>  
Kurve Imbi<sup>1</sup>  
Lassi Margit<sup>1</sup>  
Mortimer Monika<sup>1</sup>  
Müntel, Mait  
Nutt Anu<sup>2</sup>  
Racioppi Antonio<sup>3</sup>

Rebane Liis  
Rummel Alar  
Sihtmäe Mariliis  
Timohhina Natalja  
Tõnismägi Külli  
Tšekulajev Vladimir  
Vija Heiki

### Laboratory Technicians

Agurauja Arvo  
Agurauja Reet  
Bondarenko Olesja

Heinlaan Margit  
Jefimova (Panova) Jekaterina  
Kanarbik Liina<sup>1, 2</sup>

Keskrand Kalle<sup>2</sup>  
Khanduri Himani<sup>2</sup>  
Kiirend Ene<sup>1</sup>



Kivisaar Vambola  
 Kooskora Helgi<sup>1</sup>  
 Laas Pilvi  
 Livenson Ilja<sup>2</sup>  
 Pahapill Jüri  
 Peitel Maire<sup>1</sup>  
 Putting Valter<sup>2</sup>

Pöder Reio<sup>1</sup>  
 Reinhold Andres  
 Saaremäe Merle<sup>2</sup>  
 Sihver Arvo<sup>1</sup>  
 Simm Aia<sup>2</sup>  
 Tepp Kersti  
 Tiko Andres

Toim Ain  
 Tolk, Tõnu  
 Tuherm Tiit  
 Uleksin Taaniel  
 Varikmaa /Karu Minna  
 Vija Sirje

### Graduate (Doctorate) Students

Aruoja Villem<sup>1</sup>  
 Bondarenko Olesja<sup>1</sup>  
 Heinlaan Margit<sup>1</sup>  
 Khanduri Himani<sup>2</sup>  
 Kurvet Imbi<sup>1</sup>  
 Käkinen Aleksandr<sup>1</sup>

Livenson Ilja  
 Mortimer Monika<sup>1</sup>  
 Panova Jekaterina  
 Pöder Reio<sup>1</sup>  
 Rebane Liis  
 Sihtmäe Mariliis

Tepp Kersti  
 Tiko Andres<sup>2</sup>  
 Timohhina Natalja  
 Varikmaa / Karu Minna

### Undergraduate Students

Filippova Irina  
 Juganson Katre

Kanarbik Liina  
 Uleksin Taaniel

### Administration

Laigar Aili<sup>1</sup>  
 Raba Mari  
 Saar Ene  
 Saluvere Tiit

Stern Raivo  
 Suursalu Urmas  
 Sülluste Kristian  
 Till Mare

Valdmann Ene  
 Vallner Tatjana  
 Välimäe Toomas<sup>2</sup>

### Technical Staff

Aldur Niina  
 Bahurinskaja Svetlana<sup>1</sup>  
 Boitsova Jevgenia<sup>1</sup>  
 Jesaar Rein  
 Keemann Elle<sup>1</sup>

Kristal Silvia<sup>1</sup>  
 Kristal Valdur  
 Lepp Rein  
 Lillemägi Adolf  
 Nurme Reet<sup>1</sup>

Ploom Leili  
 Zahharenkova Jelena  
 Tammist Aino<sup>1</sup>  
 Tomson Jüri  
 Torn Toivo<sup>1</sup>

1 – worked part-time

2 – worked part of the year

3 – post-doc in NICPB

4 – post-doc in CERN

5 – post-doc in ETH, Zürich

6 – post-doc in UCLA

7 – post-doc in University of Pisa

## VI PUBLICATIONS

### Original articles

1. Adamson J, **Irha N**, **Adamson K**, Steinnes E, **Kirso U**. Effect of oil shale ash application on leaching behavior of arable soils: an experimental study. *Oil Shale*, 2010, 27 (3): 250-257
2. Antchev G, **Lippmaa E**, **Rummel A**, **Trummal A** et al. The TOTEM detector at LHC. Conference Information: 11th Pisa Meeting on Advanced Detectors, MAY 24-30, 2009 Isola Elba, Italy, Nuclear Instruments & Methods In Physics Research Section A-Accelerators Spectrometers Detectors And Associated Equipment, 2010, 617 (1-3): 62-66
3. **Blinova I**, **Ivask A**, Heinlaan M, **Mortimer M**, **Kahru A**. Ecotoxicity of nanoparticles of CuO and ZnO in natural water. *Environmental Pollution*, 2010, 158 (1): 41-47
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5. Christjanson P, **Pehk T**, Paju J. Structure and curing mechanism of resol phenolformaldehyde prepolymer resins. *Proc. of the Est. Acad. of Sci*, 2010, 59 (3): 225-232
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## Books

**Pihlak, Arno-Toomas.** Kilde isesüttimise protsesside ja õhuhapniku probleemide uurimise ajaloost Eestis, Tallinn, Aura Trükk Publishing, 2009, 61 pages (in Estonian)

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## Book Chapters and Articles in Proceedings

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3. Derewiński, Mirosław; Pashkova, Veronika; **Sarv, Priit.** Assembling protozeolitic nanoclusters of MFI type into a mesostructured material of wormhole-layered arrangement and acidic properties. Stud. Surf. Sci. Catal., Elsevier/North-Holland 2010, 111-112
4. Monge, Cells Claire; Guzun, Rita; **Tepp, Kersti; Timohhina, Natalja; Varikmaa, Minna; Sikk, Peeter; Käämbre, Tuuli; Saks, Valdur.** Mitochondrial Interactosome in Health and Disease: Structural and Functional Aspects of Molecular System Bioenergetics of Muscle and Neuronal Cells. Mitochondria: Structure, Functions and Dysfunctions, Ed. Oliver L. Svensson, Nova Science Publisher Inc. 2010, 7-10
5. **Siigur, Jüri; Siigur, Ene.** Activation of Factor X by Snake Venom Proteases. Toxins and Hemostasis. From Bench to Bedside, (Eds Kini, R.M.; Clemetson, K.J.; Markland, F.S.; Morita, T.), Springer 2010, 447-464
6. Anelli, G.; **Lippmaa, E.; Rummel, A.; Trummal, A.** et al. The TOTEM Experiment at the CERN Large Hadron Collider. The CERN Large Hadron Collider: Accelerator and Experiments, The TOTEM Collaboration, 2, CERN/LHCC, CERN, Geneva, Switzerland, 2009, 1-107
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8. Chatrchyan, S.; **Hektor, A.; Kadastik, M.; Kannike, K.; Lippmaa, E.; Müntel, M.; Raidal, M.; Rebane, L.** et al. The CMS experiment at the CERN LHC. The CERN Large Hadron Collider: Accelerator and Experiments, The CMS Collaboration, 2, CERN/LHCC, CERN, Geneva, Switzerland, 2009, 1-334
9. Kahru A. A chapter on situation of gender balance in Estonian science decision making. Widmer, M., Raudma, T. (Rapporteurs) Mapping the Maze: Getting More Women to the Top in Research. Luxembourg: Office for Official Publications of the European Communities, 2008, pp 44 – 45

## Other Publications (Dissertations)

1. Heinlaan, Margit. Ecotoxicological evaluation of synthetic nanoparticles and particulate environmental samples. PhD, Estonian University of Life Sciences, 2010
2. Trummal, Aleksander. Computational Study of Structural and Solvent Effects on Acidities of Some Brønsted Acids. PhD, University of Tartu Tartu, Tartu University Press, 2009
3. Heinsalu, Els. Normal and anomalously slow diffusion under external fields. PhD, University of Tartu, TU Press, 2008

4. Hektor, Andi. Neutrino physics beyond the Standard Model. PhD, University of Tartu, TU Press, 2008
5. Huvonen, Dan. Terahertz Spectroscopy of Low-Dimensional Spin Systems. PhD, Tallinn University of Technology, TUT Press, 2008
6. Kadastik, Mario. Doubly charged Higgs boson decays and implications on neutrino physics. PhD, Tallinn University of Technology, TUT Press, 2008
7. Kannike, Kristjan. Implications of Neutrino Masses. PhD, University of Tartu, TU Press, 2008
8. Müntel, Mait. Detection of doubly charged Higgs boson in the CMS detector. PhD, University of Tartu, TU Press, 2008
9. Anmann, Tiia. Integrated and Organized Cellular Bioenergetic Systems in Heart and Brain. PhD, Tallinn University of Technology, TUT Press, 2007
10. Trummal, Katrin. Purification, Characterization and Specificity Studies of Metalloproteinases from *Vipera lebetina* Snake Venom. PhD, Tallinn University of Technology, TUT Press, 2007
11. Mägi, Reelika. Application of a new analytical method for analysis of environmental discharges of oil shale processing. MSc (Second prize in category of master thesis), Tallinn University of Technology, 2010
12. Saaremäe, Merle. The expression of  $\beta$ -tubulin isoforms and their role in the regulation of permeability of mitochondrial outer membrane. MSc, Tallinn University of Technology, TUT Press, 2010
13. Adamson, Jasper. Fluoride-Free Cross-Coupling Methodology Using Disiloxanes: Synthesis of Terminal Aryl Acetylenes and Biaryl Compounds. MSc, Magdalene College, University of Cambridge, UK, 2009
14. Kurvet, Imbi. Natural and recombinant bioluminescent bacteria for high throughput toxicity screening. MSc, Tallinn University of Technology, TUT Press, 2009
15. Tõnismägi, Külli. Comparative study of snake venom l-amino acid oxidases. MSc, Tallinn University of Technology, TUT Press, 2008
16. Varikmaa, Minna. Model systems of dopamine transporter for the pharmacological characterization of ligands. MSc, University of Tartu, TU Press, 2008
17. Vija, Heiki. Separation of toxic peptides from *Amanita phalloides* and *Amanita virosa*. MSc, Tallinn University of Technology, TUT Press, 2008
18. Timohhina, Natalja. A Study Of Origination Of Characteristic Elements Of Foucault' Cardiogram. MSc, University of Tartu, TU Press, 2007
19. Panova, Jekaterina. The Fenton chemistry and its combination with coagulation for treatment of dye solutions. MSc, Tallinn University of Technology, 2007

## VII VISITING RESEARCHERS

No	Visitor's name and title	Visitor's affiliation	Visited member /unit of NICPB	Time
1.	Claire Monge, Ph.D, research scientist	Laboratory of Fundamental and Applied Bioenergetics, INSERM E221, Joseph Fourier University, Grenoble, France	Laboratory of BE	June 2009
2.	Prof. Pierre DosSantos	Service Pr-Clementy, Hôpital Haut-Lévêque, avenue Magellan, 33600 Pessac, INSERM Bordeaux France	Laboratory of BE	April 2009
3.	<i>Dr. C.A.M. (Kees) van Gestel</i>	Department of Animal Ecology, Institute of Ecological Science, Vrije Universiteit Amsterdam, The Netherlands	Laboratory of MG	May 2009
4.	Dr. Sc. Professor Irina Perminova	Department of Chemistry, Lomonosov Moscow State University	Laboratory of CP, Environmental Chemistry Group	June 2009
4.	Dr. Anita Jemec	National Institute of Chemistry, Ljubljana, Slovenia	Laboratory of MG	Dec 2009
5.	Dr. Pu-Chun Ke	Laboratory of Single-Molecule Biophysics and Polymer Physics, Department of Physics and Astronomy, Clemson University, US	Laboratory of MG	March and Dec 2010
6.	Dr. Olli-Pekka Penttinen	University of Helsinki Department of Environmental Sciences, Finland	Laboratory of MG	March, May, Oct 2010
7.	Anna Kiiski, MSc	University of Helsinki, Palmenia Centre for Continuing Education, Finland	Laboratory of MG	March, May, Oct 2010
8.	Dr. Suzanne Kadereit	Stemcell Group, Doerenkamp-Zbinden Chair for in vitro Toxicology and Biomedicine, University of Konstanz, Germany	Laboratory of MG	Sept 2010
9	Prof. Damjana Drobne	Department of Biology, Biotechnical faculty, University of Ljubljana, Slovenia	Laboratory of MG	Dec 2010



## VIII OTHER ACTIVITIES

During the period of 2007-2010 our employees have participated at dozens of conferences worldwide, they have taken part in tens of various co-operation events and have spent more than 1,400 days researching abroad or domestically in other scientific institutions. The activities are summarised in table 7 below.

Table 7 Summary of conference, co-operation and research activities of NICPB personnel 2007 - November 2010

Event	2007		2008		2009		2010	
	Participations	Days	Participations	Days	Participations	Days	Participations	Days
Internat. conferences	74	454	77	526	94	612	59	446
Nat conferences	33	68	81	140	10	15	66	103
Internat. Co-operation.	14	79	16	104	17	130	7	41
Nat. Co-oper.	7	7	8	10	3	8	3	3
Internat. research	22	303	34	301	26	388	43	491
Nat. Research	12	26	8	14	9	11	12	59

