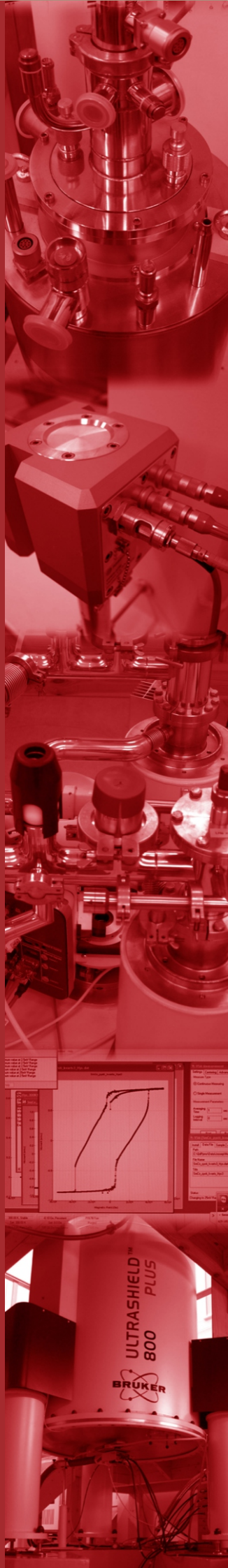
National Institute of
Chemical Physics and Biophysics

Keemilise ja Bioloogilise Füüsika Instituut

Activity Report 2011–2014

NICPB 1980–2015



National Institute of Chemical Physics and Biophysics

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Based on the Thomson Reuters Web of Knowledge (TR WoK) Essential Science Indicators NICPB is among the top 1% most cited research institutions in physics since May 1, 2013.

2015

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Kujundus OÜ Vali Press

NICPB Mission Statement

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 new generations of scientists in accordance with association 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.

Preamble

The foundation of the Institute (started originally inside the Institute of Cybernetics), the Laboratory of Chemical Physics (LCP) celebrated its 50th anniversary in 2011 and then gave birth to the Laboratory of High Energy and Theoretical Physics (LHETP), based on a workgroup in the LCP. By now the youngest lab – also youngest by the average age of its members - has grown bigger than any other lab except its parent lab.

In the fall of 2012 the former Laboratory of Molecular Genetics was renamed the Laboratory of Environmental Toxicology (LET). Tuuli Käämbre was elected the Head of the Laboratory of Bioenergetics as Prof Valdur Saks retired from the post but carries on as a research professor.

An important milestone for the Institute was the on-site visit of the Institute's International Science Advisory Board (SAB) and evaluation of the research in the Institute in June 2012. The evaluation involved an in depth review of the main research programs, tours of the facilities and laboratories, discussions with younger researchers and potential leaders, and a panel discussion on new initiatives and strategy.

The SAB concluded that: "The Institute is sound and well run, with a good relationship between the Staff and the Director. Over the last few years, the NICPB is evolving a strategy and direction that will be beneficial for the Institute and for Estonia as a whole, and despite some structural and financial impediments, is performing well scientifically. There are many high quality science programs, of international calibre, across the disciplines but including high energy physics, quantum condensed matter physics, NMR spectroscopies, toxicology, and bio-energetics. These programs increasingly make interdisciplinary links within the Institute, and some also support substantial national and international collaborations."

The recommendations given by the SAB were duly considered by the Scientific Board, which then adopted Institute's new Strategic Research Programmes for the period 2013 to 2020.

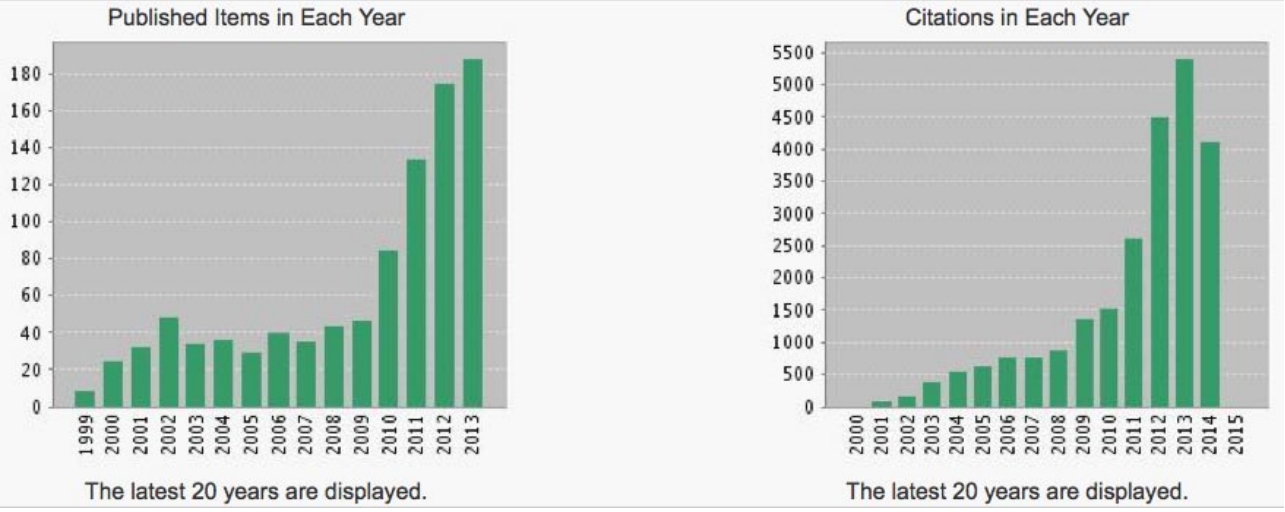

Figure 1. Published items and yearly citations (except 2014) by NICPB in TR WoK database.

Based on the Thomson Reuters Web of Knowledge (TR WoK) Essential Science Indicators NICPB is among the top 1% most cited research institutions in physics since May 1, 2013.

During the past years the Institute has slightly grown in size but at the same time has also been rejuvenated. At the end of 2010, the Institute employed 113 people with the average age of 53 years, whereas at the end of 2014 we were 124-strong with the average age of 47 years.

I Research and Development

The Institute's **Strategic Research Programmes** (**SRP**'s) are directly linked to the goals and priorities of both Framework 7 and Horizon 2020 and result from the key recommendations of the Institute's International Science Advisory Board (SAB) of July 28, 2012.

During the past few years the national framework of financing of science has undergone major changes. The largest and most important part, the targeted financing, has been replaced by so-called institutional research funding (IRF, Estonian abbreviation: IUT; typically for a 6 year period) that should enable research and development institutions to fund high-level research and development activities and to modernise and maintain the necessary infrastructure. Towards that end the IUT is complemented with a 28% financial support. The personal research grants (PRF, Estonian abbreviation PUT, typically for a 4 year period) have also undergone changes and are now allocated as a start grant for graduates, research grant for high level research or as a post-doc grant. These two (IRF and PRF) are the largest funding instruments provided by the Estonian Research Council, the new national agency. Both institutional and personal funding instruments are competition-based grants.

NICPB applied for IRF of 9 different themes in 2013 and we were successful to secure financing of 7 of them for the period of 2014 to 2019 (PIs: Ivo Heinmaa, Mario Kadastik, Anne Kahru, Tuuli Käämbre, Martti Raidal, Aleksander Rebane and Toomas Rõõm), although to a substantially lesser extent than anticipated. All the 7 themes are in concert with the recommendations of the SAB of 2012.

In addition, we have applied for 6 personal grants (3 start and 3 research grants). Due to very heavy competition of 10 to 1 and to somewhat voluntary bending of the rules we were able to score only 1 PRF in the fall of 2013. All in all we have 2 PRF (Raivo Stern PUT210 (2013-2016) and Dan Hüvonen (PUT451 for 2014-2017).

Furthermore, we have applied for 3 new IRF in 2014, namely "The role of diversity in complex systems" (PI Els Heinsalu, IUT39-1), "Interaction mechanism of bioactive compounds with various cell types" (PI Anu Aaspõllu, IUT39-2) and "Novel phases in strongly frustrated magnets" (PI Raivo Stern, IUT39-3). Eventually, Dr Heinsalu's application was the only one to get funding (for 2015-2020), albeit to much lesser extent than asked for.

Besides funding from national sources the Institute has acquired funding from European Social Fund, mediated by Estonian agencies, in the form of four (4) Mobilitas programme Top Researcher grants (hereinafter MTT) plus funding of a Centre of Excellence.

Finally, the Institute was engaged in 18 R&D projects, including two FP7 (Nanovalid and MODERN; see SRP4.1) and one INTEREG IVA (RIMA, see SRP4.1) project, 8 co-operative R&D projects under different national programmes funded by ESF and 6 industry-oriented projects.

SRP1. 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). Current programme includes both theoretical work and numerous international experiments in particle physics and cosmology. The strategy of the Institute is to be involved both in the development of new theories and in their experimental testing in forthcoming experiments.

1.1 Experimental High Energy Physics

The sub-programme "Experimental high energy physics at the CMS experiment at LHC" is currently funded from IUT23-6.

The sub-programme is also co-funded from MTT59 (Top Researcher Andrea Giammanco)

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In the experimental side NICPB is a member of the CMS collaboration of the forthcoming Large Hadron Collider at CERN. NICPB is the coordinator of Estonian scientists and summer students at CERN. As a spin-off of the experimental particle physics programme, a distributed computing concept Grid is under development and NICPB participates in it at both Estonian and European level. The Institute houses a Tier-2 computing centre, which is one of the biggest computing centres for the CMS experiment in Europe.

Currently the most important goal for the LHC experiments is to measure the properties of a recently discovered Higgs-like particle. The project aims to probe the Yukawa coupling between the Higgs boson and a top quark, which is an excellent test of the Standard Model. A good understanding of top-quark physics is achieved by studying the single top quark production that enables access to polarisation information and also gives a handle to probe physics beyond the Standard Model. Performing a search for a doubly charged Higgs boson provides a direct test for the possibility of an extended Higgs sector.

Researchers

Mario Kadastik, PhD

Andrea Giammanco, PhD

Liis Rebane, PhD

Nicolo de Filippis, PhD

Mait Müntel, PhD (left NICPB on June 16, 2013)

Venkat Kaushik, PhD

PhD Students

Andres Tiko (UT)

Degrees Defended
Rebane, Liis. Measurement of the W- >tau nu cross section and a search for a doubly charged Higgs boson decaying to tau-leptons with the CMS detector. PhD, University of Tartu, 2012

Selected Publications

1. **Calpas, Betty; Giammanco, Andrea; Kadastik, Mario; Murumaa, Marion; Raidal, Martti; Rebane, Liis; Tiko, Andres** et al. (2014). Constraints on the Higgs boson width from off-shell production and decay to Z-boson pairs. Phys.Lett., B736, 64
2. **Calpas, Betty; Giammanco, Andrea; Kadastik, Mario; Murumaa, Marion; Raidal, Martti; Rebane, Liis; Tiko, Andres** et al. (2014). Evidence for the direct decay of the 125 GeV Higgs boson to fermions. Nature Phys., 10, 1
3. Barbieri, Riccardo; Buttazzo, Dario; **Kannike, Kristjan**; Sala, Filippo; Tesi, Andrea (2013). One or more Higgs bosons? Physical Review D, 055011
4. **Giammanco, Andrea; Kadastik, Mario; Kannike, Kristjan; Murumaa, Marion; Müntel, Mait; Raidal, Martti; Rebane, Liis; Tiko, Andres; Strumia, Alessandro** et al (CMS Collaboration) (2012). Observation of a new boson at a mass of 125 GeV with the CMS experiment at the LHC. Physics Letters B, 716, 30
5. **Giammanco, Andrea; Kadastik, Mario; Müntel, Mait; Raidal, Martti; Rebane, Liis; Tiko, Andres** et al. (CMS Collaboration) (2012). A search for a doubly-charged Higgs boson in pp collisions at sqrt(s)=7

TeV. European Physical Journal C, 2189
6. **Giammanco, Andrea; Hektor, Andi; Kadastik, Mario; Müntel, Mait; Raidal, Martti; Rebane, Liis; Tiko, Andres** et al (CMS Collaboration) (2012). Combined results of searches for the standard model Higgs boson in pp collisions at sqrt(s) = 7 TeV. Phys.Lett., B710, 26-48
7. **Gabrielli, Emidio; Kannike, Kristjan**; Mele, Barbara; **Racioppi, Antonio; Raidal, Martti** (2012). Fermiophobic Higgs boson and supersymmetry. Physical Review D, 86(055014), 1 - 15
8. **Hektor, Andi; Kadastik, Mario; Kannike, Kristjan; Müntel, Mait; Raidal, Martti; Rebane, Liis** et al (CMS collaboration) (2011). Observation and studies of jet quenching in PbPb collisions at nucleon-nucleon center-of-mass energy = 2.76 TeV. Physical Review C, 84, 024906

1.2 Theoretical Particle Physics

The sub-programme "**The Origin of Mass**" is currently funded from IUT23-06

The sub-programme is also co-funded from MTT8 (Alessandro Strumia) and MTT60 (Emidio Gabrielli)

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The direction of the theoretical work in NICPB is phenomenological, and relies on availability of experimental data. Experimental neutrino physics and cosmology are currently and in the near future under fast development. This motivates the NICPB group to develop neutrino mass models and connecting them to experimental data. The neutrino masses might be directly connected to the expansion of the Universe shortly after the Big Bang. A fundamental problem in understanding the genesis and existence of the Universe is the emergence of asymmetric matter, or why there are ten orders of magnitude more matter than antimatter. One explanation goes through the leptogenesis, and NICPB participates in this work. Another priority of the NICPB group is the connection of the inflation of the Universe to the elementary particle theory.

The focus of the current research topic is to study the origin of mass of our Universe. In particular, our aim is to find the possible connection between the Higgs boson physics and the dark sector that presumably has a complicated structure. To address this question, we study results of dark matter direct and indirect detection experiments, analyse measurements of the cosmic microwave background, search for dark matter direct production at the LHC, and interpret cosmological observations and simulations for structure formation. To carry out this research, we develop scientific Grid and Cloud computing that will be our contribution to Estonian info-technology sector. At institutional and national level the aim of this proposal is to sustain the well functioning theoretical and astroparticle physics research team, to maintain the scientific computing centre, and to educate new generation of scientists that, eventually, guarantees the sustainability of this research field in Estonia.

Researchers

Martti Raidal, PhD

Andrew Fowlie, PhD

Emidio Gabrielli, PhD

Andi Hektor, PhD

Matti Heikinheimo, PhD

Els Heinsalu, PhD

Kristjan Kannike, PhD

Marco Patriarca, PhD

Antonio Racioppi, PhD

Christian Spethmann, PhD

Alessandro Strumia, PhD

Elmo Tempel, PhD
(left on October 31, 2014)

Degrees Defended
Tuvi, Taavi. Production mechanism of cosmic rays by supernova remnants. MSc, University of Tartu, 2014
Ainsaar, Siim. Fermion condensate as dark matter. MSc, University of Tartu, 2011

Selected Publications
1. **Gabrielli, Emidio; Heikinheimo, Matti; Kannike, Kristjan; Racioppi, Antonio; Raidal, Martti; Spethmann, Christian** (2014). Towards Completing the Standard Model: Vacuum Stability, EWSB and Dark Matter. Physical Review D, 89(1), 015017-1 - 015017-14.
2. **Heikinheimo, Matti; Raidal, Martti; Spethmann, Christian** (2014). Testing Right-Handed Currents at the LHC. The European Physical Journal C - Particle and Nuclear Physics, 10, 3017
3. **Hektor, Andi; Raidal, Martti; Tempel, Elmo** (2013). Evidence for indirect detection of dark matter from galaxy clusters in Fermi gamma-ray data. The Astrophysical Journal Letters, 762, L22
4. Belanger, Genevieve; **Kannike, Kristjan**; Pukhov, Alexander; **Raidal, Martti** (2013). Z3 Scalar Singlet Dark Matter. Journal of Cosmology and Astroparticle Physics, 1301, 022
5. **Heikinheimo, Matti; Racioppi, Antonio; Raidal, Martti; Spethmann, Christian**; Tuominen, Kimmo (2013). Dark Supersymmetry. Nuclear Physics B, 876, 201 - 214.
6. **Mario Kadastik, Kristjan Kannike, Antonio Racioppi, Martti Raidal**. Implications of the 125 GeV Higgs boson for scalar dark matter and for the CMSSM phenomenology. Journal of High Energy Physics 1205 (2012) 061
7. **Elmo Tempel, Andi Hektor, Martti Raidal**. Fermi 130 GeV gamma-ray excess and dark matter annihilation in sub-haloesand in the Galactic centre. Journal of Cosmology and Astroparticle Physics 1209 (2012) 032, Addendum-ibid. 1211 (2012) A01
8. Giardino, Pier Paolo; **Kannike, Kristjan; Raidal, Martti; Strumia, Alessandro** (2012). Is the resonance at 125 GeV the Higgs boson? Physics Letters B, 718, 469 - 474.

SAB recommendations on High Energy Physics and Theoretical Physics

The SAB recommends strongly to continue and support these activities and to help them flourish and grow in their national and pan-European frameworks.

The SAB also noted that:

- the established links to CERN, and the participation in a centre of excellence in high energy physics, are a strong opportunity for high profile science investment, which brings benefits in technology applications as well as public appreciation of science;
- the "big data" applications of a CERN tier 2 centre have already played out into national grid infrastructure and this could be amplified in different disciplines.

Centre for Excellence for Dark Matter in (Astro)particle Physics and Cosmology

The Laboratory of High Energy Physics and Computational Physics also houses the national **Centre of Excellence for Dark Matter in (Astro)particle Physics and Cosmology**

Head of the Centre of Excellence (CoE): Prof Martti Raidal, PhD

The CoE combines local Estonian competence in theoretical and experimental particle physics, in cosmology and in high-performance computing to carry out systematic interdisciplinary research of Dark Matter (DM) of the Universe. The aim is to search for the DM in terrestrial and satellite based experiments, to explain the origin and properties of DM and to analyse the implications of those results on particle physics and on cosmology. This research involves participation in 4 major international collaborations, the LHC CMS at CERN, Planck mission of the ESA, EGI and WLCG. The CoE develops Grid and Cloud computing in collaboration with Estonian info-technology companies and Enterprise Estonia. The CoE members teach and supervise PhD and MSc students in the University of Tartu, organise summer schools and train high-school physics teachers at CERN, and promote science via popularisation in written and electronic media.

SRP2. Physics of Condensed Matter and Materials Science

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.

2.1 New Spin Materials

Spin is a fundamental property of an elementary particle that is described properly only by laws of quantum mechanics. Despite the deep quantum nature spin has practical implications in material science. 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 coherent action of many electron spins. Even more, in multiferroics it is possible to reorient the spins with electric field. This reduces the amount of Joule heating of write operations in magnetic memories. Magneto-electric interaction between spin and polarisation waves in multiferroics is a cornerstone for new THz devices. Spin plays an important role in pairing of charge carriers in high-Tc superconductors . Superconductivity and magnetism are the driving forces of the exploration of quantum phase transitions in materials with strong electron correlations and Bose-Einstein condensation of magnons (spin waves). Among strongly correlated electron materials the heavy fermion systems are the source of unconventional superconductivity, novel magnetism, and hidden order.

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 infrared 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.

2.1.1 Interaction of THz radiation with magnetic excitations

The sub-programme is currently funded from IUT23-3 (PI Toomas Rõõm) and also from PUT451 (D. Hüvonen)

Principal Investigator: Toomas Rõõm, PhD
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THz spectroscopy is one of the most powerful methods for probing magnetic excitations in solids. We use this method to study magnetoelectric coupling in multiferroics and critical effects in different classes of magnetic materials. Magnetoelectric interaction in multiferroics mutually couples magnetisation and polarisation to electric and magnetic fields, thus offering new design concepts for memories and other electronic devices. We use THz spectroscopy in combination with high magnetic fields (beyond 30T) and low temperatures down to the milli-Kelvin range.

Researchers

Toomas Rõõm, PhD

Dan Hüvonen, PhD

Min Ge, PhD (left on May 24, 2011)

Tika Katuwal, PhD (left on August 31, 2013

Urmas Nagel, PhD

Liis Seinberg, PhD

Anna Šugai, PhD

Degrees Defended

Peedu, Laur. Infrared Spectroscopy of Molecular Hydrogen Quantum Motion in Endohedral Fullerene $H_2@C_{70}$. MSc, Tallinn University of Technology, 2013

Uleksin, Taaniel. Terahertz Spectroscopy in High Magnetic Fields at milli-Kelvin Temperatures. MSc, Tallinn University of Technology, 2012

Selected Publications

1. Szaller, Dávid; Bordács, Sándor; Kocsis, Vilmos; **Rõõm, Toomas; Nagel, Urmas**; Kézsmárki, István (2014). Effect of spin excitations with simultaneous magnetic- and electric-dipole character on the static magnetoelectric properties of multiferroic materials. Physical Review B, 89, 184419
2. Kézsmárki, I.; Szaller, D.; Bordács, S.; Kocsis, V.; Tokunaga, Y.; Taguchi, Y.; Murakawa, H.; Tokura, Y.; Engelkamp, H.; **Rõõm, T.; Nagel, U.** (2014). One-way transparency of four-coloured spin-wave excitations in multiferroic materials. Nature Communications, 5, 3203
3. Lago, J.; Zivkoviç, I.; Piatek, J. O.; Alvarez, P.; **Hüvonen, D**.; Pratt, F. L.; Diaz, M.; Rojo, T. (2014). Glassy dynamics in the low-temperature inhomogeneous ferromagnetic phase of the quantum spin ice Yb2Sn2O7. Physical Review B, 89, 024421
4. Thede, M.;Mannig, A.; Mansson, M.; **Hüvonen, D**.; Khasanov, R.; Morenzoni, E.; Zheludev, A. (2014). Pressure-Induced Quantum Critical and Multicritical Points in a Frustrated Spin Liquid. Physical Review Letters, 112, 087204
5. **T. Rõõm, L. Peedu, Min Ge, D. Hüvonen, U. Nagel**, Shufeng Ye, Minzhong Xu, and Z. Bacic, S. Mamone, M. H. Levitt, M. Carravetta, J. Y.-C. Chen, Xuegong Lei, N. J. Turro, Y. Murata, K. Komatsu (2013). Infrared spectroscopy of small-molecule endofullerenes. Phil. Trans. R. Soc. A, 371, 20110631
6. **U. Nagel**, Randy S. Fishman, T. Katuwal, H. Engelkamp, D. Talbayev, Hee Taek Yi, S.-W. Cheong, **T. Rõõm** (2013). Terahertz Spectroscopy of Spin Waves in Multiferroic $BiFeO_3$ in High Magnetic Fields. Phys. Rev. Lett 110, 257201
7. **U. Nagel, T. Uleksin, T. Rõõm**, R.P.S.M. Lobo, P. Lejay, C.C. Homes, J. Hall, A.W. Kinross, S. Purdy, T.J.S. Munsie, T.J. Williams, G.M. Luke, T. Timusk (2012). The normal state of URu_2Si_2: spectroscopic evidence for an anomalous Fermi liquid. PNAS (Proceedings of the National Academy of Sciences of USA), 109, 1916119-165
8. C. Beduz, M. Carravetta, J. Y.-C. Chen, M. Concistrè, M. Denning, M. Frunzi, A. J. Horsewill, O. G. Johannessen, R. Lawler, X. Lei, M. H. Levitt, Y. Li, S. Mamone,Y. Murata, **U. Nagel**, T. Nishida, J. Ollivier, S. Rols, **T. Rõõm**, R. Sarkar, N. J. Turro, Y. Yang (2012). Quantum rotation of ortho and para-water encapsulated in a fullerene cage. PNAS, 109, 12894-12898
9. J.S. Hall, **U. Nagel, T. Uleksin, T. Rõõm, T**. Williams, G. Luke, T. Timusk (2012). Observation of Multiple-Gap Structure in Hidden Order State of URu_2Si_2 from Optical Conductivity, Phys. Rev. B, 86, 035132
10. K. Penc, J. Romhányi, **T. Rõõm, U. Nagel**, Á. Antal, T. Fehér, A. Jánossy, H. Engelkamp, H. Murakawa, Y. Tokura, D. Szaller, S. Bordács, I. Kézsmárki, Spin-stretching modes in anisotropic magnets: spin-wave excitations in the multiferroic $Ba_2CoGe_2O_7$ (2012). Phys. Rev. Lett., 108, 257203
11. S. Bordács, I. Kézsmárki, D. Szaller, L. Demkó, N. Kida, H. Murakawa, Y. Onose, R. Shimano, **T. Rõõm, U. Nagel**, S. Miyahara, N. Furukawa, Y. Tokura (2012). Chirality of Matter Shows Up via Spin Excitations, Nature Physics, 8, 734-738
12. **Ge, Min**, **Nagel, U**., **Hüvonen, D**., **Rõõm, T**., Mamone, S., Levitt, M. H., Carravetta, M., Murata, Y., Komatsu, K., Lei, Xuegong, Turro, N. J. (2012). Infrared spectroscopy of endohedral HD and D_2 in C_{60}. J. Chem. Phys., 135, 114511
13. **M. Ge**, **D. Hüvonen**, **U. Nagel**, **T. Rõõm**, S. Mamone, M. H. Levitt, M. Carravetta,. Y. Murata, K. Komatsu, J. Y.-C. Chen and N. Turro, Interaction potential and infrared absorption of endohedral H_2 in C_{60} (2011). J. Chem. Phys., 134, 054507
14. Salvatore Mamone, Judy Y.-C. Chen, Rangeet Bhattacharyya, Malcolm H. Levitt, Ronald G. Lawler, Anthony J. Horsewill, **Toomas Rõõm**, Zlatko Bacic, Nicholas J. Turro (2011). Theory and Spectroscopy of an Incarcerated Quantum Rotor. The Infrared Spectroscopy, Inelastic Neutron Scattering and Nuclear Magnetic Resonance of $H_2@C_{60}$ at Cryogenic Temperatures, Coordination Chemistry Reviews, 255, 938-948

2.1.2 Novel phases in strongly frustrated magnets

Funded partially from PUT210 (R. Stern). Application for IUT funding was denied in 2014.

The sub-programme is also co-funded form MTT77 (Alexander Tsirlin).

Principal Investigator: Raivo Stern, PhD
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Frustrated spin systems exhibit a variety of behaviours ranging from exotic ground states and novel types of magnetic excitations, to the magnetocaloric effect and multiferroicity. A corollary of the vibrant research in this field is new frustrated materials that hold promise for novel phases, interesting physics, and potentially useful properties. We propose comprehensive studies of these materials aiming to provide an insight to their physics on the phenomenological as well as the microscopic level. This combined approach gives us the opportunity to obtain new experimental results, understand them within a suitable theoretical framework, and use this insight for the design of new materials. Our working methods include low-temperature thermodynamic measurements, NMR, x-ray and neutron scattering, and state-of-the-art electronic-structure calculations combined with microscopic modelling. Most of these methods are available in Estonia and rest upon the previous experience of our team.

Researchers

Raivo Stern, PhD

Himani Khanduri, PhD (left June 30, 2013)

Alexander Tsirlin, PhD

Oleg Janson, PhD

Joseph Law, PhD

Degrees Defended
Khanduri, Himani. Magnetic Properties of Functional Oxides. PhD, Tallinn University of Technology, 2013

Selected Publications

1. Mazurenko, V. V.; Valentyuk, M. V.; **Stern, R.**; **Tsirlin, A. A**. (2014). Nonfrustrated Interlayer Order and its Relevance to the Bose-Einstein Condensation of Magnons in $BaCuSi_2O_6$. Physical Review Letters, 112, 107202
2. Potocnik, Anton; Ganin, Alexey Y.; Takabayashi, Yasuhiro.; McDonald, Martin T.; **Heinmaa, Ivo**; Jeglic, Peter; **Stern, Raivo**; Rosseinsky, Matthew J.; Prassides, Kosmas; Arcon, Denis. (2014). Jahn-Teller orbital glass state in the expanded fcc Cs_3C_{60} fulleride. Chemical Science, 5(8), 3008 – 3017
3. Kukli, Kaupo; Kemell, Marianna; **Dimri Chandra, Mukesh**; Puukilainen, Esa; Tamm, Aile; **Stern, Raivo**; Ritala, Mikko; Leskelä, Markku (2014). Holmium titanium oxide thin films grown by atomic layer deposition. Thin Solid Films, 565, 261 – 266
4. **Khanduri, Himani; Dimri, Mukesh Chandra**; Vasala, Sami; Leinberg, Silver; Lõhmus, Rünno; Ashworth, TV; Mere, Arvo; Krustok, Jüri; Karppinen, Maarit; **Stern, Raivo** (2013). Magnetic and structural studies of LaMnO3 thin films prepared by atomic layer deposition. Journal of Physics D: Applied Physics, 46 (17), 175003
5. Krämer, Steffen; Laflorencie, Nicolas; **Stern, Raivo**; Horvatić, Mladen; Berthier, Claude; Nakamura, H.; Kimura, Tsuyoshi; Mila, Frederic (2013). Spatially resolved magnetization in the Bose-Einstein condensed state of $BaCuSi_2O_6$: Evidence for imperfect frustration. Physical Review B, 87 (18), 180405(R)
6. **Khanduri, H.;Chandra Dimri, M.; Kooskora, H.; Heinmaa, I.**; Viola, G.; Ning, H.; Reece, M. J.; Krustok, J.; **Stern, R.** (2012). Structural, dielectric, magnetic, and nuclear magnetic resonance studies of multiferroic Y-type hexaferrites. Journal of Applied Physics, 112, 073903
7. **Dimri, Mukesh Chandra; Khanduri, Himani; Kooskora, Helgi**; Kodu, Margus; Jaaniso, Raivo; **Heinmaa, Ivo**; Mere, Arvo; Krustok, Juri; **Stern, Raivo** (2012). Room-temperature ferromagnetism in Ca

and Mg stabilized cubic zirconia bulk samples and thin films prepared by pulsed laser deposition. Journal of Physics D: Applied Physics, 45, 475003 – 475009
8. Sheptyakov, D.V.; Pomjakushin, V.Yu.; **Stern, R.; Heinmaa, I**.; Nakamura, H.; Kimura, T. (2012). Two types of adjacent dimer layers in the low-temperature phase of $BaCuSi_2O_6$. Physical Review B, 86 (1), 014433
9. **Dimri, M. Chandra; Khanduri, H.; Kooskora, H.; Heinmaa, I; Joon, E.; Stern, R**. (2011). Magnetic properties and 57Fe NMR studies of U-type hexaferrites. Journal of Magnetism and Magnetic Materials, 323, 2210 – 2213
10. **Janson, O**., Chen, S., **Tsirlin, A. A**., Hoffmann, S., Sichelschmidt, J., Huang, Q., Zhang, Z.-J., Tang, M.-B.; Zhao, J.-T., Kniep, R., Rosner, H. Structure and magnetism of $Cr_2[BP_3O_{12}]$: Towards, he quantum-classical crossover in a spin-3/2 alternating chain. Physical Review B, 87, 064417 (2013)
11. **Tsirlin, A. A**., **Janson, O**., Lebernegg, S., Rosner, H. Square-lattice magnetism of diaboleite $Pb_2Cu(OH)_4Cl_2$. Physical Review B, 87, 064404 (2013)

SAB recommendations on New Spin Materials
This group is truly world-leading in the application of these methods, and expansion of the THz work to milliKelvin temperatures and 12T fields will continue this. The committee was shown strong work on multiferroic materials, hidden order in a heavy fermion compound, and endohedral small molecule fullerenes. The group has many international collaborations, beyond those necessary to acquire samples. It links well to solid-state NMR techniques at the Institute. Future work on 2-photon spectroscopy (Rebane) and in particular interactions with incoming young scientists Hüvonen and Tsirlin in the area of quantum magnetism will further enhance the intellectual strength of this area, and provide links to theory, and to neutron scattering.

The SAB also noted that the strong fundamental condensed matter program could be complemented by an applied materials effort that connected to applications and the emerging industry of "materials for energy applications" - such an effort could interact well with University programs in materials and chemical engineering.

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

The sub-programme "NMR investigations of the local structure and dynamics in solids and solutions" is currently funded from IUT23-07. However, PRF applications for biochemical applications (PUT41, Jarvet 2013) and theoretical quantum chemical approach (PUT482, Trummal 2014) have been rejected.

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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 programme. Structural analyses and control of the 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.

Yet another focus of the solid state NMR is structure determination of solid organic compounds at natural abundance of ^{13}C by using 2D NMR correlation spectroscopy using the cryoMAS probe with high sensitivity and quantum chemical calculations.

Researchers

Ivo Heinmaa, PhD

Jüri Jarvet, PhD

Enno Joon, PhD

Jaan Past, PhD

Tõnis Pehk, PhD

Indrek Reile, PhD

Priit Sarv, PhD

Raivo Stern, PhD

Juhan Subbi, PhD

Risto Tanner, PhD

Aleksander Trummal, PhD

Rando Tuvikene, PhD

PhD Students

Radu Prekup (TUT)

Degrees Defended

Kalda, Alan. NMR Study of the Local Structure of Quantum Magnets $CdCu_2B_2O_6$ and $Na_3Cu_2SbO_6$. MSc, Tallinn University of Technology, 2013

Veske, Mihkel. NMR Studies of the Magnetic Structure of the Spin-Peierls compound $TiPO_4$. MSc, Tartu University, 2013

Prekup, Radu. Carbon through-bond connectivity of natural solid organic materials using NMR spectroscopy. MSc, Tallinn University of Technology, 2012

Selected Publications

1. Tarkanovskaja, Marta; Välbe, Raul; Põhako-Esko, Kaija; Mäeorg, Uno; Reedo, Valter; Hoop, Andres; Saal, Kristjan; Krumme, Andres; Kink, Ilmar; **Heinmaa, Ivo**; Lõhmus, Ants (2014). Novel homogeneous gel fibers and capillaries from blend of titanium tetrabutoxide and siloxane functionalized ionic liquid. Ceramics International, 40(6), 7729 - 7735
2. Salvatore Mamone, Maria Concistre, **Ivo Heinmaa**, Marina Carravetta, Ilya Kuprov, Gary Wall, Mark Denning, Xuegong Lei, Judy Y.-C. Chen, Yongjun Li, Yasujiro Murata, Nicholas J. Turro, and Malcolm H. Levitt. Nuclear Magnetic Resonance of Hydrogen Molecules Trapped inside C_{70} Fullerene Cages. ChemPhysChem (2013), 14, 3121 – 3130
3. Parve, O.; Reile, I.; Parve, J.; Kasvandik, S.; Kudrjashova, M.; Tamp, S.; Metsala, A.; Villo, L.; **Pehk, T.; Jarvet, J**.; Vares, L. (2013). An NMR and MD Modeling Insight into Nucleation of 1,2-Alkanediols; Selective Crystallization of Lipase-Catalytically Resolved Enantiomers from the Reaction Mixtures. Journal of Organic Chemistry, 78(24), 12795-12801
4. Robert, Tsanev; Kalju, Vanatalu; **Jüri, Jarvet; Risto, Tanner**; Kristi, Laur; Piret, Tiigimägi; Birthe B. Kragelund; Torben Østerlund; Priit, Kogerman. (2013). The Transcriptional Repressor Domain of Gli3 Is Intrinsically Disordered. PlosOne, 8(10), e76972
5. Beckett, P.; Denning, M.S.; **Heinmaa, I.; Dimri, M.C.**; Young, E.A.; **Stern, R.**; Carravetta, M. (2012). High resolution ^{11}B NMR of magnesium diboride using cryogenic magic angle spinning. The Journal of Chemical Physics, 137(11), 114201
6. Anna Mihhalevski, **Ivo Heinmaa**, Rainer Traksmaa, **Tõnis Pehk**, Arvo Mere, Toomas Paalme, Structural Changes of Starch during Baking and Staling of Rye Bread. J. Agric. Food Chem., 60, 8492−8500 (2012)
7. J. M. Law, C. Hoch,1 R. Glaum, **I. Heinmaa, R. Stern**, J. Kang, C. Lee, M.-H. Whangbo, and R. K. Kremer. Spin-Peierls transition in the S = 1/2 compound $TiPO_4$ featuring large intrachain coupling. Physical Review B 83, 180414(R) (2011)

8. L. J. M. Davis, **I. Heinmaa**, B. L. Ellis, L. F. Nazar, G. R. Goward. Influence of particle size on solid solution formation and phase interfaces in Li0.5FePO4 revealed by P-31 and Li-7 solid state NMR spectroscopy. Physical Chemistry Chemical Physics, 13, 5171-5177 (2011)

SAB recommendations
The quality of the NMR research program is very good. The international visibility could become even larger by focusing on a few themes of high interest, for instance, magnetic materials and solid oxide fuel cells, where the unique MAS probes can be exploited. The development of novel hyperpolarisation or dynamic nuclear polarisation techniques is encouraged. The SAB recommends strong support to the continued development of the MAS probes in the framework of the Estonian Magnet Laboratory planned in NICPB, and encourages the materials physics programmes that use the unique equipment, knowhow and infrastructure available in NICPB. Protection of the IP rights by patenting is also encouraged.

The SAB also noted that the established and internationally prominent programmes in advanced NMR techniques provide a possible entry for an Estonian Magnet Lab to be one of the five pillars of the European Magnet Lab - this could bring sophisticated users from across the EU and beyond; applied materials and NMR - both probe- and magnet-development - produce natural synergies.

2.3 Energy materials

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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 and thermogravimetric measurements of those compounds. Solid state NMR studies at extremely low (10K) and high (1200K) temperatures allow to investigate charge localization in high temperature superconductors, local structure and vacancy dynamics in fuel cell components. We are also active in the development of commercially usable SOFC elements with our commercial partner Elcogen Ltd.

Researchers

Juhan Subbi, PhD

Ivo Heinmaa, PhD

Enno Joon, PhD

Jüri Pahapill, MSc

PhD Students

Reio Põder (TUT)

Selected Publications

1. **Põder, Reio; Subbi, Juhan; Kooskora, Helgi; Heinmaa, Ivo** (2014). Vacancy association energy in scandium doped ceria: ^{45}Sc MAS NMR and 2D exchange spectroscopy study. Solid State Ionics, 267, 49 – 53
2. **Subbi, Juhan; Heinmaa, Ivo; Põder, Reio; Kooskora, Helgi** (2013). Solid state NMR spin-lattice relaxation investigation of oxygen dynamics in scandium doped ceria from 60 to 1073 K. Solid State Ionics, 239, 15 – 20
3. **Subbi, Juhan; Heinmaa, Ivo; Põder, Reio; Kooskora, Helgi** (2012). Solid state NMR investigation of oxygen dynamics in scandium doped ceria in 50 K to 1073 K temperature range. Solid State Ionics, 225, 488 – 492
4. **Joon, E** (2012). In-gap states in high T_c superconductors. Physica C-Superconductivity and its Applications. Volume: 479 Pages: 123-125

5. **Dimri, Mukesh Chandra; Khanduri, Himani; Kooskora, Helgi; Subbi, Juhan; Heinmaa, Ivo**; Mere, Arvo; Krustok, J; **Stern, Raivo** (2012). Ferromagnetism in rare earth doped cerium oxide bulk samples. Physica Status Solidi A - Applications and Materials Science, 353 – 358
6. **Dimri, Mukesh Chandra; Kooskora, Helgi; Pahapill, Jüri; Joon, Enno; Heinmaa, Ivo; Subbi, Juhan; Stern, Raivo** (2011). Search for ferromagnetism in manganese-stabilized zirconia. Physica Status Solidi A - Applications and Materials Science, 208(1), 172 - 179

SAB recommendations
The SAB recommends to support strongly the SOFC development, and to encourage the close collaboration with the NMR group. It is also recommended to refine the policy of NICPB in the protection of Intellectual Property rights by encouraging patenting, either alone or together with the firm.

SRP3. Macromolecular interactions

3.1 Molecular System Bioenergetics

The sub-programme "Mechanisms of regulation of integrated energy metabolism in tumour and muscle cells" is currently funded from IUT23-01 (T. Käämbre)

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Recently developed approach, Molecular System Bioenergetics SMSB), being an important part of Systems Biology, is aimed to study intracellular structural interactions in the regulation of energy metabolism in healthy cells as well as in pathology. System Biology paradigm aims to quantitatively describe complicated biological systems at different levels and to study properties arising through interactions between subsystems, absent in macromolecules in isolation.

The programme gives us theoretical background to understand the bioenergetics of healthy muscle cells. It will also shed light to the causes of changes taking place in it in cases of cellular pathologies like ischemia, heart failure, myocardial infarction, neurodegenerative diseases, to bioenergetic mechanisms of cancer, and to the mechanisms of reperfusion injury.

As previous research in our laboratory on cardiac muscle cell bioenergetics has shown, the effective functioning of cardiomyocyte requires the kinetic co-functioning of the system comprising of respiratory chain, ATP sythasome in the mitochondrial inner membrane (including ATP synthase, adenosine-nucleotide translocase and phosphate transporters), mitochondrial creatine kinase, porine channel in the mitochondrial outer membrane (through which the metabolites are exchanged to cytosol) and protein factors modulating the channel, one of which is assumed to be tubulin heterodimer.

Alterations of intracellular structural interactions and formation of mature energy metabolism during postnatal development is an ideal model to identify the structure of the highly organised intracellular system, where the bioenergetic regulation of cell varies according to the development of functional interaction between complexes involved in the ATP production and energy transfer. One the other hand, changes in cell bioenergetics are one of the first signs of cell pathology, therefore the studies of the bioenergetics of the malignant cells are of great importance.

The aim of current research is to define the mechanisms that cause critical shifts in the regulation of energy metabolism and the alterations in the cytoskeleton structure in tumour cells in comparison with normal cells. There is evidence indicating the existence of mitochondrial respiratory supercomplexes in certain type of cancer tissue that may represent a way by which cancer cells avoid apoptosis. The exact nature of the phenomena needs future study.

The methodology of MSB and its research methods, such as metabolic control analysis, proteomics and metabolomics techniques, will be used to identify and quantify the cellular regulation and to map tumour-specific bioenergetic profiles. The crucial benefit in this case and the great significance for further diagnostic purposes lies in the use of *in vivo* studies in cooperation with The North Estonia Medical Centre. The project is a continuation of our prior fundamental studies within the framework of MSB (SF0180114Bs08) directed on the clarification of the regulation of bioenergetic processes in muscle and cancer cells *in situ*.

Researchers

Tuuli Käämbre, PhD

Valdur Saks, DSc

Kersti Tepp, PhD

Vladimir Tšekulajev, PhD

Tiia Anman (Left NICPB on August 20, 2013)

Igor Ševtšuk, PhD

Natalja Timohhina, PhD

Minna Varikmaa, PhD (left on March 27, 2014)

PhD Students

Andrus Kaldma, Andre Koit, Kati Mädo, and Ljudmila Õunpuu (TUT).

Manana Kandashvili (TU)

Degrees Defended

Klepinin, Aleksandr. Comparative analysis of mitochondrial metabolism in differentiated and undifferentiated neuroblastoma cells. MSc, Tallinn University of Technology, 2014

Varikmaa, Minna Structural and functional studies of mitochondrial respiration regulation in muscle cells. PhD, Tallinn University of Technology, 2013

Timohhina, Natalja. Molecular System Bioenergetics of the Heart Cells: Mitochondrial Interactsome. PhD, Tallinn University, 2011

Tepp, Kersti. Molecular System Bioenergetics of Cardiac Cells: Quantitative Analysis of Structure-Function Relationship. PhD, Tallinn University of Technology, 2011

Simm, Aia. Comparative bioenergetics of nerve cells. MSc, Tallinn University, 2011

Selected Publications

1. **Klepinin, Aleksandr; Chekulayev, Vladimir; Timohhina, Natalja; Shevchuk, Igor; Tepp, Kersti; Kaldma, Andrus; Koit, Andre; Saks, Valdur; Kaambre, Tuuli** (2014). Comparative analysis of some aspects of mitochondrial metabolism in differentiated and undifferentiated neuroblastoma cells. Journal of Bioenergetics and Biomembranes, 46(1), 17 - 31.
2. **Varikmaa, M.**; Bagur, R.; **Kaambre, T.**; Grichine, A.; **Timohhina, N.; Tepp, K.; Shevchuk, I.; Chekulayev, V.**; Metsis, M.; Boucher, F.; **Saks, V.**; Kuznetsov, A. V.; Guzun, R. (2014). Role of mitochondria-cytoskeleton interactions in respiration regulation and mitochondrial organization in striated muscles. Biochimica et Biophysica Acta-Bioenergetics, 1837(2), 232 - 245.
3. **Varikmaa M**, Guzun R, Grichine A, Gonzalez-Granillo M, Usson Y, Boucher F, **Kaambre T, Saks V**. (2013) Matters of the heart in bioenergetics: mitochondrial fusion into continuous reticulum is not needed for maximal respiratory activity. Journal of Bioenergetics and Biomembranes, 45 (4), 319-331
4. **Kaambre, T., V. Chekulayev, I. Shevchuk, K. Tepp, N. Timohhina, M. Varikmaa, R. Bagur, A. Klepinin, T. Anmann, A. Koit, A. Kaldma, R. Guzun, V. Valvere and V. Saks (2013).** Metabolic control analysis of respiration in human cancer tissue. Frontiers in Physiology, 4: 151
5. **Kaambre, T., Chekulayev, V., Shevchuk, I., Karu-Varikmaa, M., Timohhina, N.; Tepp, K.**, Bogovskaja, J.; Kütner, R., Valvere, V., **Saks, V**. (2012) Metabolic control analysis of cellular respiration *in situ* in intraoperational samples of human breast cancer. J Bioenerg. and Biomembr, 44 (5), 539–558
6. Gonzalez-Granillo, M., A. Grichine, R. Guzun, Y. Usson, K**. Tepp, V. Chekulayev, I. Shevchuk, M. Karu-Varikmaa,** A. V. Kuznetsov, M. Grimm, **V. Saks and T. Kaambre** (2012) Studies of the role of tubulin beta II isotype in regulation of mitochondrial respiration in intracellular energetic units in cardiac cells. J Mol Cell Cardiol, 52(2): 437-447

7. **Saks, V**., Kuznetsov, A.V., Gonzalez-Granillo, M., **Tepp, K., Timohhina, N., Varikmaa-Karu, M., Käämbre, T**., Dos Santos, P., Guzun, R. (2012) Intracellular Energetic Units regulate metabolism in the cardiac cells. J Mol Cell Cardiol, 52 (2): 419-436
8. Kuznetsov, A. V., R. Guzun, F. Boucher, R. Bagur, **T. Kaambre and V. Saks** (2012) Mysterious Ca(2+)-independent muscular contraction: deja vu. Biochem J, 445(3): 333-336
9. Aliev, M., R. Guzun, **M. Karu-Varikmaa, T. Kaambre**, T. Wallimann and **V. Saks** (2011). Molecular system bioenergics of the heart: experimental studies of metabolic compartmentation and energy fluxes versus computer modeling. Int J Mol Sci, 12(12): 9296-9331.
10. **Tepp K., Shevchuk I., Chekulayev V., Timohhina N**., Kuznetsov A.V., Guzun R., **Saks V., Kaambre T.** (2011) High efficiency of energy flux controls within mitochondrial interactosome in cardiac intracellular energetic units. Biochim Biophys Acta, 1807 (12), 1549-61
11. Guzun, R., **N. Timohhina, K. Tepp**, M. Gonzalez-Granillo, **I. Shevchuk, V. Chekulayev**, A. V. Kuznetsov, **T. Kaambre and V. A. Saks** (2011) Systems bioenergetics of creatine kinase networks: physiological roles of creatine and phosphocreatine in regulation of cardiac cell function. Amino Acids, 40(5): 1333-1348
12. Guzun, R., **M. Karu-Varikmaa**, M. Gonzalez-Granillo, A. V. Kuznetsov, L. Michel, C. Cottet-Rousselle, **M. Saaremae, T. Kaambre**, M. Metsis, M. Grimm, C. Auffray and **V. Saks** (2011) Mitochondria-cytoskeleton interaction: distribution of beta-tubulins in cardiomyocytes and HL-1 cells. Biochim Biophys Acta, 1807(4): 458-469

SAB recommendations
Research in the Saks group continues at the international forefront of studies of catabolic control, even though some of the current proposals still seem hypothetical and will require adequate controls before acceptance. Phosphorous NMR studies of the creatine phosphate system on the *in vivo* level in collaboration with the Institute's NMR lab are recommended as a future development, and the SAB recommends continuing support for this group.

3.2 Interactions of Biomolecules

The sub-programme "**Snake venom components affecting haemostasis and cancero-genesis**" did not get funding under application IUT23-02 (PI Jüri Siigur) nor did a new application, "**Interaction mechanism of bioactive compounds with various cell types**", admitted in 2014 (PI Anu Aaspõllu) nor a PRF application.

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Cellular processes and their regulation are based on recognition, binding and co-operation of bioactive molecules, and are determined by fundamental interactions in a very special cellular medium that is highly crowded with biomolecules. These basic interactions tend to yield non-traditional and unexpected manifestations.

The aim of the programme is to understand the interactions and to give their predictable description combining experimental studies with corresponding theoretical modelling of processes based on structural data.

Basic principles of molecular recognition and complex formation are studied in systems: protein-protein, protein-DNA, protein-cell membrane, protein-bioactive peptide, and protein low molecular ligands.

Our focus in these studies is finding and isolating new catalytic, gene regulating, diagnostic and pharmacological active substances from different natural sources and the overall biochemical characterization of these substances.

The results of the studies have fundamental character as they clarify the mechanism of molecular recognition between proteins and other signalling molecules in normal and pathological processes. The practical importance of the investigations is based on the potential role of the new unique proteins in understanding and resolving of contemporary health problems such as cancer, neurodegenerative, heart and blood diseases. The knowledge of the structure - function relationships of biomolecules is necessary in medicine and in pharmacology for designing new drugs and diagnostics and these data are helpful for synthesis of new bioactive substances.

Integrated approaches of modern genomics, transcriptomics and proteomics in conjunction with classical cell culture techniques open new frontiers for studies of bioactive compounds. Snake venoms are rich sources of diverse bioactive components, which can target various tissues and cell types and have therefore tremendous potential for treating wide variety of human diseases. The main goal of the project is to obtain new scientific knowledge for better understanding of mechanisms of interaction of venomous components, especially present in minor quantities, with various cell types. Specific targets are different biological processes such as haemostasis, cancerogenesis and angiogenesis. For this reason components from *V. lebetina*, *V. berus* and *N. oxiana* will be used. The outcome of the project is the better understanding of essential processes in cell biology related to human health and the evaluation of the role of specific components as potential drug candidates.

Researchers

Anu Aaspõllu, PhD

Ene Siigur, PhD

Katrin Trummal, PhD

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Mari Samel, PhD

Jüri Siigur, PhD

Heiki Vija, MSc

Degrees Defended

Vassiljeva, Olga. Structure and function of hyaluronidase from *Vipera lebetina* venom. MSc, Tallinn University of Technology, 2013

Selected Publications

1. **Trummal, K., Aaspõllu, A, Tõnismägi, K., Samel, M., Subbi, J., Siigur, J., Siigur, E.** (2014). Phosphodiesterase from *Vipera lebetina* venom - Structure and characterization. Biochimie, 106, 48 - 55.
2. **Samel, Mari; Vija, Heiki; Kurvet, Imbi; Künnis-Beres, Kai; Trummal, Katrin; Subbi, Juhan; Kahru, Anne; Siigur, Jüri** (2013). Interactions of PLA2-s from *Vipera lebetina*, *Vipera berus berus* and *Naja naja oxiana* Venom with Platelets, Bacterial and Cancer Cells. Toxins, 5, 203 – 223
3. **Siigur, Jüri; Siigur, Ene** (2013). Lebetase. Neil D. Rawlings; Guy S. Salvesen (Eds.). Handbook of Proteolytic Enzymes 3rd Edition (1054 - 1057) Elsevier Sci
4. Siigur, Ene; Trummal, Katrin; Tõnismägi, Külli; Aaspõllu, Anu; Siigur, Jüri. (2012). *Vipera Lebetina* Venom Nucleases and Nucleotidases. Toxicon, 60 (2, Special Issue), 200-200
5. **Samel, Mari; Trummal, Katrin; Siigur, Ene; Siigur, Jüri** (2012). Effect of HUVEC apoptosis inducing proteinase from *Vipera lebetina* venom (VLAIP) on viability of cancer cells and on platelet aggregation. Toxicon, 60, 648 – 655
6. **Siigur, Ene; Tõnismägi, Külli; Trummal, Katrin; Samel, Mari; Vija, Heiki; Aaspõllu, Anu**; Rönnholm, Gunilla; **Subbi, Juhan**; Kalkkinen, Nisse; **Siigur, Jüri**. (2011). A new tyrosine-specific chymotrypsin-like and angiotensin-degrading serine proteinase from *Vipera lebetina* snake venom. Biochimie, 93, 321 - 330

SAB recommendations

The SAB recommends that the group should focus on this (*specific anti-cancer treatment -Ed.*) and other aspects of possible future use of snake venom components in diagnostics and cancer therapy, and considers this group well worthy of continued support.

3.3 Two-photon Absorption (2PA) in Biomolecules

The sub-programme "**Multi-photon functional optical sensing materials**" is currently funded from IUT23-09 (A. Rebane) and FP7 Grant No 264362 TOPBIO

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Two-photon fluorescence microscopy is becoming one of the standard and most informative methods in biological research because it facilitates increased spatial resolution and increased depth of tissue penetration. These useful attributes occur due to special physical properties of two-photon absorption (2PA) phenomena, which include quadratic dependence of the excitation probability on instantaneous photon flux density, and which also allow using near-infrared wavelengths to excite visible fluorescence.

There is however at least one more unique physical property of 2PA that can and should be exploited to obtain important novel information, especially in order to address numerous critical questions regarding structure and function of biopolymers. Namely, because 2PA constitutes a higher-order interaction between light and molecular chromophore, the probability of this process depends not only on transition dipole moments between different molecular energy levels, but also depends on the value of permanent electric dipole moments of the same chromophore, which itself varies as a function of local electric field. Recently it was shown that quantitative measurement of 2PA cross section in biological chromophores such as fluorescent proteins can be used to determine accurate value of the corresponding dipole moment difference parameter, and thus determine the strength and direction of the local electric field acting inside 3-nm diameter barrel protein. This type of novel physical measurement is uniquely valuable because it allows beginning shedding light on the very fundamental, but still largely unknown properties of local electrostatic interactions in- and between biopolymers on nanometre scale.

The first goal is to continue developing physical principles of local electric field sensing by two-photon spectroscopy and microscopy. This is addressed by investigating 2PA properties in broad range of different fluorescent as well as non-fluorescent biomolecular constructs and probes, in order to create and characterisation novel type of molecular multi-photon optical sensors that are specially designed to detect and quantify local electric fields. The second and at this time a more distant goal is to initiate R&D level work on specialised hardware and software that, in combination with the specialised 2PA-optimised molecular probes can be used by other researches' for a broad range of biomolecular investigations.

We will implement new experimental tools that will allow for the first time direct measurement of local electrostatic interactions in- and between molecules on nanometer-scale. Knowledge of how charges move inside molecules along with knowledge of the strength and direction of local electric fields is critical for understanding of key life processes. We take advantage of two-photon absorption (2PA) properties of specially-designed fluorescent chromophores, which consist in quantitative relationship between 2PA cross section and the amount of change of dipole moment that the chromophore undergoes upon optical excitation from ground- to excited electronic state, and where the last quantity serves as direct probe of the local static electric field strength. We will use these unique attributes of 2PA spectroscopy, in combination with NMR spectroscopy, to study light-induced charge-transfer and associated symmetry breaking in specially-designed organic and organo-metallic chromophores.

Researchers

Aleksander Rebane, PhD

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PhD Students

Sophie Maria Teresa Gronlier Marinucci De Reguardati Di Castelfranco, MSc

Selected Publications

1. Goswami, Subhadip; Wicks, Geoffrey; **Rebane, Aleksander**; Schanze, Kirk S. (2014). Photophysics and non-linear absorption of Au(I) and Pt(II) acetylide complexes of a thienyl-carbazole chromophore. Dalton Transactions, 43(47), 17721 - 17728.
2. Wu, Jiahui; Abdelfattah, Ahmed; Miraucourt, Loïs; Kutsarova, Elena; Ruangkittisakul, Araya; Zhou, Hang; Ballanyi, Klaus; Wicks, Geoffrey; Drobizhev, Mikhail; **Rebane, Aleksander**; Ruthazer, Edward; Campbell, Robert (2014). A long Stokes shift red fluorescent Ca2+ indicator protein for two-photon and ratiometric imaging. Nature Communications, 5, 5262
3. Nikolay S Makarov, Mikhail Drobizhev, Geoffrey Wicks, Elena A Makarova, Evgeny A Lukyanets and **Aleksander Rebane**. Alternative selection rules for one- and two-photon transitions in tribenzotetraazachlorin: Quasicentrosymmetrical π-conjugation pathway of formally non-centrosymmetrical molecule. J. Chem. Phys. 138, 214314 (2013)
4. G. G. Dubinina, R. Price, K.A. Abboud, G. Wicks, P. Wnuk, Yu. Stepanenko, M. Drobizhev, **A. Rebane**, K. Schanze. Phenylene vinylene platinum(II) acetylides with prodigious two-photon absorption. J. Am. Chem. Soc. 134(47), pp. 19346-19349 (2012)
5. Starkey, Jean R; Makarov, Nikolay S; Drobizhev, Mikhail; **Rebane, Aleksander**. Highly sensitive detection of cancer cells using femtosecond dual-wavelength near-IR twophoton imaging. Biomedical Optics Express, 3(7), pp. 1534-1547 (2012)
6. **A. Rebane**, M.Drobizhev, N. S. Makarov, E. Beuerman, J. E. Haley, D. M. Krein, A. R. Burke, J. L.Flikkema, Th. M. Cooper. Relation between two-photon absorption and dipolar properties in a series of fluorenyl-basedchromophores with electron donating or electron withdrawing substituents. J. Phys. Chem A 115 (17), pp. 4255–4262 (2011)
7. Drobizhev, M.; Makarov, N.S.; Tillo, S.E.; Hughes, T.E.; **Rebane, A**. Two-photon absorption properties of fluorescent proteins. NATURE Methods, 8 (5), 393 – 361 (2011)

SAB recommendations
This is a new programme and was not presented for evaluation.

SRP4 Environmental Toxicology and Chemistry

SPR4.1 Environmental toxicology

The sub-programme "**Nano(eco)toxicology and beyond (ToxBe)**" is currently funded from IUT23-02 (A. Kahru) and is performed in Laboratory of Environmental Toxicology

In addition, two EC FP7 projects (NANOVALID; Development of reference methods for hazard identification, risk assessment and LCA of engineered nanomaterials, 2011-2014 and MODERN; MODeling the EnviRonmental and human health effects of Nanomaterials, 2013-2015) and one INTEREG IVA project (RIsk Management and remediation of chemical Accidents (RIMA), 2011-2013) remarkably contributed to research done in the Laboratory of Environmental Toxicology.

Principal Investigator: Anne Kahru, PhD, Research Professor, Head of the Laboratory
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e-mail: anne.kahru@kbfi.ee
Web: http://www.kbfi.ee/?id=2

Research of 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 strategic goal of the environmental toxicology program is to elucidate the hazard of (industrial) chemicals that are already in the environment or that 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 tonne per year (estimated number exceeds 100 000) have to be characterised in terms of toxicity. It is a considerable burden for the European chemical industry (including Estonian chemical industry), since the responsibility of assessments lies on the manufacturer.

The latter aspect is especially crucial due to the implementation of REACH - a regulation of the European Union, adopted to improve the protection of human health and the environment from the risks that can be posed by chemicals, while enhancing the competitiveness of the EU chemicals industry. According to REACH by year 2018 all chemical substances produced in excess of 1 tonne per year (more than 200 000 chemical entities altogether) have to be characterised in terms of hazardous properties. REACH regulation also covers synthetic nanoparticles (particles with at least one dimension less than 100 nm). Rapidly developing nanotechnologies offer the mankind countless benefits and synthetic nanoparticles are already produced in large scale. However, the information on their potential harmful effects is just emerging. The research in environmental toxicology in NICPB, especially the studies of environmental hazards of metal oxide nanoparticles initiated in 2004 have been groundbreaking in the world as reflected in the number of citations as well as in the successful participation in the FP6 and FP7 projects of the European Union. It should be noted that the Estonian state science award of 2011 in geo- and biosciences "Ecotoxicology and toxicity mechanisms of synthetic nanoparticles" was bestowed to Anne Kahru.

One direction of the strategic program of environmental toxicology is 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 nanoparticles using fast, high-throughput systems. As a rule, the toxicity of chemicals is related to adverse effects on cell membranes and processes of basal metabolism, which can be predicted reliably using *in vitro* assays (including tests with e.g., bacteria, protozoa and invertebrates). Quantitative Structure-Activity Relationships (QSARs) are widely used for the prediction of chemical toxicity, but only beginning to emerge for nanoparticles as the latter are considerably more difficult to model compared to conventional chemicals.

The research in the Laboratory of Environmental Toxicology (including under the IUT 23-5 project ToxBe) is focused on evaluating the existing and obtaining new scientific knowledge on chemical and nanoparticle (NP) safety. For that, we will first critically analyse the existing literature on environmental hazards of NPs, e.g., identify potential descriptors for QSAR models. Targeted (eco)toxicological testing will be used (i) to fill the data gaps on environmental hazard of NPs and (ii) to generate homogenous training sets for QSARs. Further, the toxicological pathways of hazardous NPs – solubilisation, induction of reactive oxygen species, interference with biomembranes and -molecules will be identified by refining the existing and designing new cost-effective bioassays. To increase the environmental relevance, environmentally more relevant species, test conditions and simplified laboratory food chains will be used.

Researchers

Anne Kahru, PhD

Irina Blinova, PhD

Margit Heinlaan, PhD

Kaja Kasemets, PhD

Monika Mortimer, PhD

Villem Aruoja, PhD

Olesja Bondarenko, PhD

Angela Ivask, PhD

Kai Künnis-Beres, PhD

Mariliis Sihtmäe, PhD

PhD Students

Katre Juganson, Liina Kanarbik, Aleksandr Käkinen and Sandra Suppi (TUT)

Degrees Defended

Käkinen, Aleksandr. The role of physico-chemical properties and test environment on biological effects of copper and silver nanoparticles. PhD, Tallinn University of Technology, 2014
Bondarenko, Olesja. Development of bacterial biosensors and human stem cell-based *in vitro* assays for the toxicological profiling of synthetic nanoparticles. PhD, Tallinn University of Technology, 2012
Aruoja, Villem. Algae *Pseudokircheriella subcapitata* in environmental hazard evaluation of chemicals and synthetic nanoparticles. PhD, Estonian University of Life Sciences, 2011
Sihtmäe, Mariliis. (Eco)toxicological Information on REACH-Relevant Chemicals: Contribution of Alternative Methods to *in vivo* Approaches. PhD, Tallinn University of Technology, 2011
Mortimer, Monika. Evaluation of the Biological Effects of Engineered Nanoparticles on Unicellular Pro- and Eukaryotic Organisms. PhD, Tallinn University of Technology, 2011

Selected Publications

1. **Ivask, A.; Kurvet, I.; Kasemets, K.; Blinova, I.; Aruoja, V.; Suppi, S.; Vija, H.; Käkinen, A.; Titma, T.; Heinlaan, M.**; Visnapuu, M.; Koller, D.; Kisand, V.; **Kahru, A**. (2014). Size-dependent Toxicity of Silver Nanoparticles to Bacteria, Yeast, Algae, Crustaceans and Mammalian Cells in Vitro. PLoS ONE, 9(7), e102108
2. **Mortimer, Monika**; Gogos, Alexander; Bartolome, Nora; **Kahru, Anne**; Bucheli, Thomas; Slaveykova, Vera (2014). Potential of Hyperspectral Imaging Microscopy for Semi-quantitative Analysis of Nanoparticle Uptake by Protozoa. Environmental Science & Technology, 48(15), 8760 – 8767
3. **Ivask, Angela; Juganson, Katre; Bondarenko, Olesja; Mortimer, Monika; Aruoja, Villem; Kasemets, Kaja; Blinova, Irina; Heinlaan, Margit**; Slaveykova, Vera; **Kahru, Anne**. (2014). Mechanisms of toxic action of Ag, ZnO and CuO nanoparticles to selected ecotoxicological test organisms and mammalian cells in vitro: a comparative review. Nanotoxicology, 8, 57 – 71
4. **Kahru, Anne; Ivask, Angela** (2013). Mapping the dawn of nanoecotoxicological research. Accounts of Chemical Research, 46(3), 823 – 833
5. **Bondarenko, Olesja; Ivask, Angela; Käkinen, Aleksandr; Kurvet, Imbi; Kahru, Anne** (2013). Particle-cell contact enhances antibacterial activity of silver nanoparticles. PLoS ONE, 8(5), e64060
6. **Bondarenko, O.; Juganson, K.; Ivask, A.; Kasemets, K.; Mortimer, M.; Kahru, A**. (2013). Toxicity of Ag, CuO and ZnO nanoparticles to selected environmentally relevant test organisms and mammalian cells *in vitro*: a critical review. Archives of Toxicology, 84, 1181 – 1200
7. **Kasemets, K., Suppi, S., Künnis-Beres, K., Kahru, A**. (2013). Toxicity of CuO nanoparticles to yeast *Saccharomyces cerevisiae* BY4741 wild-type and its nine isogenic single-gene deletion mutants. Chemical Research in Toxicology, 26(3), 356 – 367
8. **Blinova, Irina**; Niskanen, Jukka; Kajankari, Paula; **Kanarbik, Liina; Käkinen, Aleksandr**; Tenhu, Heikki; Penttinen, Olli-Pekka; **Kahru, Anne** (2013). Toxicity of two types of silver nanoparticles to aquatic crustaceans *Daphnia magna* and *Thamnocephalus platyurus.* Environmental Science and Pollution Research, 20(5), 3456 - 3463
9. **Käkinen A.**, Ding F., Chen P., **Mortimer M., Kahru A**. and Ke PC. (2013). Interaction of firefly luciferase and silver nanoparticles and its impact on enzyme activity. Nanotechnology, 24(345101), 1 – 9
10. **Blinova, I; Bityukova, L; Kasemets, K; Ivask, A; Käkinen, A; Kurvet, I; Bondarenko, O; Kanarbik, L; Sihtmäe, M; Aruoja, V**; Schvede, H; **Kahru, A**. (2012). Environmental hazard of oil shale combustion fly ash. Journal of Hazardous Materials, 229,230, 192 – 200
11. **Bondarenko, O., Ivask, A., Käkinen, A., Kahru, A**. (2012). Sub-toxic effects of CuO nanoparticles on bacteria: Kinetics, role of Cu ions and possible mechanisms of action. Environmental Pollution, 169, 81 – 89
12. **Heinlaan, Margit; Kahru, Anne; Kasemets, Kaja**; Arbeille, Birgitte; Prensier, Gérard; **Dubourguier, Henri-Charles** (2011). Changes in the *Daphnia magna* midgut upon ingestion of copper oxide nanoparticles: a transmission electron microscopy study. Water Research, 45(1), 179 – 190
13. **Aruoja, Villem; Sihtmäe, Mariliis; Dubourguier, Henri-Charles; Kahru, A**. (2011). Toxicity of 58 substituted anilines and phenols to algae *Pseudokirchneriella subcapitata* and bacteria *Vibrio fischeri*: Comparison with published data and QSARs. Chemosphere, 84, 1310 – 1320

SAB recommendations
The SAB strongly recommends support for the group to continue research on the present lines. After the mechanistic phase of studies, optimisation and validation of the tests are possible for a wider use e.g. in industry. Automation can be applied to these *in vitro* studies, and thus high throughput low-cost tests for industrial use will be possible. The future of this research is promising and should be further developed in NICPB.

SRP4.2 Environmental Chemistry

The research topic "Environmentally friendly utilization strategy of oil shale processing solid wastes" was funded from the NICPB Targeted Funding Scheme SF0690001s09 (2009-2013) and supported by industry-oriented projects.

Principal Investigator: Natalja Irha, PhD
Phone: +372 6398 307
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Web: http://kbfi.ee/?id=62

A treatment strategy for oil shale ash from combustion and retorting facilities of different types of world resources will be disclosed as the final goal of the project. Any method proposed for utilisation of oil shale waste should include also pretreatment of material by the effective way to eliminate hazardous ingredients or decrease their mobility. Synthesis of calcium-alumino-silicate hydrates from oil shale ash is chosen as the most promising treatment method for production of geopolymers, e.g., Al-substituted tobermorites or composites from similar compounds with long silicate chains and bridging sites. Thus, the research target was the preparation of the overall strategy for recycling of different oil shale solid wastes, taking into account the composition and characteristics of initial material and marketing needs and value of product. All the testing and industrial application activities have been performed in close co-operation with the energy sector in Estonia and abroad.

Subsequent work focuses on a microstructure and morphology at nano-level as well as evaluation of possible reaction mechanisms of a material synthesised by geopolymerisation of oil shale ash. The structural content of synthesised amorphous and crystalline material will be investigated by ^{29}Si, ^{27}Al and ^{23}Na MAS-NMR techniques. The NMR spectra allow determining the bonding of silicon, aluminium and sodium in the formed product. For sensible atomistic simulations the elemental ratios in formed nanostructures will also be determined by TEM-EDS. Environmental friendliness of the product will be evaluated by leaching tests.

Unfortunately, further applications for environmental (oil-shale related) chemistry funding PRF21 (2013) and PRF708 (2014) have been rejected.

Researchers

Natalja Irha, PhD

Uuve Kirso, DrSci (passed away Nov, 11, 2012)

Janek Reinik, PhD

Kaja Kasemets, PhD

Margit Lassi, MSc (part time)

PhD Students

Jekaterina Jefimova (UT)

Degrees Defended
Urb, Gary. Assessment of environmental impact of oil shale fly ash from PF and CFB. PhD, Tartu University, 2011
Piirisalu, Eero. Leaching behaviour of oil shale ash based composite materials. MSc, Tartu University, 2013

Selected Publications

1. **Reinik, Janek; Irha**, Natalya; Steinnes, Eiliv; **Piirisalu, Eero; Aruoja, Villem**; Schultz, Eija; Leppänen, Matti. (2015). Characterization of water extracts of oil shale retorting residues from gaseous and solid heat carrier processes. Fuel Processing Technology, 131, 443 - 451.
2. **Jefimova, Jekaterina; Irha, Natalja; Reinik, Janek; Kirso, Uuve**; Steinnes, Eiliv. (2014). Leaching of polycyclic aromatic hydrocarbons from oil shale processing waste deposit: a long-term field study. Science of the Total Environment, 481, 605 - 610.
3. **Reinik, Janek; Irha, Natalja**; Steinnes, Eiliv; Urb, Gary; **Jefimova, Jekaterina; Piirisalu, Eero** (2014). Release of 22 elements from bottom and fly ash samples of oil shale fueled PF and CFB boilers by a two-cycle standard leaching test. Fuel Processing Technology, 124, 147 - 154.
4. **Reinik, Janek; Heinmaa, Ivo**; Ritamäki, Johannes; Boström, Dan; Pongracz, Eva; Huutanen, Mika; Larsson, William; Keiski, Riitta; Kordas, Krisztian; Mikkola, Jyri-Pekka. (2014). Direct CO_2 sequestration onto alkaline modified oil shale fly ash. Oil Shale, 31(1), 79 – 90
5. **Reinik, Janek; Irha, Natalya**; Steinnes, Eiliv; Urb, Gary; **Jefimova, Jekaterina; Piirisalu, Eero**; Loosaar, Jüri (2013). Changes in trace element contents in ashes of oil shale fueled PF and CFB boilers during operation. Fuel Processing Technology, 115, 174-181
6. **Irha, Natalya; Reinik, Janek**; Steinnes, Eiliv; Urb, Gary; **Kirso, Uuve; Jefimova, Jekaterina** (2013). Leachability of trace elements from aged and fresh spent shale deposit - a field study. Oil Shale, 30(3), 456 – 467
7. **Jefimova, Jekaterina; Irha, Natalja**; Mägi, Reelika; **Kirso, Uuve** (2012). Application of Solid-Phase Microextraction Method to Determine Bioavailable Fraction of PAH in Hazardous Waste. Bulletin of Environmental Contamination and Toxicology, 89(4), 888 - 892
8. **Reinik, Janek; Heinmaa, Ivo; Kirso, Uuve**; Kallaste, Toivo; Ritamäki, Johannes; Boström, Dan; Pongracz, Eva; Huutanen, Mika; Larsson, William; Keiski, Riitta; Kordas, Kristian; Mikkola, Jyri-Pekka (2011). Alkaline modified oil shale fly ash: Optimal synthesis conditions and preliminary tests on CO2 adsorption. Journal of Hazardous Materials, 196, 180 - 186

II Development

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.

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 NMR measurements at present stretches from 10 K to 1200 K.

III Core Facilities

3.1 Estonian Magnet Laboratory

Estonian Magnet Laboratory (EML), housed by the Institute, is one of the 20 objects of the Estonian Research Infrastructures Roadmap 2010.

The EML is designated to be a research centre recognised world-wide and a leading magnet laboratory in Northern and Eastern Europe. Nationally it is the core spectrometry laboratory providing tools and means for research in strong magnetic fields.

The core of the EML is the existing know-how and infrastructure of the Institute and it is based on fixed- and sweep-field superconducting magnets for NMR and THz spectroscopy and PPMS.

3.1.1 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, DSci (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 1H/13C/15N PFG probehead
Dual 1H/13C PFG probehead
Solid state triple resonance 1H/13C/15N probehead
QCI CryoProbe
AVANCE II 600MHz (14.1T) instrument capable of performing advanced multidimensional experiments

Features: Triple resonance 1H/13C/15N PFG probehead
Solid state probes 1-6 mm and DOR probehead
AMX 500 (11.7T)

Features: Liquid 1H/13C probehead
AVANCE II 400MHz spectrometer attached to 8.5T or 4.7T WB-magnets
Features: Solid state low and high 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

3.1.2 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 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 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

Dan Hüvonen, PhD

Himani Khanduri, PhD

Mukesh Chandra Dimri, PhD

Taaniel Uleksin, PhD student

3.1.3 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 every-day 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. 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

Andres Reinhold, senior engineer

Tõnu Tolk, senior engineer

Vambola Kivisaar, technician

3.2 Optics

Contact person: Aleksander Rebane, PhD (sassrebane@gmail.com)

The Laboratory has a Mode-locked femtosecond Titanum Sapphire (Ti:S) laser Mira 900 pumped with 10 W frequency-doubled neodymium-doped vanadate (Nd:YVO4) 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

Girsh Blumberg, PhD

Jüri Pahapill, MSc

Sophie de Reguardati, PhD student

3.3 Quantum Chemistry High Performance Computing Facility (QCHPCF)

The facility has been established and is managed and operated by the members of research group, financed by Estonian Ministry of Education and Research (grants SF0690021s09AP, and SF0690021s09) and external sources.

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

The **hardware** for high performance parallel computing includes:

HP 32-core server

Features: Two SL250 Intel E5-2660 SMP nodes
Two NVIDIA Tesla K20X GPU-s
Total number of CUDA cores 5376
Peak theoretical performance 1.3 DP TFLOPS per GPU
DELL 96-core server

Features: Four PowerEdge R905 AMD 8435 SMP nodes
Mellanox Infiband interconnect between SMP nodes
Peak theoretical performance 1.6 TFLOPS
Precision 3500 console workstation
Major quantum chemistry **software** packages:
Accelrys Materials Studio Quantum Collection and Visualizer including:
CASTEP, NMR CASTEP, DMOL3, DFTB+, ONETEP, QMERA, GULP
Gaussian and GaussView
MOPAC
Also available
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
The 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.

3.4 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 been 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 years 2012-2015 and onwards.

Features in 2014
128 servers of Intel E5-2560 with 32 compute cores and 64GB of RAM
40 servers of AMD Opteron 6172 with 24 compute cores and 48GB of RAM
Dedicated and distributed storage amounting to 2 Pentabyte (PB, 10^6 GB) of raw capacity or 1PB of redundant capacity
A full 10GbE interconnect mesh between all servers
OpenNode cloud technology allowing for easy management of compute resources and software versions
SLURM scheduling for both local and Grid based access
Ca 100 kW of cooling capacity

3.5 Scientific Collections

Contact person: Kaja Kasemets, PhD (kaja.kasemets@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 was 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.

3.6 Workshop

Contact persons:

Andres Reinhold, senior engineer (reinhold@kbfi.ee)

Tiit Tuherm, senior engineer (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

CNC Router High-Z S-400, 3 axis, accuracy 0.010 mm

IV Education and Co-operation

NICPB has co-operation agreements with major Estonian universities, the University of Tartu, Tallinn University of Technology, Estonian University of Life Sciences and Tallinn University.

All research groups and Laboratories of the Institute actively collaborate with all the aforementioned Estonian universities either via common curricula and co-supervision of PhD students or as external examiners of thesis works or through common R&D activities, programmes and projects

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

Thesis	Total 2007-2010	2011	2012	2013	2014	Total 2011-2014
MSc	11	2	1	6	2	11
PhD	10	7	1	2	1	11
Total	21	9	2	8	3	22

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, Cambridge 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.

V Evaluations

SAB Evaluation of 2012

The International Science Advisory Board (SAB) met over a period of two days from June 26-27, 2012 in Tallinn to evaluate the scientific programme of the NICPB. The SAB members present were Professors Peter Littlewood (Chairman), Robert Kaptein, Tapio Niinikoski, Mart Saarma, Hanna Tähti and Marten Wikström. The members missing were Prof. Dmitri Basov and Prof. Carlos Ibáñez, both of whom, however, provided written input. Evaluation involved an in depth review of the main research programs, tours of the facilities and laboratories, discussions with younger researchers and potential leaders, and a panel discussion on new initiatives and strategy.

The SAB noted that: "The Institute is sound and well run, with a good relationship between the Staff and the Director. Over the last few years, the NICPB is evolving a strategy and direction that will be beneficial for the Institute and for Estonia as a whole, and despite some structural and financial impediments, is performing well scientifically. There are many high quality science programs, of international calibre, across the disciplines but including high energy physics, quantum condensed matter physics, NMR spectroscopies, toxicology, and bioenergetics. These programs increasingly make interdisciplinary links within the Institute, and some also support substantial national and international collaborations. The committee believes that there are considerable opportunities to increase the role and impact of the Institute as a major national laboratory of Estonia, as long as major strategic decisions are swiftly taken and executed."

The SAB focused not only on scientific programmes but took a critical look at the financial issues, stating that: "The Institute has considerable autonomy, but in the current form operates as an entirely soft-money organisation dependent on short-term funding via external grant income, which is not a tenable situation for a national laboratory that aspires to intellectual leadership as well as supporting permanent facilities for the benefit of the nation. There needs to be developed a different financial model that allows for seed funding of new activities, long-term support of excellence, and support of large-scale facilities for the university and commercial sector."

The assessments of individual research programmes are given above after each programme synopsis.

VI 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 and the Statute of the NICPB.

According to the Act, the management bodies of NICPB are the Director and the Science Council.

Science Council

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

The Science Council 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 and research staff. The Council is headed by a Chairperson.

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

The Science Council on December 31, 2014

Member	Affiliation
Professor Margus Lopp, Chairman of the Board	Member of the Estonian Academy of Sciences, Tallinn University of Technology
Anne Kahru, PhD, Deputy Chairman	NICPB
Professor Peeter Burk	Dean of the Faculty of Science and Technology, University of Tartu
Ivo Heinmaa, PhD	NICPB
Andi Hektor, PhD	NICPB
Angela Ivask, PhD	NICPB
Mario Kadastik, PhD	NICPB
Kaja Kasemets, PhD	NICPB
Marco Kirm, PhD	Vice-Rector for Research, University of Tartu
Tuuli Käämbre, PhD	NICPB
Urmas Nagel, PhD	NICPB
Tõnis Pehk, DSc	NICPB
Martti Raidal, PhD	NICPB
Toomas Rõõm, PhD	NICPB
Tiit Saluvere, PhD	NICPB, Deputy Director
Jüri Siigur, PhD	NICPB, Scientific Secretary
Raivo Stern, PhD	NICPB, Director
Igor Ševtšuk, PhD	NICPB
Toomas Välimäe, PhD	NICPB, Deputy Director

Directors

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 Science Council for a five year period and he/she reports to the Scientific Board.

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

The **Deputy Director** on Administrative affairs is responsible for the Institute's all ancillary 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, but also for administration and personnel. 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 Science Council 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 Advisory 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 (FIN)
Professor Marten Wikström	Institute of Biotechnology, University of Helsinki (FIN)

Structure

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

The scientific units are **laboratories** of:

Bioenergetics (BE)

Head: Tuuli Käämbre, PhD

tuuli.kaambre@kbfi.ee

Phone +372 6398 381

Bioorganic Chemistry (BOC)

Head: Jüri Siigur, PhD

juri.siigur@kbfi.ee

Phone +372 6398 360

Chemical Physics (CP)

Head: Urmas Nagel, PhD

urmas.nagel@kbfi.ee

Phone +372 6398 327

Environmental Toxicology (ET)

Head: Anne Kahru, PhD

anne.kahru@kbfi.ee

Phone +372 6398 373

High Energy and Computational Physics (HECP)

Head: Professor Martti Raidal, PhD

martti.raidal@kbfi.ee

Phone +372 6454 711

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

VII Facts and Figures

Outline of the financing of science in Estonia

In Estonia R&D activities are funded from the state budget, budgets of local authorities, targeted donations, income earned from the economic activities of R&D institutions, and from other sources. The financing instruments of the Estonian R&D funding system are:

Baseline funding;

Research funding;

Development funding;

Support for centres of excellence;

National research and development programme;

Compensation of costs of maintenance of the infrastructure of a R&D institution.

Baseline financing involves the financing of R&D institutions that have been positively evaluated during last regular evaluation with the aim of realising 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 Ministry of Education and Research (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. In 2014 total 8.4 million euro (M€) € are allocated for baseline financing.

The **research funding** is managed by the Estonian Research Council (ERC, Estonian acronym ETAg), a state foundation which organises and carries out assessment of the applications. Basically there are two kinds of grants:

Institutional research funding (IRF) is support allocated for financing high-level research and development, and related activities (research themes) of an institution involved with the aforementioned activities. The aim is to ensure the consistency of the research and development of an R&D institution, and to upgrade, supplement and maintain the infrastructure necessary for this purpose. The total amount allocated for IRF in 2014 is 19.3 M€, which is supplemented by additional 28% of the lump sum or 5.4 M€ for the compensation of the costs of maintenance of the infrastructure. Total amount of the instrument is thus 24.7 M€.

Personal research funding (PRF) is a contribution to the costs of high-level R&D activities carried out by researchers or small research groups who are employed by a research and development institution. Personal research funding comprises two categories of grants: exploratory research grants and start-up research grants. In 2014 PRF amount to 3.6 M€ (calls of 2012 and 2013).

Additionally, the Estonian Research Council funds post-doctoral fellows in programmes ERMOS (COFUND) and Mobilitas (ESF). The latter is also used to fund top scientists from abroad in order to launch their own research groups in Estonian R&D institutions.

The funds prescribed for **development funding** in the state budget are allocated via the budget of the Ministry of Economic Affairs and Communications to the appropriate foundation established by the state.

Internationally highly regarded research groups that work under common leadership and have clearly defined common goals are financed through the Development of Research **Centres of Excellence** measure.

The measure is aimed at creating the preconditions for strengthening cooperation in the field of research as well as improving the competitiveness of Estonian research in the European research area through supporting local top scientific research. The support sums are allocated from the ERDF.

Estonian Research Infrastructures Roadmap was prepared by the Ministry of Education and Research and Estonian Academy of Sciences and approved by the Government in 2010. Following research development trends in the world and in Estonia, the need for upgrading already existing research infrastructures as well as the initiatives for setting up new research infrastructures were mapped. A roadmap is a long term (10-20 years) planning instrument which will be updated regularly (at an interval of 3 years). The roadmap lists 20 research infrastructures of national importance, either new or in need of upgrading. However, only 9 of the 20 objects have received direct and substantial funding and 4 more indirectly through an internationalisation programme initiated in 2011 by the MER. The latter does not, as a rule, foresee investments into infrastructure.

The implementation of EU Structural Funds for supporting research and development activities is mostly governed by the MER and takes place through the Archimedes Foundation's Implementing Agency of Structural Support. The total cost of measure 4.1 "Internationalisation of Estonian R&D and participation in pan-European networks" will through the period of 2014-2020 be around 225 M€ of which investments into infrastructure including equipment amount to 136 M€.

Funding of NICPB

Table 1 Funding of NICPB 2009 – 2014 (Financial Statements, €)

Source of Finance	2009	2010	2011	2012	2013	2014 *
National budget	1 759 114	1 738 034	1 985 785	1 863 780	1 926 937	2 607 000
External Funding	412 601	728 542	1 278 424	2 005 469	2 001 476	2 214 138
Other Revenue	333 033	824 808	388 774	297 253	333 352	251 673
Grand Total	2 504 748	3 291 384	3 652 983	4 166 502	4 261 765	5 072 811
* - Budget						

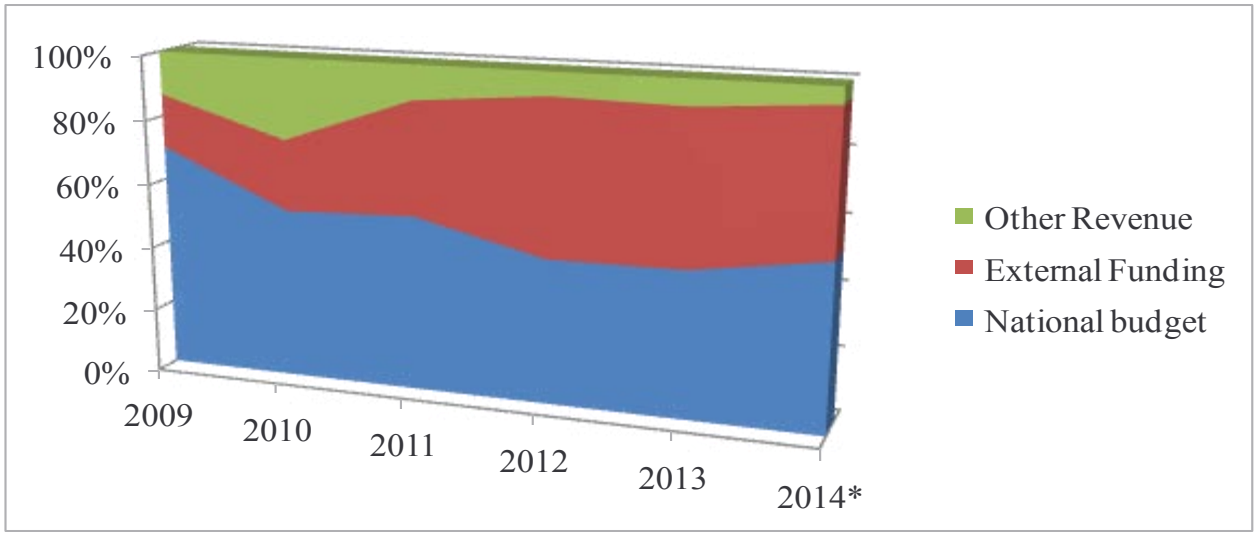


Figure 2. Share of different financing sources (according to financial statements, except 2014)

The table below describes the domestic funding of NICPB by different financial instruments, either directly from the national budget or via different foundations or agencies.

Table 2 Funding of NICPB from national budget (Financial Statements, €)

Financial Instrument	2009	2010	2011	2012	2013	2014*
Baseline financing	189 072	145 642	125 670	150 370	210 930	299 290
IRF (ETAg)	886 638	849 514	841 610	837 530	854 270	1 265 500
PRF (ETAg)	223 295	211 923	203 567	208 199	259 015	269 907
Targeted Financing of Infrastructure	246 969	244 047	243 804	242 914	219 151	353 707
Targeted financing for equipment (VAT)	0	79 636	103 650	32 823	52 431	94 410
Targeted financing for renovation	0	0	76 151	70 846	0	0
Estonian Participation in CERN	129 414	162 187	348 571	313 815	325 301	319 558
Other targeted financing	10 867	11 531	9 208	6 182	5 839	4 628
Non-earmarked financing	72 859	33 554	33 554	1 101	0	0
National Budget Total	1 686 255	1 704 480	1 952 231	1 862 679	1 926 937	2 607 000
* - Budget						

The following figure depicts the share of various domestic financial instruments in the gross domestic funding. The institutional research grants together with personal grants account for nearly 60% of domestic funding. Furthermore, if we discard the Estonian participation in CERN, the share of competition-based research grants exceeds two thirds of domestic funding.

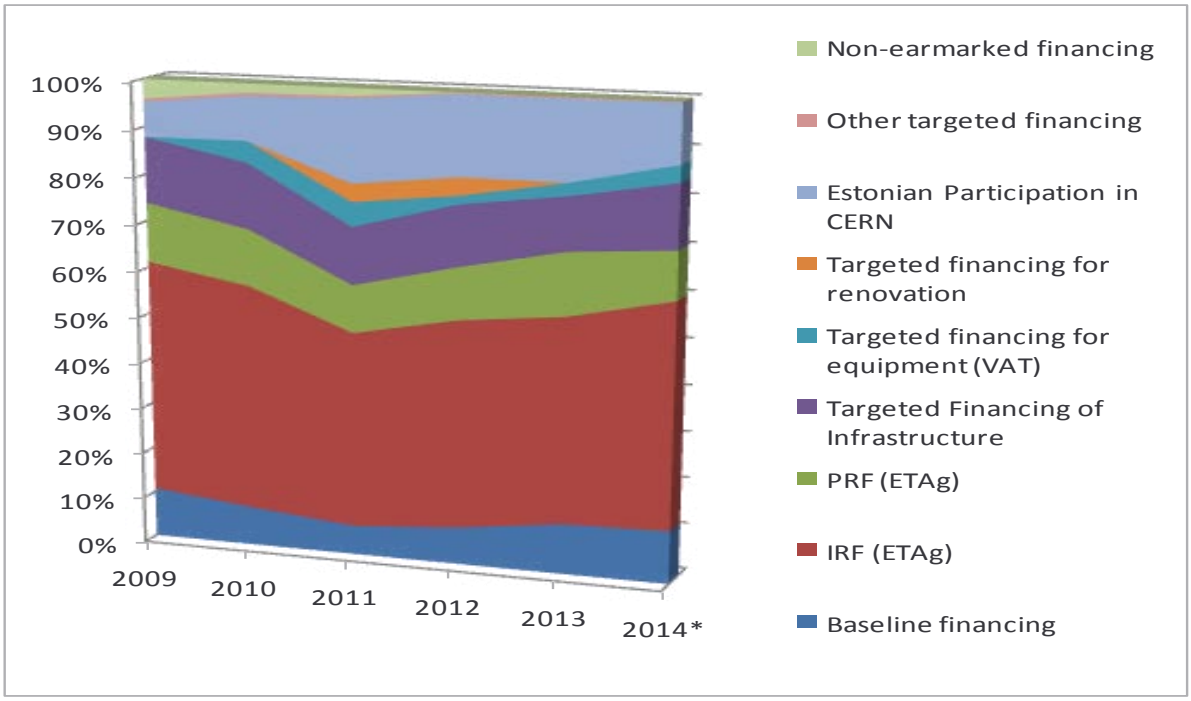


Figure 3. Share of different domestic financing instruments (according to financial statements, except 2014)

Finally, Table 3 below summarises the external project funding, which is based nearly 100% on EU funds with occasional and minute contributions from Swiss and US sources.

Table 3. Funding of NICPB from external sources (Financial Statements, €)

Source of Finance	2009	2010	2011	2012	2013	2014*
Centres of Excellence (ERDF)	0	0	84 663	291 914	419 447	294 717
Enterprise Estonia or Archimedes (Equipm)	0	401 984	628 412	281 260	373 884	447 927
EU Structural Funds (via Archimedes)	62 628	244 065	398 830	1 259 261	1 003 716	1 177 485
EU R&D Grants and Contracts (FP7, etc)	349 973	82 493	166 519	173 034	204 429	294 010
External Funding Total	412 601	728 542	1 278 424	2 005 469	2 001 476	2 214 138
* - Budget						

Personnel

Tables 4 through 6 and Figure 3 illustrate the changes in the total number of employees through the last 4 years. Although the growth has been moderate, the increase in lab technicians clearly indicates that the average age of the employees must have decreased.

Table 4. Personnel of NICPB (total number) by staff categories

Staff Category	2011	2012	2013	2014
Researchers total	64	68	64	69
Lab Technicians, incl students	28	31	38	34
Administration	11	10	9	9
Technical Staff (Ancillary Services)	13	13	13	12
Total	116	122	124	124

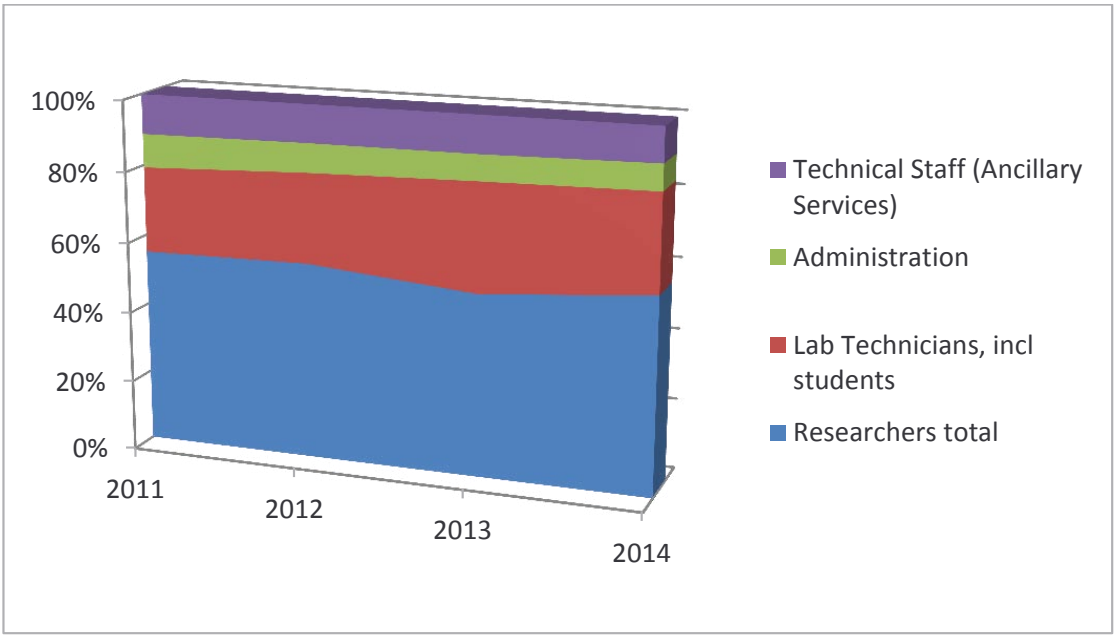


Figure 4. Proportions of staff categories (total number) in 2011 to 2014

Table 5 Personnel of NICPB (Full Time Equivalent) by staff categories

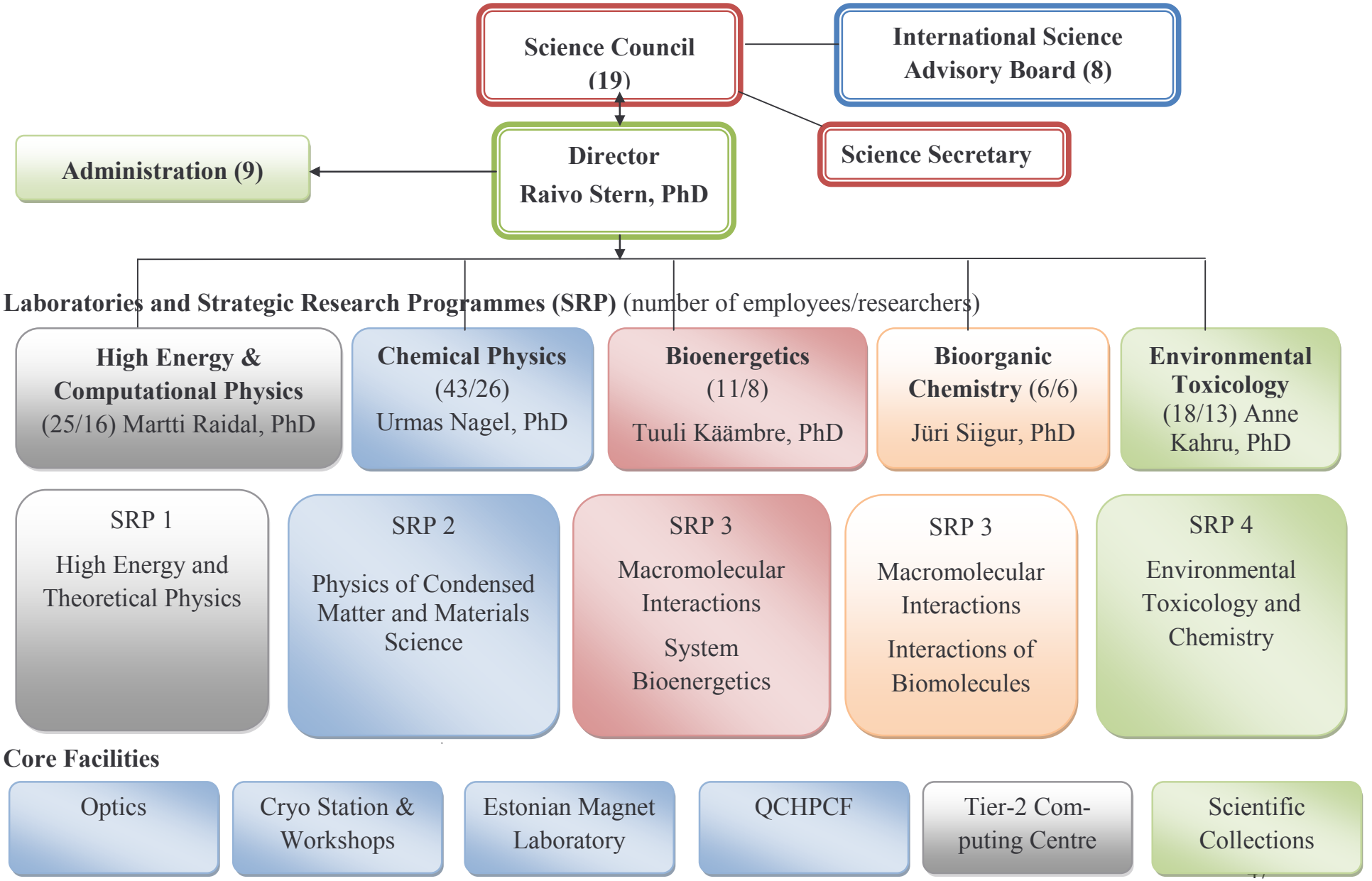
Staff Category	2011	2012	2013	2014
Researchers total	51,8	57,3	55,1	58,4
Lab Technicians, incl students	22,2	23,7	29,1	26,8
Administration	10,3	9,3	9,0	9,0
Technical Staff (Ancillary Services)	10,6	10,6	10,6	9,6
Total	94,8	100,8	103,8	103,7

Table 6. Personnel of NICPB, number of women (F) and average age of (all) employees

	2011			2012			2013			2014		
Category	Total	F	Age	Total	F	Age	Total	F	Age	Total	F	Age
Researchers	64	23	49,8	68	25	47,7	64	23	48,4	69	26	46,6
Technicians	28	13	44,9	31	12	41,8	38	12	38,8	34	8	35,9
Administr	11	6	58,1	10	5	58,9	9	4	58,4	9	4	59,4
Services	13	8	66,1	13	8	67,1	13	8	68,1	12	8	68,8
Total	116	50	51,2	122	50	49,2	124	47	48,2	124	46	46,7

The median age is 45 years.

VIII NICPB Organisation Chart



IX Administration of NICPB