TEHNOMEEDIKUM

TEADUS- JA ARENDUSTEGEVUSE AASTAARUANNE 2013

1. Struktuur

TTÜ Tehnomeedikum, TTU Technomedicum
Direktor Kalju Meigas

- **Biomeditsiinitehnika instituut, Department of Biomedical Engineering, Ivo Fridolin**
  Biomeditsiinitehnika õppetool, Chair of Biomedical Engineering, Kalju Meigas
  Meditsiinifüüsika õppetool, Chair of Medical Physics, Ivo Fridolin
- **Kardioloogiakeskus, Centre of Cardiology**
  Elektrofüsioloogia õppetool, Chair of Electrophysiology
- **Kliinilise meditsiini instituut, Department of Clinical Medicine, Ruth Sepper**
  Kliinilise meditsiini õppetool, Chair of Clinical Medicine, Ruth Sepper
  Tervishoiutehnoloogia õppetool, Chair of Health Care Technology, Peeter Ross
  NMR grupp, NMR group, Ago Samoson

2. Struktuuriüksuse T&A iseloomustus

2.1. Department of Biomedical Engineering

2.1.1. Biofluid optics group, Ivo Fridolin

Teadustöö kirjeldus

On-line monitoring of uremic toxins. Today, there is no method available for on-line monitoring of uremic toxins with different molecular size for the end stage renal disease (ESRD) therapy quality assessment. Firstly in the world, the research of prof. Fridolin proposed a solution for the optical on-line HD monitoring [Fri01, Fri02] by BFOS, enabling determination of Kt/V for urea [Uhl03]. The implementation studies during technology transfer [She08, Fri08, Lum09] led to a successful commercial technology - the first integrated HD dose monitor in the world - Option Adimea, (BBraun Avitum AG) [Cas10]. The sensor is manufactured by an Estonian SME (Ldiamon AS), demonstrating the high potential of the optical signals for monitoring and social impact to Estonian economy.

The biofluid optics research within the project is the first in the world presenting concept of a new multicomponent dialysis monitor utilising optical techniques. The multicomponent monitor incorporates on-line removal estimation of all three uremic toxins' groups (small, middle and protein bound) resulting: (i) Water soluble small molecular weight uremic toxins. Novel algorithms for measuring concentration of water soluble small molecular weight uremic toxins, urea, uric acid and creatinine, in the spent dialysate for estimation of dialysis dose and nutritional status (protein nitrogen appearance and lean body mass) on dialysis patients were developed; (ii) Middle and protein bound uremic toxins. Unique method compared to earlier known state of the art for determining middle and protein bound uremic toxins in the spent dialysate utilizing fluorescence spectroscopy was proposed, which was a base for the Estonian and international PCT patent applications. The promising results have been achievd in developing and implementing novel optical technologies to assess the small [Hol2010c] and protein bound and middle uremic toxins [Hol12, Tom12, Tom13, Jer10, pUhl2010a, pUhl2010b, pUhl11] – CVD risk and malnutrition–inflammation syndrome markers [Hol11, Enb12, Tom12, Hol13, Jia13, pUhl13], among some potential IR markers. A review of the topic

related to dialysis dose monitoring assessing uremic toxins by various optical methods [Uhl12] has been published.
Moreover, it was confirmed at first time that the light emitting diod based miniaturised optical monitor is capable to estimate dialysis dose and nutritional status without blood samples and offers a possibility for simplified mapping of the dialysis.
Analysis of uremic toxins- cardiovascular disease markers. No standard laboratory analyses are available for a number of protein bound and small uremic toxins' measurements in the biological fluids so far. Many of the uremic toxins are candidates being cardiovascular disease markers. For this reason an appropriate high performance liquid chromatography (HPLC) method, capable to measure more uremic toxins compared to existing standard laboratory methods, was developed during the project, making it possible to: (1) show that the molecular mass of the main UV chromophores in the uremic fluids do not exceed 3 kDa; (2) identify and quantify 5 uremic toxins in the serum and in the spent dialysate (uric acid, hypoxanthine, indoxyl sulfate, indole-3-acetic acid, and hippuric acid); (3) determine the optical spectra for 16 chromophores in the uremic fluids; (4) investigate the behaviour of water soluble small molecular weight and protein bound uremic toxins, and UV-absorbance in respect to low and high flux dialyzers during hemodialysis [Aru12].

Cooperation: Laboratory of Chemical Physics, National Institute of Chemical Physics and Biophysics, Tallinn (Estonia), Centre of Nephrology, North-Estonian Medical Centre, Tallinn (Estonia), Linköping University Hospital, Linköping (Sweden).

Tähtsamad teadustulemused:

- A new approach to create prediction models for survival was established for the first time [PatApplication Fri13]. By a combination of levels of concentrations and dialysis efficiency of two waste products, UA and urea, the result showed a more accurate survival prediction of dialysis patients compared to a single variable. This is novel and ground-breaking and opens up the opportunity to add additional data to combine with UA to create prediction models, including identified risk factors, for various health problems.

- A study was undertaken to develop an optical method for the estimation of creatinine (Cr) removal during dialysis using UV-absorbance. A single wavelength (SW) and a multi-wavelength (MW) model were developed using stepwise regression utilizing Cr values from the laboratory as the dependent parameter. The reduction ratio (RR) and total removed Cr (TRCr) were estimated. In summary, creatinine removal during dialysis can be estimated as reduction ratio and total removed creatinine with the UV-absorbance technique [Tom13].

- J. Holmar, defended her PhD-thesis “Optical Method for Uric Acid Removal Assessment during Dialysis” 10th October 2013;

- In clinical practice, many events like patient blood pressure changes, needle displacement and concentrate depletion can trigger dialysis machine alarm, which will stop the treatment and give wrong information during optical dialysis dose monitoring. The competences of BME in biosensorics and RES in digital design and dependability formed the creative and synergetic basis for developing new competitive bioengineering solutions within optical dialysis monitoring. The research results in test and diagnosis

developed by RES allows coping with the complexity of dependency problems in new innovative applications proposed by BME. New methods (AVRG, SMART and SIF) for accurate dialysis dose evaluation and extrapolation by means of Kt/V from online UV-absorbance measurements were proposed [Fri13]. The algorithms have a significantly positive effect on removal the disturbances and data visualization for the doctors showing substantial improvement on both chart readability and measurement precision. The output of the monitor has higher reliability and helps to avoid false prescriptions and high-quality medical care can be offered for the patients. The final aim of the dialysis monitoring technique will be to deliver a platform for technology transfer realised as a practical toolkit for the clinicians helping obtain adequate dialysis targets meeting the individual needs of each patient and leading to "personalized healthcare" within haemodialysis.

- A study assessed removal dynamics of paracetamol (PAR), as an extraordinary chromophore in spent dialysate, upon the optical monitoring of dialysis of end-stage renal disease patients with inflammation complications [Tan13]. Peaks of UA, PAR, PAR-glucuronide, and PAR-sulphate were identified on the basis of specific mass spectra. Removal of PAR was found to be proportional to that of uric acid if intake of the drug by patient occurred half a day before dialysis. But disturbances of the UV-absorbance curves at 280 nm were observed related to rise of UA concentration in spent dialysate when PAR was taken by patients in the course of dialysis. The mechanism of such relation remains unknown. It was concluded that possible benefits and risks of treatment of uremic patients with paracetamol-containing drugs may need to be reassessed.

- A study investigated the possibility to determine the amount of removed Indoxyl Sulphate (IS) during dialysis session [Hol13]. An optical method using fluorescence spectra was used. This study indicates, that it is possible to estimate RR of IS using only fluorescence values of the spent dialysate and achieved parameter can be used for describing the elimination of protein bound uremic toxins during the dialysis procedure.

- A study explored the possibility to determine the amount of total removed Indoxyl Sulphate (TR_IS) during dialysis session, an optical method utilizing absorbance and fluorescence spectral data of the spent dialysate was used. Fluorescence and absorbance spectra of the spent dialysate were measured with spectrofluorophotometer and spectrophotometer. The spectral values were transformed into IS concentration using multiple linear regression model from the total material noted as optical method (Opt). IS concentration was estimated using high-performance liquid chromatography (HPLC) method as a reference. TR_IS values were calculated. Achieved results were compared regarding mean values and SD and collated with the amount of total removed urea value (TR_Urea) for the same dialysis procedures. Mean TR value (mg) for urea was 28 947±9 241; TR for IS was 151.4±87.3 estimated by HPLC and 149.4±84.9 estimated by Opt. The TR_IS values were not significantly different ($p \leq 0.05$). This study indicates, that it is possible to estimate TR_IS using only spectral values of the spent dialysate and the parameter can be used for quantifying the elimination of protein bound uremic toxins during the dialysis procedure.

- Totally 4 patents were published and one patent application was filed:

- Estonian Patent EE05637B1 (granted 15.02.2013). Method and device for monitoring removal of hardly diffusible uremic retention solutes during dialysis by UV-absorbance. Application P201100002 (filed 14.01.2011). Authors: Fredrik Uhlin, Jana Holmar, Ivo Fridolin. Owner: Tallinn University of Technology.

- Estonian Patent EE05622B1 (granted 15.02.2013). Optical method and device for measuring concentrations of substances in biological fluids. Applications PCT/EE2008000026 and EE201000054 (Filed: 4.12.2008). Authors: Ivo Fridolin, Jana Holmar, Kai Lauri, Merike Luman. Owner: Tallinn University of Technology.

- Estonian Patent EE05674B1 (granted 31.05.2013). Optical method and device for measuring quantitatively concentrations of urea, creatinine, and uric acid in biological fluids. Applications (Filed: 27.05.2010). Authors: I. Fridolin, J. Holmar (Jerotskaja), K. Lauri, M. Luman. Owner: Tallinn University of Technology.

- Estonian Patent EE05669B1 (granted 15.08.2013). Optical method and device for determination of middle molecules and protein bound uremic toxins in the biological fluids. Application nr P201000085 (filed 10.12.2010). Authors: Fridolin, I., Uhlin F., Jerotskaja, J., Tanner, R., Arund, J.. Owner: Tallinn University of Technology.

- Patent Appl. Ivo Fridolin, Fredrik Uhlin, Jana Holmar, Merike Luman. „Method for dialysis patients' survival prediction using small uremic markers“. US61/819508. Filed: 03/05/2013. Owner: Tallinn University of Technology..

Viis olulisemat publikatsiooni aruandeaastal:

1. Tomson, R.; Fridolin, I.; Uhlin, F.; Holmar, J.; Lauri, K.; Luman, M. (2013); „Optical Measurement of Creatinine in Spent Dialysate“ Clinical Nephrology 2013; volume 79 (2); pp. 107 - 117.
2. Fridolin, I.; Karai, D. ; Kostin, S. ; Ubar, R. (2013). Accurate Dialysis Dose Evaluation and Extrapolation Algorithms during On-line Optical Dialysis
3. Risto Tanner, Jürgen Arund, Ivo Fridolin, and Merike Luman, “Paracetamol Interference in Uric Acid Levels in Uremic Patients Revealed by Monitoring Spent Dialysate,” ISRN Nephrology, vol. 2013, Article ID 515292, 4 pages, 2013. doi:10.5402/2013/515292
4. Holmar, Jana; Uhlin, Fredrik; Ferenets, Rain; Lauri, Kai; Tanner, Risto; Arund, Jürgen; Luman, Merike; Fridolin, Ivo. (2013). Estimation of Removed Uremic Toxin Indoxyl Sulphate during Hemodialysis by Using Optical Data of the Spent Dialysate. In: Proceedings of 35th Annual International Conference of the IEEE EMBS: 35th Annual International Conference of the IEEE EMBS, Osaka, Japan, 3 - 7 July, 2013. IEEE, 2013, 6707 - 6710.
5. Ivo Fridolin, Fredrik Uhlin, Jana Holmar, Merike Luman. „Method for dialysis patients' survival prediction using small uremic markers“. US61/819508. Filed: 03/05/2013. Owner: Tallinn University of Technology.

Välisakadeemiate või muude oluliste T&A- ga seotud välisorganisatsioonide liikmed.

Jana Holmar - IEEE EMBS(IEEE Engineering in Medicine and Biology Society) liige
Jürgen Arund - IbioMep liige

2.1.2. Brain research group, Hiie Hinrikus

Teadustöö kirjeldus

The research activity is continuously aimed to development of algorithms for detection of characteristic changes in the brain electroencephalographyc (EEG) signal related to the mental disorders and the effect of external physical stressor. For this purpose, the recordings of new EEG signals from medication-free patients were initiated in cooperation with the ITK Centre of Psychiatry and family doctors. The methods of activity were approved by two new permission from Tallinn Medical Ethics Committee.
Two electroencephalogram (EEG) analysis methods, spectral asymmetry index (SASI) and Higuchi's fractal dimension (HFD), were compared for detection of depression. Linear SASI method is based on evaluation of the balance of powers in two EEG frequency bands in one channel selected higher and lower than the alpha band spectrum maximum. Nonlinear HFD method calculates fractal dimension directly in the time domain. The resting EEG signals of 17 depressive patients and 17 control subjects were used as a database for calculations. SASI values were positive for depressive and negative for control group in frontal, temporal, parietal and occipital channels ($p<0.05$). SASI indicated 88% as depressive from depressive group subjects and 82% as non-depressive from control group subjects. The calculated HFD values averaged over a group detected a small (3%) but statistically significant increase for depressive compared to control group in temporal, parietal and occipital channels ($p<0.05$). HFD indicated 94% as depressive from depressive group subjects and 76% as non-depressive from control group subjects. The rate of correct indication for both, depressive and control subjects is 85% using SASI or HFD method. Statistically significant variations were revealed between symmetric channels of the right and left hemispheres neither for SASI nor for HFD values ($p>0.05$). The results indicated that the original linear EEG analysis method SASI protected by our US patent and the nonlinear HFD method both demonstrated a good sensitivity for detection of characteristic features of depression in a single-channel EEG.

Tähtsamad teadustulemused:
The original spectral asymmetry method for EEG analysis SASI, protected by our US patent from 2012, demonstrated a sensitivity for detection of characteristic features in depression comparable and even better compared to much more complicated nonlinear Higuchi's fractal dimension method in a single-channel EEG.

Olulisim publikatsioon aruandeaastal:
Maie Bachmann, Jaanus Lass, Anna Suhhova, and Hiie Hinrikus, "Spectral Asymmetry and Higuchi's Fractal Dimension Measures of Depression Electroencephalogram," Computational and Mathematical Methods in Medicine, vol. 2013, Article ID 251638, 8 pages, 2013. doi:10.1155/2013/251638

Välisakadeemiate või muude oluliste T&A- ga seotud välisorganisatsioonide liikmed.
Hiie Hinrikus - International Academy for Medical and Biological Engineering – Fellow; European Alliance for Medical and Biological Engineering and Science – Founding Fellow

2.1.3. Cardiovascular direction research group, Kalju Meigas

Teadustöö kirjeldus

The focus in preventing and treating cardiovascular diseases (CVD) today is moving from a statistical risk factors approach (age, BP level, cholesterol, diabetes) toward direct assessment of arterial wall impairment (arterial thickness, arterial wall properties). Atherosclerosis is the main cause for deaths in Europe; unfortunately Estonia belongs to countries with highest mortality levels for CVD in Europe. Therefore availability of inexpensive non-invasive methods for diagnostics of atherosclerosis in very early stage is extremely important. The arterial wall elasticity is a major function of the aorta. Loss of elasticity leads to pulse pressure rise and to increase of pulse wave velocity (PVW). PWV, recognized recently as an independent diagnostic parameter, is widely recognized as a direct marker of arterial stiffness. In early stage the pathogenesis atherosclerotic process can be stopped to prevent serious CVD.
Availability of a range of methods and techniques allow measurement PWV and other variables related to the stiffness of arteries. Currently, measurements using tonometry, pulse wave imaging and arterial compliance using doppler ultrasonography are used to assess arterial parameters. Although some of the techniques and devices are clinically accepted, the methods applied in these devices are complicated. The application of tonometry transducers or ultrasound probes on target arteries can be rather difficult. Therefore, simpler and easier methods are required. Application of PPG for PVW measurement provides a simple method and promising solution of the problem. Modern signal processing creates a novel level of PPG signal application in PWV measurements.

Tähtsamad teadustulemused:
Developed a new methodology for early diagnosis of atherosclerosis based on optical non-invasive determination of dynamic compliance of arteries. Novelty compared to international excellence is within a dramatic improvement of time in simultaneous and quick optical registration of mechanical movements of arteries walls, pulse wave velocity and shape, and dynamics of blood pressure creates a system of parameters for estimation of dynamic compliance of arteries and to get early diagnoses of atherosclerosis.
The number of physiological signals and reference parameters (pulse waves from different locations of the body, peripheral pressure pulse wave, electrocardiographic signal, phonocardiography waves, augmentation indices and pulse wave velocity in aorta) has been measured from volunteers and atherosclerotic patients (diabetes mellitus). The novelty is in the concept for the development of the new optical method and its evaluation. The new signal processing methods have been developed and are currently under development.

Viis olulisemat publikatsiooni aruandeaastal:

- Pilt, Kristjan; Ferenets, Rain; Meigas, Kalju; Lindberg, Lars-Göran; Temitski, Kristina; Viigimaa, Margus, New Photoplethysmographic Signal Analysis Algorithm for Arterial Stiffness Estimation, The Scientific World Journal, 2013, 9 pp;
- Viigimaa M, Talvik A, Wojciechowska W, Kawecka-Jaszcz K, Toft I, Stergiou GS, Nasothimiou EG, Kotsis V, Agabiti Rosei E, Salvetti M, Dorobantu M, Martell-Claros N, Abad-Cardiel M, Hernández-Hernández R, Doménech M, Coca A, Identification of the hemodynamic modulators and hemodynamic status in uncontrolled hypertensive patients, Blood Press. 2013 Dec;22(6):362-70;
- ESH/ESC Guidelines for the management of arterial hypertension: The Task Force for the management of arterial hypertension of the European Society of Hypertension (ESH) and of the European Society of Cardiology (ESC). Authors/Task Force Members, Mancia G, Viigimaa M, et al. Eur Heart J. 2013 Jul;34(28):2159-2190;
- Pilt, Kristjan; Meigas, Kalju; Temitski, Kristina; Viigimaa, Margus, The effect of local cold and warm exposure on index finger photoplethysmographic signal waveform,

Conference proceedings of the IEEE Engineering in Medicine and Biology Society, 2013, 2300 – 2303;

- Estonian patent EE05619B1 (granted 15.02.2013). Method and device for long term variability monitoring of cardiovascular parameters based on registered electrocardiograph and pulse wave signals. Application P201100016 (filed 09.03.2011). Inventors: Kalju Meigas, Mart-Rein Rosmann, Jaanus Lass, Jüri Kaik, Kristjan Pilt, Denis Karai, Indrek Raig, Avo Tölpt.

Välisakadeemiate või muude oluliste T&A- ga seotud välisorganisatsioonide liikmed.
Margus Viigimaa - Rootsi Hüpertensiooni Ühingu auliige
Margus Viigimaa - Bulgaaria Hüpertensiooni Liiga auliige
Margus Viigimaa - Kasahstani Kardioloogide Assotsiatsiooni auliige
Margus Viigimaa - Ukraina Arstiteaduste Akadeemia Kuldmedali laureaat
Margus Viigimaa - Ungari Hüpertensiooni Ühingu auliige.

2.1.4. Sudden death research group, Jüri Kaik

Teadustöö kirjeldus

Evaluation of new generation event recorders and telemetric data transmission, including ambulatory sleep apnea monitors. Evaluation of novel heart rate and cuff-less blood circulation Holter devices (European Space Agency project: Development of the Heart Rate and Cuff-less Blood Circulation Holter Device for Non-invasive, Simultaneous and Continuous Monitoring of Cardiovascular Parameters on the Earth and in Space, stage 2).

Tähtsamad teadustulemused:
Evaluation of the dependace of various physiological parameters on the severity of sleep apnea. Application of international patent.

Olulisim publikatsioon aruandeaastal:
Shipilova, T.; Pshenichnikov, I.; Karai, D.; Ripulk, J.; Kaik, J. (2013). 24-hour Pattern of Heart Rate in Relation to Organ Damage in Women with Arterial Hypertension. Kardiologiya, 8, (1):24-27

2.2. Department of Clinical Medicine, Ruth Sepper

Teadustöö kirjeldus

- Investigations on causes and development and early diagnostics of asthma and chronic obstructive lung disease - Prof. Ruth Sepper (leader of research group),senior researcher Kaiu Prikk, post-graduates Sirje Marran, Berit Pilden;
- Project „CHROMED“ - Clinical Trials for Elderly patients with Multiple Disease – Ruth Sepper, Kaiu Prikk, Mariliis Sepper;
- E-health R&D projects:
  eMedic – Developing New Practices for Teleconsultation and Diabetes - project manager Ruth Sepper, senior researcher Peeter Ross, project coordinators Veronika Palmiste-Kallion, Mall Maasik;
- PrimCare IT - Counteracting brain drain and professional isolation of health professionals in remote primary health care through tele-consultation and tele-mentoring to strengthen social conditions in remote BSR - project manager Madis Tiik, senior researcher Peeter Ross.

Tähtsamad teadustulemused:

We demonstrated that lung function deviation and lung structural changes are present in chronic smokers before the clinical signs of airway obstruction reveal and these changes are associated with early onset of chronic obstructive pulmonary disease (COPD). Further investigations have performed to find early COPD biomarkers by use of data mining and bio-informatic approach.

Olulisemad publikatsioonid aruandeaastal:

1. Hunt, A.; Ristolainen, A.; Ross, P.; Opik, R.; Krumme, A.; Kruusmaa, M. (2013). Low cost anatomically realistic renal biopsy phantoms for interventional radiology trainees. European Journal of Radiology, 82(4), 594 – 600.
2. Ross, P. (2013). Veebipõhine ligipääs isiklikele terviseandmetele: patsiendiportaalide kasutamise ülevaade . Eesti Arst, 92(3), 145 – 151.
3. de Lusignan S, Ross P, Shifrin M, Hercigonja-Szekeres M, Seroussi B. (2013). A comparison of approaches to providing patients access to summary care records across old and new Europe: an exploration of facilitators and barriers to implementation. Studies in Health Technology and Informatics [2013, 192:397-401]. Ross P, Mill R. Digitaalsete dokumentide jagamise standardprofiilid tervishoius (Digital data sharing profiles in Healthcare). (2013). Eesti Arst 2013; 92(9):516–523.
5. Rätsep, T.; Minajeva, A.; Asser, T. (2013). Relationship between neovascularization and degenerative changes in herniated lumbar intervertebral discs. European Spine Journal, 22(11), 2474 - 2480.
6. Liik M, Paris M, Vahter L, Gross-Paju K, Haldre S. BMC Neurol. 2013 Dec 17;13:204.
7. Liik M, Vahter L, Gross-Paju K, Haldre S. Cognitive profile and depressive symptoms in patients with epilepsy. Medicina (Kaunas). 2013;49(6):254-61.

Välisakadeemiate või muude oluliste T&A- ga seotud välisorganisatsioonide liikmed.

Ruth Sepper	-	FP7 Programm Tervis programmikomitee, ekspert
		Marie Curie Individual fellowships, Panel Life, FP7, ekspert
		American Thoracic Society, liige
		Gruusia Teadusfond, ekspert
		Eur. Respir. J, Clinical Chem. Acta, retsensent
		J Proteomics, retsensent
		PloS ONE, retsensent
Kaiu Prikk	-	European Respiratory Society, liige
		American Thoracic Society, liige
Peeter Ross	-	European Society of Radiology, liige
		Finnish Society of Telemedicine and eHealth, liige
Madis Tiik	-	Finnish Society of Telemedicine and eHealth, liige
Ave Minajeva	-	Federation of the Societies of Biochemistry and Molecular Biology, (tööleping kuni 31.08.2013) liige
Katrin Gross-Paju	-	Euroopa Neuroloogia Ühingute Föderatsiooni Neurorehabilitatsiooni paneeli liige
		Advisory Board – Multiple Sclerosis – Central East Europe, liige

T&A-ga seotud tunnustused, ülevaade teaduskorralduslikust tegevusest, teadlasmobiilsusest ning hinnang oma teadustulemustele.

Kliinilise meditsiini instituudi teadus- ja arendustegevuse valdkonnad on:

- Astma ja kroonilise obstruktiivse kopsuhaiguse tekke, arengu ja varase diagnostika uurimise põhjused (*Investigations on causes and development and early diagnostics of asthma and chronic obstructive lung disease).* Teadussuuna juht prof. Ruth Sepper, kaastöötajad vanem- teadur Kaiu Prikk, doktorandid Berit Pilden ja Sirje Marran.
- E-tervise teadussuund (*E-health)*, mida juhib rahvusvaheline teadlaskond, kuhu kuuluvad Tallinna ja Helsingi Tehnikaülikooli dotsent Hanna Pohjonen, projektijuht Madis Tiik, PhD, dotsent ja vanemteadur Peeter Ross, PhD.

2.3. NMR group, Ago Samoson

Teadustöö kirjeldus

We developed a MAS NMR probe, providing in-situ study of chemical reactions at temperatures up to 300C. The rotor, constituting effectively a reaction cell, is filled by solid, catalytic substrate and fed by fluid reactants during spinning at frequencies over 10,000 Hz. The reaction products are removed from the reaction space by evacuation and directed to further chromatographic or MS analyses. We studied Fluoride and Lithium ion battery electrodes and ion conductor materials, demonstrating also an experimental possiblity to get complementary high resolution NMR and ESR data on a same set of compounds. A bio-VT NMR probe was refined to feature 4th resonance channel and improved rotor stability at 100,000 HZ spinning rates. A time-line profiling of blood serum metabolites was initiated on a cohort of volunteers, compounded by a contextually novel statistical correlation anlyses.

Olulisemad publikatsioonid aruandeaastal:

1. Bratman, V. L.; Fedotov, A. E.; Kalynov, Yu. K.; Makhalov, P. B.; Samoson, A. THz Gyrotron and BWO Designed for Operation in DNP-NMR Spectrometer Magnet. Journal Of Infrared Millimeter And Terahertz Waves. Dec. 2013. 2013, 34, 12. Pp. 837-846.

2. Agarwal, Vipin; Tuherm, Tiit; Reinhold, Andres; Past, Jaan; Samoson, Ago; Ernst, Matthias; Meier, Beat H. Amplitude-modulated low-power decoupling sequences for fast magic-angle spinning NMR. Chemical Physics Letters. Sep. 2013. Pp 1-7 2013. 5

3. Rongeat, Carine; Reddy, M. Anji; Witter, Raiker; Fichtner, Maximilian. Nanostructured Fluorite-Type Fluorides As Electrolytes for Fluoride Ion Batteries. Journal Of Physical Chemistry C. Mar 14 2013, Vol. 117, no 10. Pp. 4943-4950.

4. Witter, Raiker; Roming, Marcus; Feldmann, Claus; Ulrich, Anne S. Multilayered core-shell structure of polyol-stabilized calcium fluoride nanoparticles characterized by NMR. Journal Of Colloid And Interface Science. Jan. 15 2013, Vol 2013, no 390. Pp. 250-257.

5. Zhao-Karger, Zhirong; Witter, Raiker; Bardaji, Elisa Gil; Wang, Di; Cossement, Daniel; Fichtner, Maximilian. Altered reaction pathways of eutectic LiBH4-Mg(BH4)(2) by nanoconfinement. Journal Of Materials Chemistry A. 2013. Vol 1, no 10. Pp. 3379-3386.

Rahvusvahelised tunnustused

Ago Samoson - Invited presentations at Indian national and worldwide EUROMAR conferences.

T&A-ga seotud tunnustused, ülevaade teaduskorralduslikust tegevusest, teadlasmobiilsusest ning hinnang oma teadustulemustele.

ENMR group continued with complementing functionality the new laboratory, it features now inorganic syntheses, microprecision machining and medicinal herb-nutraceutical cultivation.