KEEMIA- JA MATERJALITEHNOLOOGIA TEADUSKONNA MATERJALITEADUSE INSTITUUDI TEADUS- JA ARENDUSTEGEVUSE AASTAARUANNE 2011

1. Instituudi struktuur

Instituudi direktor Enn Mellikov

- Füüsikalise keemia õppetool, Chair of Physical Chemistry, Andres Öpik
- Pooljuhtmaterjalide tehnoloogia õppetool, Chair of Semiconductor Materials Technology, Enn Mellikov
- Keemiliste kiletehnoloogiate teaduslaboratoorium, Laboratory of Thin Film Chemical Technology, Malle Krunks

2. Instituudi teadus- ja arendustegevuse (edaspidi T&A) iseloomustus

(NB! punktid 2.1- 2.6 täidab struktuuriüksus)

2.1 struktuuriüksuse koosseisu kuuluvate uurimisgruppide

2.1.1 teadustöö kirjeldus *(inglise keeles*);

Füüsikalise keemia õppetool, Chair of Physical Chemistry

Molecularly imprinted polymers

The experience of our research group in MIPs fabrication is based on the use of electrosynthesized polymers as matrix materials for molecular imprinting. We have introduced a novel approach and materials for producing surface imprinted polymer (SIP) microrods with selective protein-binding sites located on their surface. The proposed method is based on the electrochemical synthesis of poly-3,4-ethylenedioxythiophene (PEDOT) within the pores of protein modified polycarbonate membrane served as sacrificial microreactors for synthesis. The obtained surface-imprinted PEDOT microrods were shown to selectively recognize the template protein – avidin (Av), as demonstrated by competitive binding assays using fluorescence detection. In order to implement the possibility for the label-free detection of protein by SIPs microstructures we have developed a novel concept to generate micropatterned SIPs for protein recognition by using standard photolithographic technology.

Photoabsorbers and hybrid structures for solar cell applications

Using HVE technique CdS/CdTe solar cells were prepared. The current work is connected with preparation and activation of the CdS/CdTe PV structures with the purpose to investigate the possibility to use high work function organic layers (ECPs etc.) as back-contact for CdTe layer. Main conditions for CdS and CdTe thin films deposition and following treatment were selected from the literature data with the purpose to prepare and compare complete CdTe solar cells with standard p+Cu_xTe back contact and conductive polymer PEDOTdoped with polystyrene sulfonic acid (PEDOT/PSS) back contact. In order to prepare the complete solar cells, the appropriate deposition parameters and thickness of highly conductive polymer layers were selected experimentally. It was found that highly conductive PEDOT/PSS intermediate layer can significantly improve the back contact characteristics of CdTe. However these hybrid structures need to be further optimized to compete successfully with conventional inorganic back contacts in complete CdTe solar cells.

Preparation of $Cu_2ZnSnSe_4$ photoabsorber layers by selenization of Sn–Zn–Cu sequential films was also investigated. The stacked Sn-Zn-Cu films with a different sequence of composing metals were prepared by HVE and selenized in the elemental Se atmosphere. It was shown that the pathway to

form the $Cu_2ZnSnSe_4$ photoabsorber phase under the pressure of elemental Se and the phase composition of selenized films depends on the temperature of selenization.

Physical and chemical properties of the basic materials and developed functional structures

Until now we tried to find common behavior and common features in high temperature electrical conductivity (HTEC) isobars of these systems made by using HTEC and EPR methods. The best way to describe high temperature defect equilibrium (HTDE) is to calculate defect concentrations using experimentally determined HTEC isotherms and isobars data. EPR measurements confirm the defect structure in the systems under investigation.

Thorough analysis of electrical properties of solar cell devices has demonstrated that the impedance spectroscopy is one of the most sensitive diagnostic and analysis method for the future development of the already existing systems and structures as well as for finding new ones.

The conductivity of electrically conductive polymers is attributed to the presence of a conducting, i.e. percolating network, and the film is imagined as a percolating conductor-insulator composite. The dynamic density functional theory implemented in MesoDyn simulation code (Accelrys Inc.) has been used for theoretical modelling of such systems. In 2011 we generalized our calculations of the percolation pathways to a broad range of the PEDOT/PSS mass ratios (further called simply "the mass ratio"), doping levels and interaction parameters to get a necessary insight into the percolation behavior of this complex in the framework of the generated morphologies.

Pooljuhtmaterjalide tehnoloogia õppetool, Chair of Semiconductor Materials Technology

We have studied processes of formation kesterite $Cu_2ZnSn(Se,S)_4$ monograin powders and thin films that are used as absorbers in low-cost monograin layer (MGL) solar cells. CZTS and CZTSe are belived to be the next generation absorbers for solar cells that are composed of Earth abundant and non-toxic elements enabling thus significant cost reduction. The bacis studies are concentrated to PL studies. Information about the basic physical properties, defect structure and recombination mechanisms of studied materials was obtained. The investigated PL spectra of different kesterites had shapes from broad asymmetric bands, which are characteristic of heavily doped semiconductors, to narrow excitonic peaks with phonon replicas that implies a rather good crystal quality. Recombination related to deep donor-acceptor pairs, Fano-type resonances, excitons bound to an isoelectronic defect have also been observed. Additional information about the electronically active defects in materialsis was obtained from admittance spectroscopy of the solar cells on the base of these materials. From capacitance measurements, information about the charge carrier concentration, mobility of the carriers, defect activation energies, bulk and interface defects etc. was obtainedIt was found that the dominant recombination channel involves absorber/buffer interface states.

The vibrational properties and the phase composition of the semiconductor compounds was studied by using Raman spectroscopy. We proposed a novel method to study spatial potential fluctuations in compensated absorber materials used in solar cells. The method is based on the analysis of the temperature dependence of quantum efficiency curves in solar cells. As an example, in $Cu_2ZnSnSe_4$ spatial potential fluctuations with average energetic depth of 25 meV were determined, that is in very good agreement with the data obtained from PL analysis.

We develop a new approach of electrochemical deposition of CZTS thin films: *electrochemical molecular layer epitaxy* (EMLE). The control of films growth could be realized by using different organic solvents (as electrolyte), applying complexing agents and also by applied potential or current density. The reaction mechanisms, process parameters were investigated. The influence of different deposition parameters (potential of deposition, duration of the process and composition of solution) to the parameters of films was studied. The regularities of selenization of films at different

temperatures up to CZTS were studied for films of different composition. The path of possible reactions of formation of CZTS thin films in selenization process was proposed.

Laboratory of thin film chemical technologies

The formation chemistry of In-sulfide films in chemical spray pyrolysis (CSP) process has been studied. New Indium complex is synthesized, its elemental composition and structure determined and thermal behaviour studied. The complex compound $In(tu)_3Cl_3$ formed in aqueous solution containing InCl3 and thiourea (tu), this compound is thermally stable up to 200 °C. Upon thermal degradation in inert and oxidative atmospheres In_2S_3 forms at temperatures below 250 °C. XRD and XPS studies showed that usage of thiourea-rich spray solution with In and S parent substances molar ratio of In:S=1:6 instead of In:S=1:3 is an effective tool to retard the oxidation processes during the growth of In_2S_3 films by spray method. In_2S_3 films with [O]< 1 at.% can be grown at temperatures up to 400 °C. It has been shown that solvent has an effect on the film properties. Highly (0 0 12) oriented β-In2S3 films with Eg = 2.2 eV are obtained spraying aqueous solutions while spraying alcoholic solutions results in thinner but more compact films with reduced (0 0 12) orientation and Eg of 2.0 eV.

We showed that $CuInS_2$ films grown at low temperatures (T< 300 °C) has advantages containing low amount of oxygen ([O] < 1 at.%) and exhibiting uniform distribution of the elements in the film depth. Disadvantage is that films are composed of small crystallites (d< 10 nm). Thermal treatment of the films in H_2S atmosphere results in well-crystallized films, while Cu_xS phase, present in the films prepared by spray of Cu-rich solutions retards the formation of the CH-ordered phase.

ZnO nanorod (NR) arrays on glass substrate were prepared by CSP method,. ZnO NRs show intense UV and very weak green emission bands in PL spectra at RT. At 10K, fine structure of UV-emission related to bounded and free exciton transitions is detected and analysed. ZnO:In thin films as possible TCO layers were deposited by CSP. Electrical properties depending on the film growth temperature and solution spraying rate were determined.

The development of structural, optical and electrical properties of CBD deposited CdS films in reducing conditions of the thermal treatment process has been studied. The kinetics of the formation of the CdS film electrical properties was elaborated. CdS films were used to form CdS-CdTe solar cell.

2.1.2 aruandeaastal saadud tähtsamad teadustulemused *(inglise keeles).*

Füüsikalise keemia õppetool, Chair of Physical Chemistry

We have introduced a novel approach and materials for producing surface imprinted polymer (SIP) microrods with selective protein-binding sites located on their surface.

It was found that highly conductive PEDOT/PSS intermediate layer can significantly improve the back contact characteristics of CdTe.

Pooljuhtmaterjalide tehnoloogia õppetool, Chair of Semiconductor Materials Technology

18research papers (1.1) published or applied for the publication, 1 doctoral thesis defended

Laboratory of thin film chemical technologies

9 research papers published, 1 doctoral thesis defended.

2.2 uurimisgrupi kuni 5 olulisemat publikatsiooni läinud aastal.

Füüsikalise keemia õppetool, Chair of Physical Chemistry

1. Lautner, G.; Kaev, J.; Reut, J.; Öpik, A.; Rappich, J.; Syritski, V.; Gyurcs?nyi, R. E. (2011). Selective Artificial Receptors Based on Micropatterned Surface-Imprinted Polymers for Label-Free Detection of Proteins by SPR Imaging. Advanced Functional Materials, 21(1), 591 – 597 **The best research paper of TTU in the field of engineering and technology**
2. Jarkov, A.; Bereznev, S.; Laes, K.; Volobujeva, O.; Traksmaa, R.; Öpik, A.; Mellikov, E. (2011). Conductive polymer PEDOT:PSS back contact for CdTe solar cell. Thin Solid Films, 519(21), 7449 - 7452.
3. Adhikari, N.; Bereznev, S.; Laes, K.; Kois, J.; Volobujeva, O.; Raadik, T.; Traksmaa, R.; Tverjanovich, A.; Öpik, A.; Mellikov, E. (2011). High-Vacuum Evaporation of n-CuIn3Se5 Photoabsorber Films for Hybrid PV Structures. Journal of Electronic Materials, 40(12), 2374 - 2381.

Pooljuhtmaterjalide tehnoloogia õppetool, Chair of Semiconductor Materials Technology

1. Kask, E.; Raadik, T.; Grossberg, M.; Josepson, R.; Krustok, J. (2011). Deep defects in Cu2ZnSnS4 monograin solar cells. Energy Procedia, 10, 261 - 265.
2. Kauk, M; Muska, K; Altosaar, M; Raudoja, J; Pilvet, M; Varema, T; Timmo, K; Volobujeva, O. (2011). Effects of sulphur and tin disulphide vapour treatments of Cu2ZnSnS(Se)4 absorber materials for monograin solar cells. Energy Procedia, xxx - xxx. [ilmumas]
3. Mellikov, E.; Meissner, D.; Altosaar, M.; Kauk, M.; Krustok, J.; Öpik, A.; Volobujeva, O.; Iljina, J.; Timmo, K.; Klavina, I.; Raudoja, J.; Grossberg, M.; Varema, T.; Muska, K.; Ganchev, M.; Bereznev, S.; Danilson, M. (2011). CZTS Monograin Powders and Thin Films. Global Research and Education (8 - 13).Trans Tech Publications Ltd
4. Klavina, I.; Kaljuvee, T.; Timmo, K.; Raudoja, J.; Traksmaa, R.; Altosaar, M.; Meissner, D. (2011). Study of Cu2ZnSnSe4 monograin formation in molten KI starting from binary chalcogenides . Thin Solid Films, 519, 7399 - 7420.

Laboratory of thin film chemical technologies

1. Otto, K.; Oja Acik, I.; Tõnsuaadu, K.; Mere, A; Krunks, M. (2011). Thermoanalytical study of precursors for In2S3 thin films deposited by spray pyrolysis. Journal of Thermal Analysis and Calorimetry, 105(2), 615 - 623.
2. Otto, K.; Katerski, A.; Mere, A.; Volobujeva, O.; Krunks, M. (2011). Spray Pyrolysis Deposition of Indium Sulfide Thin Films. Thin Solid Films, 519(10), 3055 - 3060

2.3 Loetelu struktuuriüksuse töötajate rahvusvahelistest tunnustustustest.

E. Mellikov	ülemaailmse PV konverentsi programmkomitee liige

2.4 Loetelu struktuuriüksuse töötajatest, kes on välisakadeemiate või muude oluliste T&A-ga seotud välisorganisatsioonide liikmed.

E. Mellikov	PV Nordic Steering Committee
E. Mellikov	M-ERA Eesti VABARIIGI esindaja juhtkomitees
E. Mellikov	PV –Baltic liige
E. Mellikov	SET -50 materjalide töögruppi liige (ekspert)

O. Volobujeva	Eesti Vabariigi esindaja Euroopa Teadusfondi reaal ja tehnikateaduste komisjonis PESC
O. Volobujeva	PV –Baltic liige
O. Volobujeva	M-ERA Eesti Vabariigi esindaja töökomisjonis
M. Grossberg	EERA –PV Eesti Vabariigi esindaja õhukeste kilede töögrupis
D. Meissner	PV –Baltic liige

2.5 Aruandeaasta tähtsamad T&A finantseerimise allikad.

2.6 Soovi korral lisada aruandeaastal saadud T&A-ga seotud tunnustusi (va punktis 2.3 toodud tunnustused), ülevaate teaduskorralduslikust tegevusest, teadlasmobiilsusest ning anda hinnang oma teadustulemustele.

TTÜ parim arendustöö aastal 2011 "Kuluefektiivse päikesepatarei väljaarendamine"
E. Mellikov, M. Altosaar, M. Kauk, K. Timmo, T. Varema, J. Raudoja, O.Volobujeva, J, Krustok, M, Grossberg, M.Pilvet, T. Raadik
TTÜ parim teaduspublikatsioon 2011, tehnika valdkond, nimetatud veebr. 2012
Lautner, G.; Kaev, J.; Reut, J.; Öpik, A.; Rappich, J.; Syritski, V.; Gyurcs?nyi, R. E. (2011). Selective Artificial Receptors Based on Micropatterned Surface-Imprinted Polymers for Label-Free Detection of Proteins by SPR Imaging. Advanced Functional Materials, 21(1), 591 – 597
TTÜ parim teaduspublikatsioon 2010, tehnika valdkond nimetatud veebr. 2011,
M. Krunks, E. Kärber, A. Katerski, K. Otto, I. Oja Acik, T. Dedova, A. Mere, Extremely thin absorber layer solar cells on zinc oxide nanorods by chemical spray, Solar Energy Materials & Solar Cells, 94 (2010) 1191-1195

Teadustöö toimus vastavalt plaanitule. Tulemuslikuselt võis teadus-ja arendusööd hinnata väga hea hindega. Instituut on osaline kahes EV teaduse tippkeskuses. Instituut oli samuti suhteliselt edukas HTM sihtfinantseerimise konkursil (A. Öpik), infrastuktuuri nn. Väikeinfrastruktuuri projektides (E. Mellikov, M. Krunks) ja ETF grantide taotluskonkursil saades finatseerimise järgmisteks aastateks kuuele grantitaotlusele (M. Grossberg, K. Timmo, M. Kauk, L. Lott, J. Hiie, M. Krunks) Eriti aktiivselt toimus liitumine rahvusvahelise teaduskoostöö võrkudega erinevates PV ja materjalide valdkondades: M-ERA, EERA-PV ja PV-Baltic, kesteriitide alane koostöövõrk.

2.7 Instituudi teadus- ja arendustegevuse teemade ja projektide nimetused *(Eesti Teadusinfosüsteemi, edaspidi ETIS, andmetel)*

- Haridus- ja Teadusministeerium

sihtfinantseeritavad teemad:

- T714, Elektrit juhtivate polümeermaterjalide omaduste uurimine ja modifitseerimine kasutamiseks funktsionaalsete materjalidena ning elektronseadiste komponentidena, Öpik Andres
- T092, Õhukesekilelised ja nanostruktuursed materjalid keemilistel meetoditel, Krunks Malle

- T099, Uued materjalid ja tehnoloogiad tuleviku päikeseenergeetikale, Mellikov Enn

baasfinantseerimise toetusfondist rahastatud projektid (sh TTÜ tippkeskused):
- ÜPTK0, Kõrgtehnoloogilised materjalid ja seadised alternatiivsele energeetikale, Enn Mellikov
- B01, CZTS(Se) tüüpi absorbermaterjalide defektstruktuuri uuringud, Maarja Grossberg
- B07, Juhtivteadur Malle Krunksi poolt juhitava uurimisgrupi toetamine
- B08, Professor Dieter Meissneri poolt juhitava uurimisgrupi toetamine

riiklikud programmid:
- Energiatehnoloogia programm, AR10128, Uued materjalid päikeseenergeetikale, Enn Mellikov
-

- Teiste ministeeriumide poolt rahastatavad riiklikud programmid:
  ei olnud aruandeperioodil

- Uurija-professori rahastamine:
  Ei toimunud

- SA Eesti Teadusfond

grandid:
- ETF7678, $CuInSe_2$ legeerimine võõrlisanditega ja alternatiivsed puhverkihid rakendamiseks monoterakihi päikesepatareides, Kauk Marit
- ETF7718, Päikesepaneelide energiareitingu uuringud, Jagomägi Andri
- ETF7788, Sool-geeli meetodil kasvatatud metalli oksiidide kihid optoelektroonikale, Oja Acik Ilona
- ETF8147, Nelikmaterjalide kiled kalgogeniseerimisse protsessis; mehhanism ja kineetika, Volobujeva Olga
- ETF8249, Biotundlikud süsteemid pindmiste mälupesadega molekulaarselt jäljendatud elektrit juhtivatest polümeeridest, Sõritski Vitali
- ETF8282, Rekombinatsioonilised kaod CZTS(Se) päikesepatareides, Krustok Jüri
- ETF8509, Keemilise pihustuspürolüüsi meetodil kasvatatud ZnO nanovarraste areng, Dedova Tatjana
- ETF8655, Nanostruktuursete kalkogeniid-pooljuhtide süntees elektrokeemilise sadestamise meetodil, Julia Kois
- ETF8714, Hübriidsed aluskontaktid CdTe päikeseelementidele, Sergei Bereznev
- ETF8964, Päikesepatarei $Cu_2ZnSn(Se,S)_4$–tüüpi absorbermaterjalide süntees, omaduste kujundamine ja p-n siirde formeerimine, Mare Altosaar

ühisgrandid välisriigiga:
ei olnud aruandeperioodil

järeldoktorite grandid (SA ETF ja Mobilitas):
- JD98, Uued odavad materjalid ja tehnoloogiad päikeseenergeetikale, Ganchev Maxim
- MJD213, $Cu_2ZnSn(SSe)_4$ õhukesed kiled päikeseenergetikale, Revathi Naidu

tippteadlase grandid (Mobilitas):
ei olnud aruandeperioodil

- Ettevõtluse Arendamise SA

eeluuringud:

ei olnud aruandeperioodil

arendustoetused:

Kuluefektiivse päikesepatarei väljaarendamine, Enn Mellikov

- SA Archimedesega sõlmitud lepingud

infrastruktuur (nn „mini-infra“, „asutuse infra“):

- AP714, Elektrit juhtivate polümeermaterjaliide omaduste uurimine ja modifitseerimine kasutamiseks funktsionaalsete materjalidena ning elektronseadiste kopmponentidena, Öpik Andres
- AP092, Õhukesekilelised ja nanostruktuursed materjalid keemilistel meetoditel, Krunks Malle
- AP009, Uued materjalid ja tehnoloogiad tuleviku päikeseenergeetikale, Mellikov Enn
- ÜLTAP65, Nano- ja mikrostruktuursete uuringute komplekslabor , Enn Mellikov

Eesti tippkeskused:

- TAR11059, Kõrgtehnoloogilised materjalid jätkusuutlikuks arenguks, Enn Mellikov
- TAR11060, Mesosüsteemide teooria ja rakendused, Malle Krunks

riiklikud programmid:
Energiatehnoloogia progrramm

- AR10128, Uued materjalid päikeseenergeetikale, Enn Mellikov

muud T&A lepingud:

- SA Keskkonnainvesteeringute Keskusega sõlmitud lepingud:
  ei olnud aruandeperioodil

- Siseriiklikud lepingud:
  Crystalsol OÜ, Kuluefektiivse päikesepatarei väljaarendamine, Enn Mellikov

- EL Raamprogrammi projektid:

- VFP432, Development of flexible single and tandem II-VI based high efficiency thin film solar cells, Hiie Jaan

- Välisriiklikud lepingud:

- VIE395, Koostöövõrk päikeseenergeetika arendamiseks Euroopa Liidu uutes liikmesmaades, Mellikov Enn
- Connor OY(Soome), EFI (Norra), Crystalsol GmbH (Austria) Kuluefektiivse päikesepatarei väljaarendamine, Enn Mellikov

2.8 Struktuuriüksuse töötajate poolt avaldatud sihtfinantseeritava teadusteema taotlemisel arvestatavad eelretsenseeritavad teaduspublikatsioonid *(ETIS klassifikaatori alusel 1.1, 1.2, 1.3, 2.1, 2.2, 3.1, 3.2, 3.3, 4.1 ja 5.1).*

1.1

Jarkov, A.; Bereznev, S.; Laes, K.; Volobujeva, O.; Traksmaa, R.; Öpik, A.; Mellikov, E. (2011). Conductive polymer PEDOT:PSS back contact for CdTe solar cell. Thin Solid Films, 519(21), 7449 - 7452.

Leinemann, I.; Kaljuvee, T.; Traksmaa, R.; Raudoja, J.; Grossberg, M.; Altosaar, M.; Meissner, D. (2011). Copper zinc tin selenide monograin formation in molten sodium iodide starting from binary chalcogenides . Journal of Alloys and Compounds, xx - xx. [ilmumas]

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ammonium nitrate with different additives:thermodynamic analysis. Journal of Thermal Analysis and Calorimetry, 105(1), 13 - 26.

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Luckert, F.; Hamilton, D. I.; Yakushev, M. V.; Beattie, N. S.; Zoppi, G.; Moynihan, M.; Forbes, I.; Karotki, A. V.; Mudryi, A. V.; Grossberg, M.; Krustok, J.; Martin, R. W. (2011). Optical properties of high quality Cu2ZnSnSe4 thin films. Applied Physics Letters, 99, 062104

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Ganchev, M.; Iljina, J.; Kaupmees, L.; Raadik, T. ; Volobujeva, O.; Mere, A.; Altosaar, M.; Raudoja, J.; Mellikov, E. (2011). Phase composition of selenized Cu(2)ZnSnSe(4) thin films determined by X-ray diffraction and Raman spectroscopy . Thin Solid Films, 519(21), 7394 - 7398.

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1.2

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1.3, 2.1, 2.2, 3.1

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3.2, 3.3, 4.1, 5.1

2.9 Struktuuriüksuses kaitstud doktoriväitekirjade loetelu

Liina Kaupmees, materjaliteaduse instituut
Teema: *Selenization of Molybdenum as Contact Material in Solar Cells* (Molübdeeni kui päikesepatarei kontaktmaterjali seleniseerimine)
Juhendaja: juhtivteadur Mare Altosaar
Kaitses: 1.12.2011
Omistatud kraad: filosoofiadoktor (keemia- ja materjalitehnoloogia)

2.10 Struktuuriüksuses järeldoktorina T&A-s osalenud isikute loetelu *(ETIS-e kaudu esitatud taotluste alusel)*

JD98, Uued odavad materjalid ja tehnoloogiad päikeseenergeetikale, Ganchev Maxim
MJD213, Cu2ZnSn(SSe)4 õhukesed kiled päikeseenergetikale, Revathi Naidu

2.11 Struktuuriüksuses loodud tööstusomandi loetelu

3. Struktuuriüksuse infrastruktuuri uuendamise loetelu

–	Bi-destillaator,	14.01.2011,	3 963 €
–	Vaakumpump, 1	4.03.2011,	3 466 €
–	Spectroscopy Ultraviolet Photo,	6.04.2011,	49 300 €
–	Monokromaator	13.06.2011,	35 500 €
–	Impedants analüsaator,	22.08.2011,	13 395 €
–	Kuivatuskapp	30.08.2011,	4 461 €
–	Optilised lauad, komplekt 2 tk,	1.09.2011,	19 990 €
–	Ultraheli pihustuskompleks ,	10.11.2011,	29 250 €